Preface

The idea of the book entitled **"Physical Chemistry: SET PYQ's"** was born because of the lack of any comprehensive book covering all the aspects of various entry level chemistry competitive examinations in particular conducted by CSIR, GATE, TIFR State and National Eligibility Test, but not limited to.

This book covers all PYQ's with topic wise sorted question and solution

1. Quantum Chemistry,
2. Molecular Spectroscopy,
3. Group Theory,
4. Chemical Thermodynamics,
5. Statistical Thermodynamics,
6. Electrochemistry,
7. Chemical Kinetics,
8. Colloidal and Surface Chemistry,
9. Solid State,
10. Polymer Chemistry.

The ultimate purpose of this book is to equip the reader with brainstorming challenges and solution for organic chemistry and applied aspect examinations. It contains predigested information on the entire academic subject of organic chemistry for good understanding, assimilation, self-evaluation, and reproducibility. Although we have made every effort to make the book error free, we are under no illusion. We welcome comments, criticism and suggestions from the readers to evolve the contents.

Acknowledgement

First of all I would like to thank our entire students at Institute for advanced Studies (IFAS), who have helped us to learn and practice both the art and science of chemistry. We would like to thank Er. Radheshyam Choudhary, Founding CEO, IfAS Edutech Pvt. Ltd. for being a continuous source of inspiration through his positive strokes.

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This book is a team effort, and producing it would be impossible without outstanding people of IFAS publication. It was pleasure to work with many others dedicated and creative people of IFAS during the production of this book. Special thanks for Vikendra Metha who crafted our ideas to wonderful design of cover page and Kuldeep Singh Rathore for formatting and type setting.

And finally, our humble greetings to all who put their significant efforts and are unmentioned.

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QUANTUM CHEMISTRY

CHAPTER 1

HP SET

[HP-SET 2014]

1. The wave function $\sin^{-1}$ is not acceptable, because it is:-
   (A) Not continuous
   (B) Not an eigen function of kinetic energy operator
   (C) Not differentiable
   (D) Not a single valued function

[HP-SET 2014]

2. The value of the commutator $[x,{p_x}^2]$, is given by:-
   (A) $2i$ (B) $2i\hbar$
   (C) $2i\hbar x$ (D) $2i\hbar p_x$

[HP-SET 2014]

3. The first order correction to energy for the ground state of a particle in a box due to perturbation λx is would be:-
   (A) $\lambda L/2$ (B) λL
   (C) $2\lambda L$ (D) 2

[HP-SET 2014]

4. The energy levels of cyclopropenyl cation are $\alpha + 2\beta$, $\alpha - \beta$ and $\alpha - \beta$. The delocalization energy of $C_3H_3^+$ is:-
   (A) 2β (B) 0
   (C) 3β (D) β

[HP-SET 2017]

5. The zero point energy of the harmonic oscillator is:-
   (A) $h\omega$ (B) zero
   (C) $\frac{1}{2}h\omega$ (D) $\frac{2}{3}h\omega$

[HP-SET 2017]

6. The energy levels of the cyclobutadiene are $\alpha + 2\beta, \alpha, \alpha, \alpha - 2\beta$. The delocalization energy in this molecule is:-
   (A) 0 (B) -4β
   (C) -8β (D) 4α

[HP-SET 2017]

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

[HP-SET 2017]

8. When hydrogen atom is placed in an electric field along the y-axis, the orbital that mixes most with the ground state 1s orbital is:-
   (A) 2s (B) $2p_x$
   (C) $2p_y$ (D) $-2p_z$

[HP-SET 2018]

9. The separation between the adjacent energy levels of a particle in a one-dimensional box of length a is:
   (A) $n^2h^2/8ma^2$ (B) $(a/2)^{1/2}$
   (C) $(2n+1)h^2/8ma^2$ (D) $8ma^2/h^2$

[HP-SET 2018]

10. The energy of photon associated with light of wavelength 200 nm is:
    (A) 99×10^{-19} J (B) 0.9×10^{-19} J
    (C) 9.9×10^{-19} J (D) 9.0×10^{-19} J

[HP-SET 2018]

11. If $e^{\alpha x}$ is an eigen function and $d^n/\ dx^n$ is an operator, then the eigen value will be:
    (A) α^n (B) α
    (C) n (D) n^α

[HP-SET 2018]

12. A projectile of mass 1.0 g is known to within 1 μm s^{-1}. Calculate the minimum uncertainty in its position:
    (A) 5×10^{26} m s^{-1} (B) 5×10^{26} m
    (C) 5×10^{-26} m s^{-1} (D) 5×10^{-26} m

KERALA SET

[KERALA-SET 2012]

13. According to de Broglie hypothesis, the wave length of a particle is -----
    (A) Directly proportional to its mass
    (B) Directly proportional to its energy
    (C) Directly proportional to its momentum
    (D) Inversely proportional to its momentum

[KERALA-SET 2012]

14. Which among the following will have maximum wave character if they move with identical speeds?
    (A) Electrons (B) Protons
    (C) Neutrons (D) Alpha particles

[KERALA-SET 2012]

15. The energy of a particle in a one-dimensional box is given by -----

(A) $nh^2/8ma^2$ (B) $n^2h^2/8ma^2$

(C) $n^2h^2/4ma^2$ (D) $nh^2/4ma^2$

[KERALA-SET 2012]

16. The number of radial nodes for the 3s orbital of hydrogen atom is -----

(A) 0 (B) 1

(C) 2 (D) 3

[KERALA-SET 2012]

17. _____ is not a fermion.

(A) Electron (B) Proton

(C) Neutron (D) 4He

[KERALA-SET 2012]

18. What is the energy of the photon having a wavelength 3.313 A˚?

(A) 3×10^{-16} J (B) 13.254×10^{-16}J

(C) 6×10^{-16}J (D) 13.254×10^{-18}J

[KERALA-SET 2013]

19. In units of $h^2/8ml^2$, the energy difference between levels corresponding to 3 and 2 node eigen functions for a particle of mass m in a one dimensional box of length l is

(A) 1 (B) 3

(C) 5 (D) 7

[KERALA-SET 2013]

20. The momentum of a photon of frequency 5×10^{20} s^{-1} is nearly

(A) 1.1×10^{-25} Kg m s^{-1} (B) 1.1×10^{-21} Kg m s^{-1}

(C) 2.1×10^{-21} Kg m s^{-1} (D) 2.1×10^{-22} Kg m s^{-1}

[KERALA-SET 2013]

21. The equation which forms the basis of photoelectric effect is

(A) $h\nu = 1/2mv^2 - w$ (B) $1/2mv^2 = h\nu - w$

(C) $W = h\nu + mv^2$ (D) $1/2\ mv^2 = h\nu + w$

[KERALA-SET 2015]

22. The first emission line of Balmer series of He^+ spectrum has wave no. in cm^{-1}(R_H = Rydberg constant)

(A) $\frac{3}{4}R_H$ (B) $\frac{5}{36}R_H$

(C) $\frac{5}{9}R_H$ (D) $\frac{1}{4}R_H$

[KERALA-SET 2015]

23. Which of the following is an eigen function of the operator $\hat{P}_x$?

(A) e^{ikx} (B) xe^{ikx}

(C) $x^2 + 2x$ (D) $\cos 2x$

[KERALA-SET 2015]

24. The angular momentum of an electron in the 4d-orbital is

(A) $\frac{2h}{\pi}$ (B) $\sqrt{2}\frac{h}{2\pi}$

(C) $\sqrt{3}\frac{h}{2\pi}$ (D) $\sqrt{6}\frac{h}{2\pi}$

[KERALA-SET 2015]

25. The average radius of 1s orbital of H-atom is

(A) a_0 (B) $2a_0$

(C) $1.5a_0$ (D) $3a_0$

[KERALA-SET 2015]

26. The number of radial nodes present in 4f-orbitals is

(A) Zero (B) One

(C) Two (D) Three

[KERALA-SET 2015]

27 If a trial function is used to calculate the energy of a quantum mechanical system, the calculated energy is always greater than the true energy. This statement is related to

(A) Perturbation theory

(B) Variation principle

(C) Born-Oppenheimer approximation

(D) Heisenberg's uncertainty principle

[KERALA-SET 2015]

28. According to MO theory the ground state wave function including spin of H_2 molecule is represented as

(A) $\frac{1}{\sqrt{2}}\begin{vmatrix}\sigma_g1s(1)\alpha(1) & \sigma_g1s(1)\beta(1)\\ \sigma_g1s(2)\alpha(2) & \sigma_g1s(2)\beta(2)\end{vmatrix}$

(B) $\frac{1}{\sqrt{2}}\begin{vmatrix}\sigma_u1s(1)\alpha(1) & \sigma_u1s(1)\beta(1)\\ \sigma_g1s(2)\alpha(2) & \sigma_g1s(2)\beta(2)\end{vmatrix}$

(C) $\frac{1}{\sqrt{2}}\begin{vmatrix}\sigma_g1s(1)\alpha(1) & \sigma_g1s(1)\beta(1)\\ \sigma_g1s(2)\beta(2) & \sigma_g1s(2)\alpha(2)\end{vmatrix}$

(D) $\frac{1}{\sqrt{2}}\begin{vmatrix}\sigma_g1s(1)\alpha(1) & \sigma_u1s(1)\beta(1)\\ \sigma_g1s(2)\alpha(2) & \sigma_u1s(2)\beta(2)\end{vmatrix}$

[KERALA-SET 2015]

29. The angle between the two hybrid orbitals ψ_1 and ψ_2 shown below is

$\psi_1 = \frac{1}{\sqrt{3}}2s - \frac{1}{\sqrt{6}}2p_x + \frac{1}{\sqrt{2}}2p_y$

$\psi_2 = \frac{1}{\sqrt{3}}2s - \frac{1}{\sqrt{6}}2p_x - \frac{1}{\sqrt{2}}2p_y$

(A) $90°$ (B) $109.5°$

(C) $120°$ (D) $180°$

[KERALA-SET 2016]

30. Which of the following is not a linear operator?

(A) $\frac{d^2}{dx^2}$ (B) $\sqrt{\ }$

(C) $\hat{P}_x$ (D) $\hat{H}$

[KERALA-SET 2016]

31. The probability that a particle to be found in between 0 and a/2 in a one dimensional box of length 'a' is

(A) $\frac{1}{2}$ (B) $\frac{1}{3}$

(C) $\frac{1}{4}$ (D) $\frac{3}{4}$

[KERALA-SET 2016]

32. The angular momentum of an electron in the f-orbital is

(A) $\sqrt{2}\frac{h}{2\pi}$ (B) $\sqrt{6}\frac{h}{2\pi}$

(C) $\sqrt{3}\frac{h}{2\pi}$ (D) $\sqrt{12}\frac{h}{2\pi}$

[KERALA-SET 2016]

33. According to the Born-Oppenheimer approximation, which of the following relative motion may be neglected?

(A) Electron to nucleus (B) Electron to electron

(C) Nucleus to nucleus (D) All of the above

[KERALA-SET 2016]

34. For hydrogen molecule in the excited state $\sigma_g^1\sigma_u^1$, the spin part of the triplet state with $m_s = 0$ is proportional to

(A) α(1)β(2) (B) α(1)β(2) + β(1)α(2)

(C) α(1)α(2) (D) α(1)β(2) - β(1)α(2)

[KERALA-SET 2016]

35. The term symbol of a molecule with the electronic configuration

$(1\sigma_g)^2(1\sigma_u)^2\ (2\sigma_g)^2(2\sigma_u)^2(1\pi_u)^2(1\pi_u)^2(3\sigma_g)^1$ is

(A) $^1\Sigma_g^+$ (B) $^3\Sigma_g^+$

(C) $^2\Sigma_g^-$ (D) $^2\Sigma_g^+$

[KERALA-SET 2016]

36. According to Huckel MO treatment the four π-MO energies of butadiene are given by $\alpha \pm 1.62\beta$ and $\alpha \pm 0.62\beta$. The delocalization energy of butadiene is

(A) 0.62 β (B) 0.48 β

(C) 1.62 β (D) 1.48 β

[KERALA-SET 2016]

37. Which of the following is a well-behaved function? (x lies between plus and minus infinity).

(A) $y = \exp(a x^2)$ (B) $y = ax + b$

(C) $y = ax^2$ (D) $y = \exp(-a x^2)$

[KERALA-SET 2017]

38. The time dependent Schrodinger equation is

(A) $\widehat{H}\Psi = E\Psi$

(B) $i\hbar\frac{\partial\Psi}{\partial t} = \widehat{H}\Psi$

(C) $\nabla^2\Psi + V\Psi = E\Psi$

(D) $-\frac{\hbar^2\partial^2\Psi}{2m\partial x^2} + V\Psi = E\Psi$

[KERALA-SET 2017]

39. If the energy of a particle in a cubical box of edge length L is $\frac{3h^2}{8mL^2}$ the energy required for the excitation of the particle into the next higher energy level is

(A) $\frac{3h^2}{8mL^2}$ (B) $\frac{6h^2}{8mL^2}$

(C) $\frac{9h^2}{8mL^2}$ (D) $\frac{3h^2}{4mL^2}$

[KERALA-SET 2017]

40. The number of radial and angular nodes in a 4f orbital are respectively

(A) 3, 3 (B) 2, 2

(C) 0, 3 (D) 0, 2

[KERALA-SET 2017]

41. Which of the following is an eigen function of the operator P_x?

(A) e^{ikx} (B) xe^{ikx}

(C) $x^2 + 2x$ (D) e^{ikx^2}

[KERALA-SET 2017]

42. The energy of a particle in a 3D cubic box of side length L is 14 $h^2/8mL^2$. The degeneracy of the state is

(A) 4 (B) 2

(C) 6 (D) 3

[KERALA-SET 2017]

43. According to variation principle, the energy E evaluated using a trial wave function will be related to the ground state energy

(A) $E \leq E_0$ (B) $E = E_0$

(C) $E \geq E_0$ (D) $E \neq E_0$

[KERALA-SET 2017]

44. The third Hermite polynomial is

(A) 1 (B) $4\xi^2$

(C) 2ξ (D) $4\xi^2$-2

[KERALA-SET 2017]

45. According to Huckel MO treatment the six π-MO energies of benzene are given by $\alpha \pm 2\beta$ and $\alpha \pm \beta$ twice. The delocalization energy of benzene is

(A) -2β (B) 2β

(C) β (D) 4β

[KERALA-SET 2018]

46. The ground state energy of a particle in a 1D box of length 1Å is 0.6032×10^{-17} J. The energy gap between first and the second energy level is

(A) 6.032×10^{-17} J (B) 1.8095×10^{-17} J

(C) 0.2528×10^{-17} J (D) 0.6032×10^{-17} J

[KERALA-SET 2018]

47. The commutator $[\hat{L}_x.\hat{L}_y]$is equal to

(A) - ih $\hat{L}_z$ (B) $i\hbar\hat{L}_z$

(C)$-i\hbar\hat{L}_z$ (D) – $ih\hat{L}_z$

[KERALA-SET 2018]

48. The value of the spherical harmonics $Y_{1,0}(\theta,\phi)$ is

(A) $\sqrt{\frac{3}{4\pi}}sin\theta$ (B) $\sqrt{\frac{3}{4\pi}}cos\theta$

(C) $\sqrt{\frac{3}{4\pi}}sin\theta cos\phi$ (D) $\sqrt{\frac{3}{4\pi}}sin\theta sin\phi$

[KERALA-SET 2018]

49. The Huckel theory secular determinant equation for cyclobutadiene is

(A) $\begin{vmatrix} x & 1 & 0 & 1 \\ 1 & x & 1 & 0 \\ 0 & 1 & x & 1 \\ 1 & 0 & 1 & x \end{vmatrix} = 0$ (B) $\begin{vmatrix} x & 0 & 1 & 1 \\ 1 & x & 0 & 1 \\ 1 & 0 & x & 1 \\ 1 & 1 & 0 & x \end{vmatrix} = 0$

(C) $\begin{vmatrix} x & 1 & 0 & 0 \\ 1 & x & 1 & 0 \\ 0 & 1 & x & 1 \\ 0 & 0 & 1 & x \end{vmatrix} = 0$ (D) $\begin{vmatrix} x & 0 & 0 & 1 \\ 1 & x & 1 & 0 \\ 0 & 1 & x & 1 \\ 1 & 0 & 0 & x \end{vmatrix} = 0$

[KERALA-SET 2018]

50. The delocalisation energy of benzene according to Huckel MO method is

(A) 0.48β (B) 2.0 β

(C) 4.0 β (D) 4.472 β

[KERALA-SET 2018]

51. If uncertainty in position and momentum are equal, then uncertainty in velocity is

(A) $1/2m\ (h/\pi)^{1/2}$ (B) $1/m\ (h/2\pi)^{1/2}$

(C) $1/2m\ (h/4\pi^{1/2})$ (D) $1/m\ (h/2\pi)^{1/2}$

[KERALA-SET 2018]

52. If two operations commute, then

(A) They are Hermitian

(B) They are linear

(C) They have the same eigen functions

(D) They have the same eigen values

[KERALA-SET 2018]

53. Use Hückel theory to determine the energies of the π orbitals of the allyl radical system, C_3H_4.

(A) $\alpha+\beta,\alpha,\alpha-\beta$ (B) $\alpha+2\beta.\alpha,\alpha-2\beta$

(C) α,α,α (D) $\alpha+\sqrt{2}\,\beta,\alpha,\alpha-\sqrt{2}\,\beta$

[KERALA-SET 2019]

54. Which of the following observations of photoelectric effect could not be explained using classical mechanics?

I. The proportionality of the intensity of photoelectric current to the intensity of radiation.

II. Existence of a threshold frequency characteristic of the metal

III. The variation of stopping potential of photoelectrons linearly with the frequency of the radiation

IV. The absence of a time lag between the fall of radiation on the metal surface and the ejection of electrons

(A) I, II and III only (B) I, II and IV only

(C) II, III and IV only (D) I, III and IV only

[KERALA-SET 2019]

55. In Compton effect, the Compton wavelength is the $\Delta\lambda$ corresponding to the scattering angle θ equal to

(A) 90° (B) 60°

(C) 45° (D) 180°

K SET

[KSET 2013]

56. The square of the wave function in quantum mechanics represents:-

(A) A state of the system

(B) Shape of the system

(C) Probability of the system

(D) Energy of the system

[KSET 2014]

57. The zero point energy of an electron is equal to:-

(A) $\frac{h^2}{2m^{\ 2}}$ (B) $\frac{h^2}{4ma^2}$

(C) $\frac{h^2}{8ma^2}$ (D) $\frac{h^2}{16ma^2}$

[KSET 2014]

58. An acceptable wave function must be:-

(A) Continuous, have a continuous first derivative, be single valued and be square integrable

(B) Discontinuous, have a discontinuous first derivative, be single valued and be square integrable

(C) Continuous, have a continuous first derivative, be of any value and no restrictions in square integrability

(D) Both (B) and (C)

[KSET 2015]

59. Ψ^2 measures

(A) The energy of the electron in n^{th} orbit

(B) Uncertainty in the position and velocity of electron

(C) The probability of finding an electron in a given region

(D) The hybrid character of orbitals

[KSET 2015]

60. $\nabla^2 in\ \nabla^2\Psi + \frac{8\pi^2 m(E-V)}{h^2}\Psi = 0$ is known as
(A) Laplacian operator (B) Hamiltonian operator
(C) Angular momentum (D) Energy operator

[KSET 2016]

61. Hamiltonian operator (H) in $H\Psi = E\Psi$ is the operator for the ____ of the system.
(A) Potential energy of the system
(B) Kinetic energy of the system
(C) Total energy of the system
(D) Zero point energy of the system

[KSET 2017]

62. Match the following:-

List - I (Color)	**List –II**
i) Green	a) 420
ii) Red	b) 620
iii) Orange	c) 530
iv) Violet	d) 700

(A) i-d, ii- c, iii - b, iv - a
(B) i-c, ii- d, iii - b, iv -a
(C) i-a, ii - b, iii - c, iv - d
(D) i-c, ii - a, iii - b, iv-d

[KSET 2017]

63. The following data is given (p-probability):-

X	p(x)
1	0.20
3	0.25
4	0.55

The average value of x is equal to
(A) <x>= 3.15 (B) <x>=0.12
(C) <x>= 0.24 (D) <x>= 0.31

[KSET 2017]

64. Which of the following are linear operators?
$\frac{d}{dx}, \frac{d^2}{dx^2}, \sqrt{}, x^2$
(A) $\frac{d}{dx}, \frac{d^2}{dx^2}$ and x^2 (B) $\sqrt{}$
(C) $\sqrt{}$ and x^2 (D) $\frac{d}{dx}$ and $\sqrt{}$

[KSET 2013]

65. The radial and angular wave function gives:-
(A) Shape, orientation and energy, size of the orbitals respectively
(B) Energy, size and shape, orientation of the orbitals respectively
(C) Energy and size of orbitals respectively
(D) Shape and orientation of orbitals respectively

[KSET 2013]

66. According to the Schrodinger's wave equation the energy of a particle (E_n) in one dimensional box is:-
(A) $E_n = \frac{n^2h^2}{ma^2}$ (B) $E_n = \frac{n^2h^2}{4ma}$
(C) $E_n = \frac{nh}{8ma^2}$ (D) $E_n = \frac{n^2h^2}{8ma^2}$

[KSET 2013]

67. Perturbation theory is a technique that gives _____
(A) Approximate solution to Schrodinger wave equation
(B) Correct solution to Schrodinger wave equation
(C) Does not deal with Schrodinger wave equation
(D) None of the above

[KSET 2014]

68. Which one of the following statements is not true?
(A) S orbitals are spherically symmetric
(B) A harmonic oscillator obeys Hooke's law
(C) Spin quantum number, S, for an electron S = 1
(D) An azeotrope is a mixture that boils without change of composition

[KSET 2014]

69. Pick out the fermions
i) Electron
ii) Proton
iii) Neutron
iv) Deuteron
(A) iv is correct
(B) i and iv are correct
(C) iii and iv are correct
(D) i, ii and iii are correct

[KSET 2014]

70. An even function is
i) f(–x) = f(x)
ii) Product of two even functions
iii) Product of two odd functions
iv) Product of an even and an odd function
(A) i, ii and iii are correct (B) iv is correct
(C) ii and iv are correct (D) i and iv are correct

[KSET 2014]

71. Linear momentum of photon of wavelength 350 nm is equal to
(A) 0.189×10^{-27} kgms^{-1}
(B) 1.89×10^{-27} kgms^{-1}
(C) 1.89×10^{-26} kgms^{-1}
(D) 1.89×10^{-28} kgms^{-1}

[KSET 2014]

72. Match the following:-

i) Bohr frequency condition	a) $\ominus = \frac{h\nu}{k}$
ii) Debye temperature	b) ΔE = hν
iii) Linear momentum	c) ΩΨ = wΨ
iv) Eigen value equation	d) h/λ

(A) i – b, ii – a, iii – d, iv – c
(B) i – c, ii – a, iii – d, iv – b
(C) i – a, ii – b, iii – c, iv – d
(D) i – d, ii – b, iii – a, iv – c

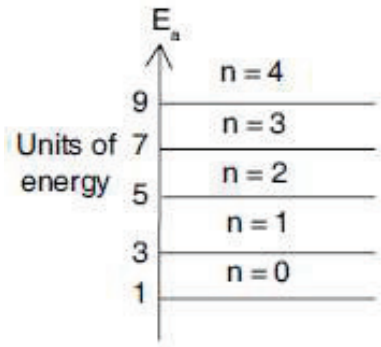
[KSET 2015]

73. For a particle in a one-dimensional box of length L, in the region $0 \leq x \leq \frac{1}{4}$, the probability of the state is given by $p = \frac{1}{4} - \frac{sin\left(\frac{n\pi}{2}\right)}{2\pi}$ Then the probability for the particle in the state n = 2 and n = 1 are respectively:-

(A) 0.125 and 0.25 (B) 0.375 and 0.0908
(C) 0.25 and 0.0908 (D) 0.75 and 0.25

[KSET 2015]

74. The figure shown in the energy level diagram corresponding to:-



(A) Particle in a box (B) Particle tunneling
(C) Harmonic oscillator (D) Hydrogen atom

[KSET 2015]

75. The selection rules for hydrogenic atom are:-

(A) ΔI= ±1 Δm_l = 0, ±1 (B) ΔI=±1 Δm_l =± 1/2
(C) ΔI=0 Δm_l =± ½ (D) ΔI=±1 Δm_l = - ½

[KSET 2015]

76. Choose the correct statement(s)

i) Bosons are particles with half integral spin.
ii) Symmetry number of NH_3 is 3.
iii) The stiffer the bond, the greater is the force constant.
iv) An aerosol is a dispersion of a liquid in a gas

(A) ii, iii and iv are correct (B) i and ii are correct
(C) i is correct (D) iii and iv are correct

[KSET 2016]

77. The simplest ground state VB wave function of a HCI molecule is given as

$\Psi = \Psi_H$ (1s, 1) Ψ_{CI} ($3p_z$, 2) + B , where B represents

(A) Ψ_{CI} (1s, 1) Ψ_H ($3p_z$,3) (B) Ψ_H ($3p_z$,3) Ψ_{CI} (1s,3)
(C) Ψ_{CI} (2s, 2) Ψ_H (1s, 1) (D) Ψ_H (1s, 2) Ψ_{CI} ($3p_z$,1)

[KSET 2016]

78. The unperturbed energy levels of a system are $E_0 = 0$, $E_1 = 2$ and $E_2 = 4$. The second order correction to energy for the ground state in the presence of the perturbation V for which $V_{10} = 2$, $V_{20} = 4$ and $V_{12} = 6$, is found to be

(A) + 6 (B) - 6
(C) – 8 (D) + 8

[KSET 2016]

79. When a particle of mass 9.10 x 10^{-28}g in a certain 1-D box goes from n = 5 level to the n=2 level, it emits a photon of frequency 6.0 10^{14} cm^{-1}. The length of the box is:-

(A) 1.8 x 10^{-7}m (B) 1.8 x 10^{-7} cm
(C) 8.1 x 10^{-7} cm (D) 8.1 x 10^{-7}m

[KSET 2017]

80. Which of the following is incorrect about the de Broglie relationship?

(A) $h = \lambda P$ (B) $E = \frac{hC}{\lambda}$
(C) $\lambda = \frac{h}{mC}$ (D) $E_{knetic} = \frac{2h\nu}{\lambda}$

[KSET 2017]

81. According to the Schrodinger's wave equation, the wave function (Ψ_n) of a particle in one dimensional box is:-

(A) $\Psi_n = A \cdot sin\left(\frac{n\pi x}{a}\right)$ (B) $\Psi_n = A \cdot \sin(n\pi x)$
(C) $\Psi_n = A \cdot sin\left(\frac{n\pi}{a}\right)$ (D) $\Psi_n = A \cdot x \sin(n\pi a)$

[KSET 2017]

82. Indicate which of the following function is acceptable as wave functions?

(A) Ψ = x (B) $\Psi = e^x$
(C) $\Psi = e^{-x}$ (D) $\Psi = e^{-x^2}$

[KSET 2017]

83. In time independent perturbation theory, the perturbation is:-

(A) Always present and unvarying
(B) Not present and unvarying
(C) Always present and varying
(D) Not present and varying

[KSET 2017]

84. The wave function for the bonding molecular orbital for a heteronuclear diatomic XY molecule. Assuming that the electron on an average spends 70% of its time on nucleus X and 30% of its time on nucleus Y is:-

(A) $\Psi_{MO} = 0.70\phi_x + 0.30\phi_y$

(B) $\Psi_{MO} = 0.84\phi_x + 0.55\phi_y$

(C) $\Psi_{MO} = 0.30\phi_x + 0.70\phi_y$

(D) $\Psi_{MO} = 0.55\phi_x + 0.84\ \phi_y$

[KSET 2018]

85. $$\nabla^2 in\ \nabla^2\Psi + \frac{8\pi^2 m}{h^2}(E - V)\Psi = 0$$

is known as

(A) Hamiltonian operator (B) Laplacian operator

(C) Angular momentum (D) Energy operator

[KSET 2018]

86. If the function $f = e^{-ax}$ is acted upon by the operator $\frac{d}{dx}$, the eigen value and eigen function respectively are

(A) $-a$ and e^{-ax} (B) 2a and e^{ax}

(C) ax and e^{-2x} (D) $\frac{d}{dx}$ and e^{ax}

[KSET 2018]

87. The quantum mechanical operator for kinetic energy of a particle moving in three directions is

(A) $\frac{-h^2}{8\pi^2 m}\nabla^2$ (B) $\frac{h}{2\pi i}\nabla$

(B) $\frac{h}{8\pi^2 m}\nabla^2$ (D) $\frac{8\pi^2 m}{h^2}\nabla^2$

[KSET 2018]

88. According to Schrodinger equation the energy of a particle (En) in one dimensional

(A) $E_n = n^2h^2/ma^2$ (B) $E_n = n^2h^2/4ma$

(C) $E_n = n^2h^2/8ma^2$ (D) $E_n = nh/8ma^2$

[KSET 2020]

89. The filling of molecular orbitals takes place according to

(A) The Aufbau principle

(B) Pauli Exclusion principle

(C) Hund's rule of maximum multiplicity

(D) All of the mentioned above

[KSET 2020]

90. Which of the following is not a Huckel approximation in Huckel Molecular Orbital Theory (HMOT)?

(A) HMOT is applicable to planar molecules

(B) The overlap integrals S_{ij} are taken as δ_{ij}

(C) The energy integrals H_{ij} are taken as alpha

(D) The energy integrals H_{ij} are taken as either beta or zero

[KSET 2020]

91. For a free particle in one direction which of the following is correct?

(A) The energy is quantized

(B) The energy can take any negative value

(C) The wave function can be normalized

(D) The energy can take any positive value

[KSET 2020]

92. Which of the following is true for the acceptable wave function for bound state?

(A) The wave function must be real

(B) The wave function must be even Function

(C) The wave function must be quadratically integrable

(D) The wave function must anti-symmetric with respect to interchange of any two particles

[KSET 2020]

93. For a function f(x) = Ae^{-2ix} for $1 \leq x \leq 5$, which one of the following is the value A such that the function is normalised for the given range of values?

(A) Zero (B) One

(C) Two (D) Three

MH SET

[MHSET 2011]

94. The de Broglie wavelength of an electron in a Bohr orbit with radius *r* and quantum number *n* is proportional to:

(A) *nr* (B) 1/*nr*

(C) *n/r* (D) *r/n*

[MHSET 2011]

95. Which of the following conditions is *not* essential for an eigen function of the Hamiltonian operator to be an acceptable wave function?

(A) Continuous (B) Normalized

(C) Always positive (D) Single valued

[MHSET 2011]

96. The number of nodes in a 3*s* orbital is:

(A) 0 (B) 1

(C) 2 (D) 3

[MHSET 2011]

97. The energy of an orbital in the hydrogen atom depends on the quantum number:

(A) *n* (B) *l*

(C) *m* (D) *s*

[MHSET 2011]

98. The three unpaired electrons on the nitrogen atom is ascribed to:

(A) Pauli's exclusion principle
(B) Aufbau principle
(C) Hund's rule
(D) Uncertainty principle

[MHSET 2013]

99. An atom with a single electron has an atomic number of *z*. *m* and *e* are the mass and charge of an electron, respectively. *n* is the principal quantum number of a circular orbit of the electron, around the nucleus. Considering the electrostatic attraction between the electron and the nucleus to be balanced exactly by the centrifugal force arising from the circular motion of the electron, the radius of the orbit of *n* = 2 is:

(A) $\frac{4(h/2\pi)^2}{mze^2}$ (B) $\frac{2(h/2\pi)^2}{mze^2}$
(C) $\frac{4mze^2}{(h/2\pi)^2}$ (D) $\frac{2mze^2}{(h/2\pi)^2}$

[MHSET 2013]

100. The number of quantum numbers of a free electron (one that is not bound to a nucleus) is:

(A) 0 (B) 1
(C) 2 (D) 4

[MHSET 2015]

101. The average value of r^2 (i.e., $< r^2 >$) in the 1s orbital of hydrogen atom is (a_0 is the Bohr radius)

(A) a_0 (B) 0.5 ${a_0}^2$
(C) $3{a_0}^2$ (D) 1.5 ${a_0}^3$

[MHSET 2016]

102. The hydrogenic orbital having two radial nodes and one angular node in their appropriate representations is:

(A) 3d (B) 4p
(C) 5d (D) 5p

[MHSET 2016]

103. The hydrogenic orbital with its (unnormalized) spherical harmonic part being $sin^2\theta\ sin^2\phi$ represents which of the following orbital?

(A) $d_{x^2-y^2}$ (B) d_{z^2}
(C) d_{yz} (D) d_{xy}

[MHSET 2013]

104. An electron of mass 'm' is confined to a 1-D box of length 'L'. It makes a radiative transition from second excited state to ground state. The wavenumber of the photon emitted is:

(A) $\frac{h}{mL^2c}$ (B) $\frac{2h}{mL^2c}$
(C) $\frac{9h}{mL^2c}$ (D) $\frac{3h}{mL^2c}$

[MHSET 2013]

105. The wave function of a 1-D harmonic oscillator between x = –∞ and x = +∞ is given by:

$$\Psi(x) = \text{N exp}\left(-\frac{\beta x^2}{2}\right).$$

$$\left(\int_0^\infty e^{-ax^2}\frac{1}{2}\left(\frac{\pi}{a}\right)^{1/2}\right)$$

The value of N, that normalizes the function $\Psi(x)$, is:

(A) $\left(\frac{\beta}{\pi}\right)^{1/2}$ (B) $\left(\frac{\beta}{\pi}\right)^{1/4}$
(C) $\left(\frac{\beta}{2\pi}\right)^{1/2}$ (D) $\left(\frac{\pi}{\beta}\right)^{1/4}$

[MHSET 2013]

106. The molecular orbitals of 1, 3-butadiene (not in proper order) are given below: (f_1, f_2, f_3, f_4 are the 2pz orbitals on carbon atoms 1, 2, 3 and 4 respectively).

$\psi_1 = 0.372f_1 – 0.602f_2 + 0.602f_3 – 0.372f_4$.
$\psi_2 = 0.602f_1 + 0.372f_2 – 0.372f_3 – 0.602f_4$.
$\psi_3 = 0.372f_1 + 0.602f_2 + 0.602f_3 + 0.372f_4$.
$\psi_4 = 0.602f_1 – 0.372f_2 – 0.372f_3 + 0.602f_4$.

The HOMO and LUMO in the ground state of 1, 3-butadiene are respectively:

(A) ψ_2 and ψ_3 (B) ψ_3 and ψ_2
(C) ψ_2 and ψ_4 (D) ψ_2 and ψ_1

[MHSET 2013]

107. The Slater determinant (un-normalized) for the ground state of lithium atom is:

(A) $\begin{vmatrix} 1s(1)\alpha(1) & 1s(1)\beta(1) & 2s(1)\alpha(1) \\ 1s(2)\alpha(2) & 1s(2)\beta(2) & 2s(2)\alpha(2) \\ 1s(3)\alpha(3) & 1s(3)\beta(3) & 2s(3)\alpha(3) \end{vmatrix}$

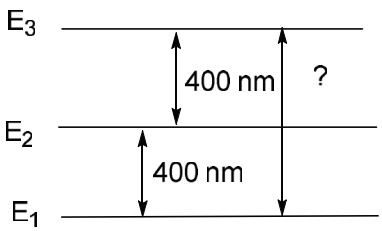
(B) $\begin{vmatrix} 1s(1)\alpha(1) & 1s(1)\beta(1) & 1s(1)\alpha(1) \\ 1s(2)\alpha(2) & 1s(2)\beta(2) & 1s(2)\alpha(2) \\ 1s(3)\alpha(3) & 1s(3)\beta(3) & 1s(3)\alpha(3) \end{vmatrix}$

(C) $\begin{vmatrix} 1s(1)\alpha(1) & 1s(1)\beta(1) & 1s(1)\beta(1) \\ 1s(2)\alpha(2) & 1s(2)\beta(2) & 1s(2)\beta(2) \\ 1s(3)\alpha(3) & 1s(3)\beta(3) & 1s(3)\beta(3) \end{vmatrix}$

(D) $\begin{vmatrix} 1s(1)\alpha(1) & 2s(1)\alpha(1) & 2s(1)\beta(1) \\ 1s(2)\alpha(2) & 2s(2)\alpha(2) & 2s(2)\beta(2) \\ 1s(3)\alpha(3) & 2s(3)\alpha(3) & 2s(3)\beta(3) \end{vmatrix}$

[MHSET 2013]

108. The separation between E_1 and E_3 in the following energy level diagram will be:



(A) 800 nm (B) 400 nm
(C) 200 nm (D) 300 nm

[MHSET 2013]

109. The commutator of $[x^2, p_x]$ is equal to:
(A) $\frac{hx}{\pi i}$ (B) $\frac{2hx}{\pi i}$
(C) $\frac{hx^2}{2\pi i}$ (D) $-\frac{hx}{\pi i}$

[MHSET 2013]

110. The life time of a state that gives rise to a spectral line of width 0.1 cm^{-1} is:
(A) 53 nm (B) 53 pm
(C) 33 nm (D) 33 pm

[MHSET 2013]

111. The wave function for a particle in a 1-D box of length 'L' is given as $\psi = A \sin \frac{\pi x}{L}$. The value of 'A' for a box of length 50 nm is:
(A) $5\sqrt{2}\ (nm)^{1/2}$ (B) $0.2\ (nm)^{-1/2}$
(C) $0.2\ (nm)^{1/2}$ (D) $\sqrt{5}/10\ (nm)^{-1/2}$

[MHSET 2013]

112. The quantum state of a particle in a circular path in a plane is given by:
$\Psi_m(\phi) = \left(\frac{1}{\sqrt{2\pi}}\right) e^{-im\phi}$, m = 0, ±1, ± 2, …….
When a perturbation H' = P cos θ is applied (P is a constant), what will be the first order correction to the energy of the m^{th} state?
(A) 0 (B) P/(2π)
(C) P/(4π) (D) $Pm^2/(4\pi^2)$

[MHSET 2013]

113. The molecular orbitals of 1, 3-butadiene (not in proper order) are given below:
(f_1, f_2, f_3, f_4 are the 2pz orbitals on carbon atoms.)
$\psi_1 = 0.372f_1 - 0.602f_2 + 0.602f_3 - 0.372f_4$
$\psi_2 = 0.602f_1 + 0.372f_2 - 0.372f_3 - 0.602f_4$
$\psi_3 = 0.372f_1 + 0.602f_2 + 0.602f_3 + 0.372f_4$
$\psi_4 = 0.602f_1 - 0.372f_2 - 0.372f_3 + 0.602f_4$
The correct order of the orbitals with increasing energy is:
(A) $\psi_1 < \psi_2 < \psi_3 < \psi_4$
(B) $\psi_3 < \psi_2 < \psi_4 < \psi_1$
(C) $\psi_3 < \psi_4 < \psi_1 < \psi_2$
(D) $\psi_4 < \psi_3 < \psi_2 < \psi_1$

[MHSET 2015]

114. The number of nodes of any orbital of hydrogen atom, other than the origin and at infinity, is given by
(A) $n - l - 1$
(B) $n - 1$
(C) n
(D) $n + l$

[MHSET 2015]

115. An electron in the ground state of hydrogen atom is excited to a level having principle quantum no. n. It was found to absorb at wavelength λ of the electromagnetic spectrum. The value of n is (R = Rydberg constant)
(A) $\sqrt{\frac{R}{\lambda - 1}}$ (B) $\sqrt{R\lambda(\lambda - 1)}$
(C) $\sqrt{\frac{R\lambda}{R\lambda - 1}}$ (D) $\sqrt{\frac{R\lambda - 1}{R\lambda}}$

[MHSET 2015]

116. Based on Huckel treatment of π electron in conjugated cyclic hydrocarbons, which of the following statements is incorrect.
(A) Lowest energy level in all such system is degenerate.
(B) Ground state of cyclobutadiene is a triplet.
(C) Delocalization energy of benzene is about 150 kJ mol^{-1}.
(D) The value of resonance integral between neighbouring atoms is β.

[MHSET 2015]

117. States arising from two p electrons are (symbols have their usual meaning)
(A) ^3P, ^3D, ^1S (B) ^2D, ^1P, ^1S
(C) ^1S, ^3P, ^1P (D) ^3P, ^1D, ^1S

[MHSET 2015]

118. The Ms = 0 component of triplet state arising from two electrons is (symbols have their usual meaning)
(A) $\alpha(1)\,\beta(2)$
(B) $\alpha(2)\,\beta(1)$
(C) $\frac{1}{\sqrt{2}}[\alpha(1)\,\beta(2) + \beta(1)\,\alpha(2)]$
(D) $\frac{1}{\sqrt{2}}[\alpha(1)\,\beta(2) - \beta(1)\,\alpha(2)]$

[MHSET 2015]

119. The degeneracy of the energy level that corresponds to energy $\frac{19}{m}\left(\frac{\pi\hbar}{a}\right)^2$ of a particle in a cubic box of length 'a' is:
(A) 3 (B) 6
(C) 9 (D) 1

[MHSET 2015]

120. The delocalization energy of butadiene molecule within the HMO framework of theory (β being the empirical parameter therein) is given by:
(A) β (B) $0.472\,\beta$
(C) $2\,\beta$ (D) $4\,\beta$

[MHSET 2015]

121. The most probable distance of 2s electron (in Å) in the ground state of H atom is:
(A) 1.058 (B) 2.116
(C) 0.529 (D) 0.794

[MHSET 2016]

122. The trial function for the particle in 1D box (with $0 \leq x \leq a$) leading to the best possible ground state energy employing the variational method should be
(A) $x^{\alpha}(a-x)^{\beta}$ (B) $\sin\left(\frac{\pi x}{a}\right)$
(C) x(a-x) (D) $x^2(a-x)^2$

[MHSET 2016]

123. The commutator $[\hat{x}, \hat{p}_x]$ is equal to:
(A) -i$\hbar$ (B) 0
(C) $\hat{p}_z$ (D) 1

[MHSET 2016]

124. The average separation of $2p_z$ electron of the H atom from the nucleus will be (a_0 Bohr radius):
(A) $3a_0/2$ (B) $5a_0$
(C) $4a_0$ (D) a_0

[MHSET 2016]

125. Which of the following statement is not correct about the quantum mechanical harmonic oscillator?
(A) The amplitude of a quantum mechanical harmonic oscillator in its ground state will not exceed its classical value in lower energy states.
(B) The average values of <x> and <p> are zero.
(C) In highly excited states the quantum mechanical oscillator behaves as a classical oscillator
(D) The wave function for quantum mechanical harmonic oscillator is always either odd or even

[MHSET 2017]

126. To every observable in classical mechanics there exists a corresponding linear ……. in quantum mechanics.
(A) Hamiltonian operator (B) Probability function
(C) Hermitian operator (D) Non-commutator

[MHSET 2017]

127. Which of the following statements is not true for quantum mechanical harmonic oscillator?
(A) The smaller the mass of the oscillation particle, the greater will be its zero-point energy, for a fixed force constant.
(B) The frequency is the same as that of a classical oscillator with the same mass and force constant.
(C) Increasing the force constant increases the spacing between adjacent energy levels.
(D) The vibrational potential energy is a constant of motion.

[MHSET 2017]

128. The spin multiplicity of an atom in its ground state and having the outershell configuration $4s^2 3d^7$ is:
(A) 19 (B) 15
(C) 7 (D) 4

[MHSET 2017]

129. Which of the following is a prediction that would result from a simple HMO treatment of the butadienyl cation, $C_4H_6^+$?
(A) The ESR coupling constant is larger for hydrogens attached to the two inner carbons.
(B) The central C-C bond has a higher π-bond order than it has in the neutral molecule.
(C) The positive charge resides mostly on the two central carbons.
(D) The MO coefficients on the central pair of carbons are larger in all of the π MOs than they are in the neutral molecule.

[MHSET 2017]

130. Which of the following is/are acceptable quantum mechanical wave functions?
(i) $f(X) = X^2 + 1$, for all values of X
(ii) $\Psi = 1 / (4 - X)$; $0 \leq X \leq 10$
(iii) $\Psi = 1 / (4 - X)$; $0 \leq X \leq 3$
(A) (ii) and (iii) (B) (i) only
(C) (i) and (iii) (D) (iii) only

[MHSET 2017]

131. The ionization energy for hydrogen atom is 13.6 eV. The ionization energy for the ground state of Li^{2+} is :
(A) 27.2 eV (B) 6.8 eV
(C) 122.4 eV (D) 40.8 eV

[MHSET 2017]

132. Which of the following is not a feature of Born Oppenheimer approximation?
(A) Nuclear coordinates remain unchanged during electronic transitions
(B) Excited and ground electronic states have the same internuclear distance
(C) Electronic and vibrational motions are separable
(D) Amplitude of nuclear vibrations is smaller than that of electrons

[MHSET 2018]

133. A particle in a one-dimensional box of length L can be excited from n = 1 to n = 2 state with frequency. If the box length is doubled, the frequency needed to achieve this transition is:
(A) v/4 (B) v/2
(C) 2v (D) 4v

[MHSET 2018]

134. If operator $\widehat{D}^n$(n times differentiate with respect to x) operates on eigen function e^{ax}, the eigenvalue would be:
(A) $n\alpha$ (B) n^α
(C) α^n (D) n ! α

[MHSET 2018]

135. The eigen functions of a rigid rotator are:
(A) Spherical harmonics
(B) Laguerre polynomials
(C) Hermite polynomials
(D) Legendre transformers

[MHSET 2018]

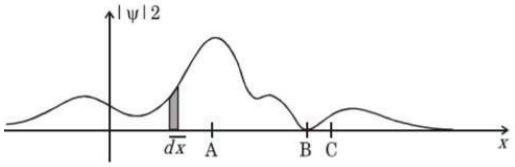
136. According to Hund's rule, most stable state for np^2 configuration is ...
(A) $^1S_0$ (B) $^3P_0$
(C) $^3P_1$ (D) $^3P_2$

[MHSET 2018]

137. According to simple HMO theory, which one of the following statements about butadiene is true?
(A) It has a non-bonding MO
(B) Exciting an electron from the HOMO to the LUMO will not change the π bond orders
(C) Exciting an electron from the HOMO to the LUMO will not change the π charge densities
(D) It is most likely to undergo electrophilic substitution at one of the two inner carbons

[MHSET 2018]

138. Given below is the wave function of a particle: Which of the following is correct?



(A) The particle is more likely to be found near B
(B) The particle is more likely to be found near A
(C) The shaded area represents the energy of the particle when it travels through a distance dx
(D) The shaded area represents the amplitude of the particle in an area dx

[MHSET 2018]

139. The de Broglie wavelength of an electron travelling with 1% speed of light is about:
(mass of electron and speed of light are 9.109×10^{-31} kg and 2.998×10^8 ms^{-1} respectively):
(A) 243 m (B) 243 cm
(C) 243 Å (D) 243 pm

[MHSET 2019]

140. If the radius of the hydrogen atom is 53 pm, the radius of the He+ ion will be close to:
(A) 75 pm (B) 38 pm
(C) 106 pm (D) 27 pm

[MHSET 2019]

141. Which of the following equations corresponds to photoelectric effect?
(A) h_λ = W_0 + K.E (B) $h\nu$ = W_0 - K.E
(C) $h\nu$ = W_0 + K.E (D) h_λ = W_0 - K.E

[MHSET 2019]

142. The momentum operator in one-dimension is ...
(A) $-\hbar \frac{\partial}{\partial x}$ (B) $-i\left(\frac{\hbar \partial}{\partial t}\right)$ - $\hbar \frac{\partial}{\partial t}$
(C) $-i\hbar \frac{\partial}{\partial x}$ (D) i- $\hbar \frac{\partial}{\partial t}$

[MHSET 2020]

143. Which of the following is correct?
(A) In X-ray photoelectron spectroscopy valence electrons are ejected.
(B) K. E of photoelectrons increase when the intensity of the incident X-rays is increased.
(C) K. E of photoelectrons decreases when the oxidation state of the surface is increased.
(D) Number of photoelectrons emitted increases with frequency of the incident X-rays.

[MHSET 2020]

144. A particle can occupy either the ground state at E = 0 or an excited state at E > 0. At a temperature T, the probability of the particle being in the excited state is:
(A) 0 (B) $1 + \exp\left(-\frac{E}{K_B T}\right)$
(C) $\frac{\exp\left(-\frac{E}{K_B T}\right)}{1 + exp\left(-\frac{E}{K_B T}\right)}$ (D) $\frac{1}{1 + exp\left(-\frac{E}{K_B T}\right)}$

[MHSET 2020]

145. According to Einstein's photoelectric equation, the slope of the plot of kinetic energy of the photoelectrons vs. the frequency of the incident radiation:
(A) Will depend upon the nature of the metal that emits the photoelectrons
(B) Will depend on the intensity of the incident radiation
(C) Will depend on both the intensity of the radiation and the nature of the metal
(D) Will be the same for all metals and independent of intensity of radiation

[MHSET 2020]

146. for a simple harmonic oscillator:
(A) Potential energy varies linearly with displacement from equilibrium
(B) Spacing between energy levels increases with increasing energy
(C) Spacing between energy levels decreases with increasing energy
(D) Number of nodes of the wave function increases with increase in energy

[MHSET 2020]

147. Which of the following is correct for H_2^+ ion?
(A) A possible trial wave function for the ion is $\Psi = C_1\ 1S_A \pm C_2\ 1S_B$
(B) The coefficients of the trial wave function are not equal
(C) A possible trial wave function is $\Psi = C_1\ 1S_A / C_2\ 1S_B$
(D) The 1S orbitals are not normalised

[MHSET 2020]

148. Which of the following is true according to variation theorem?
(I) the ground state energy of a quantum mechanical system is zero.
(II) $\frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\ |\Psi\rangle} \geq E_0$
(III) $\frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\ |\Psi\rangle} = E_0$
(IV) The ground state energy of a quantum mechanical system is infinite.
(A) (I) and (II) (B) (II) only
(C) (III) only (D) (I) and (IV)

[MHSET 2021]

149. The ratio of the energy of the electron in the ground state of hydrogen atom to that of the electron in the first excited state of Be3+ is :
(A) 1 : 4 (B) 1 : 8
(C) 2 : 9 (D) 1 : 16

[MHSET 2021]

150. A proton is 1836 times heavier than an electron. The ratio of the de Broglie wavelengths, λ_e/λ_P is :
(A) 1 : $(1836)^2$ (B) $(1836)^{1/2}$: 1
(C) 1836 : 1 (D) $(1836)^2$: 1

[MHSET 2021]

151. The energy of a particle in a three-dimensional box of equal side lengths is given as :

$$E = \frac{h^2}{8ma^2}\left(n_x^2 + n_y^2 + n_z^2\right)$$

The degeneracy of energy for the levels nx ny nz = 1, 1, 1, 2, 1, 1 and 3, 2, 1 respectively are:
(A) 3, 4, 6 (B) 1, 1, 1
(C) 1, 3, 6 (D) 1, 3, 3

[MHSET 2021]

152. Ionization energy of hydrogen atom is 13.6 eV; the ionization energy for the ground state of Li^{2+} is approximately:
(A) 27.2 eV (B) 40.8 eV
(C) 54.4 eV (D) 122.4 eV

TAMILNADU SET

[TAMILNADU]

153. For an Eigen function α^{ihx} of linear momentum operator $\dot{P}x$ the Eigen value is
(A) *ik* (B) *i*
(C) *i* (D) $\hbar$

[TAMILNADU]

154. _____ is Laplacian operator.
(A) $\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ (B) $i\frac{\partial}{\partial x} + j\frac{\partial}{\partial y} + k\frac{\partial}{\partial z}$
(C) $\hat{A}\psi = \alpha\psi$ (D) $\hat{A}\widehat{A^n} - \widehat{A^n}A$

TELANGANA SET

[TELANGANA 2012]

155. The value of the Planck's constant is
(A) 6.626×10^{-34} J-s (B) 6.626×10^{-27} J-s
(C) 1.380×10^{-23} JK^{-1} (D) 9.109×10^{-31} Kg

[TELANGANA 2012]

156. If an arbitrary wave function is used to calculate the energy of a quantum mechanical system the calculated energy is never less than the true energy of the system. This statement is
(A) Heisenberg uncertainty principle
(B) Perturbation theory
(C) Law of conservation of energy
(D) Variation principle

[TELANGANA 2013]

157. When the label of any two identical fermions are exchanged, the total wave function changes sign, when the labels of any two identical Bosons are exchanged the total wave function retains the same sign. This statement is
(A) Pauli principle
(B) Heisenberg uncertainty principle
(C) Variation principle
(D) Perturbation theory

[TELANGANA 2013]

158. Because the nuclei are so much more massive than the electrons, an electronic transition takes place very much faster than the nuclei can respond. This is the
(A) Heisenberg uncertainty principle
(B) Franck Condon principle
(C) Pauli principle
(D) Born-Oppenheimer approximation

[TELANGANA 2013]

159. The Balmer series in the spectrum of atomic H arise from the transitions $\left(\nabla = R_H\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)\right)$
(A) $n_1 = 1$ (B) $n_1 = 2$
(C) $n_1 = 3$ (D) all of the above

[TELANGANA 2013]

160. In the orbital approximation where each electron occupies its own orbital $\psi(r_1, r_2, r_3 ...)$ =
(A) $\psi_1(r_1) + \psi_2(r_2) + \psi_3(r_3) + ...$
(B) $-\psi_1(r_1) - \psi_2(r_2) - \psi_3(r_3) ...$
(C) $\psi_1(r_1).\psi_2(r_2).\psi_3(r_3) ...$
(D) $\psi_1(r_1) + \psi_2(r_2) - \psi_3(r_3) ...$

[TELANGANA 2014]

161. The number of radial nodes for a 3s orbital is
(A) 0 (B) 1
(C) 2 (D) 3

[TELANGANA 2014]

162. Wave function of a particle at some point x has the value ψ , then the probability of finding the particle between x and x + dx is proportional to
(A) $|\psi|\,dx$ (B) $|\psi|^3 dx$
(C) $|\psi|^2\,dx$ (D) $|\psi|$

[TELANGANA 2014]

163. Zero-point energy (E_o)of a harmonic oscillator is
(A) $E_o = h^2/8\,mL^2$ (B) $E_o = ½\,h\,\nu$
(C) $E_o = 0$ (D) $E_o = 4h^2 / 8\,m$

[TELANGANA 2014]

164. The ground state term symbol of Li is
(A) $^2S_{\frac{1}{2}}$ (B) $^2P_{\frac{1}{2}}$
(C) $^1S_{\frac{1}{2}}$ (D) $^1D_2$

[TELANGANA 2017]

165. If uncertainty in position and momentum are equal, then uncertainty in velocity is:
(A) $1/2m\sqrt{h/\pi}$
(B) $1/m\sqrt{h/\pi}$
(C) $1/3m\sqrt{h/2\pi}$
(D) $1/4m\sqrt{h/\pi}$

[TELANGANA 2017]

166. The degeneracy of a quantum particle in cubic box having energy four times that of the lowest energy is:
(A) 3 (B) 1
(C) 6 (D) 4

[TELANGANA 2017]

167. Which of the following is not linear operator?
(A) d^2/dx^2 (B) $\hat{P}_x$
(C) $\hat{H}$ (D) $\sqrt{}$

[TELANGANA 2017]

168. According to Huckel MO treatment the four π-MO energies of butadiene are given by $\alpha \pm 1.62\beta$ and $\alpha \pm 0.62\beta$. The delocalization energy of butadiene is:
(A) 0.62β (B) 0.48β
(C) 1.62β (D) 1.48β

[TELANGANA 2017]

169. If a trial wave function is used to calculate the energy of a quantum mechanical system, the calculated energy is always greater than the true energy. The statement is related to:
(A) Perturbation theory
(B) Variation principle
(C) Born-Oppenheimer approximation
(D) Heisenberg uncertainty principle

[TELANGANA 2012]

170. Huckel MO energy levels of ethylene are
(A) $\alpha + 2\beta; \alpha - 2\beta$ (B) $\alpha + \beta; \alpha - \beta$
(C) $\alpha + 1/2\beta; \alpha - 1/2\beta$; (D) $\alpha + 3\beta; \alpha - 3\beta$

[TELANGANA 2012]

171. Match the following :

List I	**List II**
I. $H\psi = E\psi$	1. Planck
II. $E = h\nu$	2. Born
III. $\|\psi\|^2$	3. Dirac
IV. $\lambda = h/mV$	4. De Broglie
	5. Schrodinger

	I	II	III	IV
(A)	5	1	2	4
(B)	1	2	3	4
(C)	4	5	2	1
(D)	3	2	4	1

[TELANGANA 2012]

172. In quantum mechanical tunnelling the transmission coefficient
(A) Increases with the thickness of the barrier
(B) Decreases exponentially with the thickness of the barrier

(C) Decreases with the square of the thickness of the barrier

(D) Does not depend on the thickness of the barrier

[TELANGANA 2012]

173. Example of fermions are

(A) Electron and proton (B) Photon and proton

(C) Electron and photon (D) Photons

[TELANGANA 2012]

174. Lowest allowed energy is equal to zero for a

(A) Harmonic oscillator

(B) Particle in a two dimensional box

(C) A rigid rotator

(D) Hydrogen atom

[TELANGANA 2012]

175. An electron of mass 'm' is confined to a one dimensional box of length 'l'. The frequency of the radiation absorbed during its excitation from its second energy level to third level is

(A) $\frac{5h}{8ml^2}$ (B) $\frac{h}{8ml^2}$

(C) $\frac{3h}{8ml^2}$ (D) $\frac{4h}{8ml^2}$

[TELANGANA 2013]

176. Match the following

List – I	List – II
I) Planck	1) 6.023×10^{23} mol^{-1}
II) Rydberg	2) 1.381×10^{-23} JK^{-1}
III) Boltzman	3) 1.0974×10^{5} cm^{-1}
IV) Avogadro	4) 6.626×10^{-34} J-s
V) Faraday	

	1	2	3	4
(A)	V	III	II	I
(B)	IV	III	II	I
(C)	III	II	I	IV
(D)	IV	V	I	II

[TELANGANA 2013]

177. The correct statements among the following are

1) An acceptable wave function must be continuous
2) An acceptable wave function must be single valued
3) An acceptable wave function must not be square integrable
4) An acceptable wave function must have continuous first derivative

(A) 1, 2, 4 (B) 1, 2, 3

(C) 2, 3, 4 (D) 1, 3, 4

[TELANGANA 2013]

178. Identify the eigen function of the operator d/dx from the following

(A) x^2 (B) e^x

(C) x (D) $x^2 - x$

[TELANGANA 2013]

179. If an arbitrary wave function is used to calculate the energy using variation theory, the value calculated is

(A) Never greater than the true energy

(B) Never less than the true energy

(C) Always equal to the true energy

(D) Always equal to zero

[TELANGANA 2014]

180. The Hamiltonian for the internal motion of a hydrogen like atom is given by

(A) $\frac{-\hbar^2}{2\mu}\nabla^2 - \frac{Ze^2}{4\pi\epsilon_0 r}$ (B) $\frac{-\hbar^2}{2\mu}\nabla^2 + \frac{Ze^2}{4\pi\epsilon_0 r}$

(C) $\frac{-\hbar^2}{2\mu}\nabla^2$ (D) $\frac{-\hbar^2}{2\mu}\nabla^2 + {}^1/_2\, kx^2$

[TELANGANA 2014]

181. The correct statements among the following are:

1) Angular momenta of 1s, 2s and 3s orbitals are same
2) Energies of 1s, 2s and 3s orbitals are same
3) Angular momenta of 1s, 2s and 3s orbitals are different
4) Energies of 1s, 2s and 3s orbitals are different

(A) 1, 2 (B) 2, 3

(C) 3, 4 (D) 1, 4

[TELANGANA 2014]

182. The perturbation Hamiltonian $H^{(1)}$, for the first order correction to the ground-state energy for a particle in a box with a variation in the potential v = – ϵ sin (πx/L) is given by

(A) – ϵ sin (πx/L) (B) $\epsilon^2 \sin^2$ (πx/L)

(C) $\epsilon^3 \sin^3$ (πx/L) (D) ϵ^3

[TELANGANA 2014]

183. A particle of mass 'm' is confined between two walls of a box at x = 0 and x = 2L. The potential energy is zero inside this one dimensional box but rises abruptly to infinity at the walls. The energy of this particle (E) is given by

(A) $\frac{n^2h^2}{8mL^2}, n = 1,2 \ldots$ (B) $\frac{n^2h^2}{32mL^2}, n = 1,2 \ldots$

(C) $\frac{n^2h^2}{16mL^2}, n = 1,2 \ldots$ (D) $\frac{n^2h^2}{18mL^2}, n = 0,1,2 \ldots$

[TELANGANA 2014]

184. The energies E+ of bonding and E– of antibonding orbitals of a homonuclear diatomic molecule are given by the secular determinant $\begin{vmatrix} a-E & \beta-ES \\ \beta-ES & a-E \end{vmatrix}$ the solutions of this equations are

(A) $E_{\pm} = \frac{a \mp \beta}{S}$ (B) $E_{\pm} = \frac{a \mp \beta}{1-S}$

(C) $E_{\pm} = \frac{a\beta}{1 \pm S}$ (D) $E_{\pm} = \frac{a \pm \beta}{1 \pm S}$

[TELANGANA 2014]

185. Match the following

List – I

I. Orbital angular momentum quantum number

II. Magnetic quantum number

III. Spin quantum number

IV. Total angular momentum quantum number

List – II

1. M_l
2. l
3. j
4. S

	1	2	3	4
(A)	I	II	III	IV
(B)	I	III	II	IV
(C)	II	I	IV	III
(D)	III	IV	I	II

[TELANGANA 2014]

186. Which one of the following spin wave functions (Ψ_{spin}) is antisymmetric?

(A) Ψ_{spin} = [α(1)β (2) – β (1) α(2)]

(B) Ψ_{spin} = β (1)β (2)

(C) Ψ_{spin} = α(1) α(2)

(D) Ψ_{spin} = [α(1)β (2) + β (1)α(2)]

[TELANGANA 2014]

187. According to HMO theory, the possible energy levels for ethylene in terms of coulombic (α) and exchange (β) integrals are

(A) (α+β) and (2α + β) (B) (α+β) and (α – 2β)

(C) (α+2β) and (α –2β) (D) (α+β) and (α – β)

[TELANGANA 2017]

188. What is the order of energies of 4s, 4p, 4d and 4f orbitals of hydrogen atom?

(A) 4s > 4p > 4d > 4f (B) 4s < 4p < 4d < 4f

(C) 4s > 4p < 4d < 4f (D) 4s = 4p = 4d = 4f

[TELANGANA 2017]

189. The valence bonding molecular orbital of a hydrogen chloride HCl molecule may be described as the linear combination of the hydrogen 1s and chloride 3p atomic orbitals.

$\Psi = 0.23\Psi_H + 0.77\Psi_{Cl}$. Calculate the probability of finding an electron in a 1s orbital on hydrogen is:

(A) 8.2%

(B) 23%

(C) 77%

(D) 54%

[TELANGANA 2017]

190. Calculated the probability that an electron described by a hydrogen atomic 1s wave function will be found within one Bohr radius of the nucleus.

(A) 33.3% (B) 50%

(C) 32.3% (D) 23%

[TELANGANA 2017]

191. The expression for the following operator $\left(\frac{d}{dx} + x\right)^2$ is:

(A) $\frac{d^2}{dx^2} + x\frac{d}{dx} + x^2 + 1$ (B) $\frac{d^2}{dx^2} + 1 + x^2$

(C) $\frac{d^2}{dx^2} + 1 - x^2$ (D) $\frac{d^2}{dx^2} + 2x\frac{d}{dx} + x^2$

[TELANGANA 2017]

192. The lowest allowed energy is equal to zero for:

(A) Hydrogen atom

(B) A particle in a three dimensional box

(C) An harmonic oscillator

(D) A rigid rotor

[TELANGANA 2018]

193. According to Huckel Molecular Orbital Theory (HMO) the possible energy in terms of Coulombic (α) and exchange (β) integrals are

(A) $(\alpha + \beta)$, α, $(2\,\alpha + \beta)$, $(2\,\alpha - \beta)$

(B) $(\alpha + 2\beta)$, 2α, $(\alpha - 2\beta)$, $(2\,\alpha + \beta)$

(C) $(\alpha + 2\beta)$, α, α, $(\alpha - 2\beta)$

(D) α, α, $(\alpha + \beta)$, $(\alpha + 2\beta)$

[TELANGANA 2018]

194. The average position of a particle in one dimensional box of length L is

(A) L (B) L/2

(C) 2L (D) 12L

[TELANGANA 2018]

195. Average distance for 2s orbital of He+ is

(A) 1A° (B) 2A°

(C) 3A° (D) 4A°

[TELANGANA 2018]

196. The radial function 'R' depends on

1. n
2. l
3. m
4. s

(A) 1, 2 (B) 1, 4

(C) 2, 3 (D) 3, 4

WBSET

[WBSET 2015]

197. The average value of r^2 (i.e., $< r^2 >$) in the 1s orbital of hydrogen atom is (a_0 is the Bohr radius)
(A) a_0 (B) 0.5 a_0^2
(C) $3a_0^2$ (D) 1.5 a_0^3

[WBSET 2017]

198. The wave function of the electron in the lowest energy state of hydrogen atom is proportional to exp(–r/a_o) where a_o is a constant. The relative probability of finding the electron inside a volume d_v at a_o relative to nucleus is:
(A) 14·2 (B) 13·6
(C) 0·71 (D) 7·1

[WBSET 2017]

199. The set of angular parts of 2pz, 2px, 2py orbitals of hydrogen atom are:
(A) cosθ, – sinθ$e^{i\varphi}$, sinθ$e^{-i\varphi}$
(B) cosθ, – sinθ$e^{i\varphi}$, sinθ$e^{i\varphi}$
(C) sinθ, – cosθ$e^{i\varphi}$, sinθ$e^{-i\varphi}$
(D) cosθ, sinθ cosφ, sinθ sinφ

[WBSET 2017]

200. For a hetero nuclear diatomic molecule which of the following statements is true?
As the energy difference between the two interacting atomic orbitals increases
(A) both bonding and antibonding effects increases.
(B) both bonding and antibonding effects decreases.
(C) bonding effect decreases but anti bonding effect increases.
(D) bonding effect increases but anti bonding effect decreases.

[WBSET 2015]

201. The number of nodes of any orbital of hydrogen atom, other than the ones at the origin and at infinity, is given by
(A) $n-1-1$ (B) $n-1$
(C) n (D) $n+1$

[WBSET 2015]

202. An electron in the ground state of hydrogen atom is excited to a level having principal quantum no. n. It was found to absorb at wavelength 2 of the electromagnetic spectrum. The value of n is
(R = Rydberg constant)
(A) $\sqrt{\frac{R}{\lambda-1}}$ (B) $\sqrt{R\lambda(\lambda-1)}$
(C) $\sqrt{\frac{R\lambda}{R\lambda-1}}$ (D) $\sqrt{\frac{R\lambda-1}{R\lambda}}$

[WBSET 2015]

203. Based on Hückel treatment of π it electrons in conjugated cyclic hydrocarbons, which of the following statements in incorrect.
(A) Lowest energy level in all such systems is degenerate.
(B) Ground state of cyclobutadiene is a triplet.
(C) Delocalization energy of benzene is about 150 kJ / mole
(D) The value of resonance integral between neighbouring atoms is B

[WBSET 2015]

204. The M_S = 0 component of triplet state arising from two electrons is (symbols have their usual meaning)
(A) $\alpha(1)\,\beta\,(2)$
(B) $\alpha\,(2)\,\beta\,(1)$
(C) $\frac{1}{\sqrt{2}}\,[\alpha(1)\,\beta\,(2) + \beta\,(1)\,\alpha(2)]$
(D) $\frac{1}{\sqrt{2}}[\alpha(1)\,\beta\,(2) - \beta\,(1)\,\alpha(2)$

[WBSET 2017]

205. Which of the following trial wave functions may be used to calculate the first excited state of harmonic oscillator by variational method with a as a parameter?
(A) e^{-ax^2} (B) xe^{-ax^2}
(C) $(x^2-1)e^{-ax^2}$ (D) xe^{-ax}

[WBSET 2017]

206. The wavelength of a charged particle (λ),varies with potential difference (E) through which it is acclarated as:
(A) $\lambda \propto \frac{1}{E}$ (B) $\lambda \propto E$
(C) $\lambda \propto E^{-1/2}$ (D) $\lambda \propto \sqrt{E}$

[WBSET 2017]

207. If someone recognizes that $p(x) = Ce^{-2/2x^2}$ is an even function, then the value of C is determined to be:
(A) $\left(\frac{\pi a^2}{2}\right)^{1/2}$ (B) $\frac{1}{2\pi a^2}$
(C) $\frac{1}{(\pi a^2)^{1/2}}$ (D) $\frac{1}{(2\pi a^2)^{1/2}}$

[WBSET 2017]

208. If e^{ax} is an eigenfunction of the operator d^n/dx^n, the eigenvalue is found to be:
(A) a^n (B) a
(C) na (D) $\frac{1}{a^n}$

209. The probability of finding a particle in an one-dimensional box of length a is found to be:
(A) between $-a/2$ to $a/2$ (B) between 0 and $-a/2$
(C) 0 (D) a
[WBSET 2018]

210. The degree of degeneracy for an energy level $\frac{17h^2}{8ml^2}$ of a particle in a cubical box of side 'L' is
(A) 5 (B) 3
(C) 4 (D) 2
[WBSET 2018]

211. A particle of mass 'm' moving in one – dimension between x=a and x=b is described by a wave function $\Psi = \frac{N}{x}$ where N is normalization constant. The average value of x is
(A) $\frac{b}{a}$ (B) $\frac{ab}{b-a}e^{b/a}$
(C) $\frac{ab}{b-a}\ln\frac{a}{b}$ (D) $\frac{ab}{b-a}$ [lnb-lna]
[WBSET 2018]

212. Ψ_1 and Ψ_2 are normalized and are mutually orthogonal to each other. The normalization constant for the function $\Psi_1 + \sqrt{3}\Psi_2$ is
(A) $\frac{\sqrt{3}}{2}$ (B) 1
(C) $\frac{1}{2}$ (D) $\frac{3}{2}$
[WBSET 2018]

213. Which of the following is correct wave function for helium atom?
(A) 1s(1) 2s(2) ($\alpha_1\beta_2 - \beta_1\alpha_2$)
(B) [1s(1) 2s(2) – 2s(1) 1s (2)] ($\alpha_1\beta_2 - \beta_1\alpha_2$)
(C) 1s(1) 2s(2) $\alpha_1\beta_2$ – 2s (1) 1s (2) $\beta_1\alpha_2$ + 1s(1) 2s(2) $\beta_1\alpha_2$ -2s (1) 1s(2) $\alpha_1\beta_2$
(D) [1s(1) 2s(2) – 2s(1) 1s(2)] ($\alpha_1\beta_2 - \beta_1\alpha_2$)
[WBSET 2018]

214. The degeneracy of the most probable energy level for an atom of mass 'm' of one mole of an ideal das at TK and pressure P atm, assuming that the atom can be treated as a particle in a three-dimensional cubical box is
(A) $\frac{2\sqrt{3mKT}}{h}(\frac{RT}{P})^{\frac{1}{3}}$ (B) $\frac{2l\sqrt{3mKT}}{h}$
(C) $\frac{\sqrt{3mKT}}{h}(\frac{RT}{P})^{\frac{1}{2}}$ (D) $\frac{2l\sqrt{mKT}}{h}$
[WBSET 2018]

215. A normalized trial function for a particle in a one-dimensional box of length 'L' is $\Psi = Nx(L - x)$
Where N is normalization constant. The upper bound to the ground state energy of the system
(A) $\frac{Nh^2}{8ml^2}$ (B) $\frac{N^2h^2}{8ml^2}$
(C) $\frac{N^2h^2l^3}{6m}$ (D) $\frac{N^2h^2l^3}{8m}$
[WBSET 2018]

216. exp ($-\alpha x^2$) is an eigen function of $-\frac{d^2}{dx^2} + x^2$ provided
(A) $\alpha = \frac{1}{2}$ (B) $\alpha = 1$
(C) $\alpha = \frac{1}{\sqrt{2}}$ (D) $\alpha = 2$
[WBSET 2020]

217. A quantum particle in a two-dimensional square box is in a state described by n1 = 1 and n2 = 7. State(s) in accidental degeneracy with this state is feasible with
(A) $n_1 = 7, n_2 = 1$
(B) No permissible integral values of n_1 and n_2
(C) $n_1 = 5, n_2 = 5$
(D) both of ($n_1 = 7, n_2 = 1$) and ($n_1 = 5, n_2 = 5$)
[WBSET 2020]

218. The operator $\left(\frac{d}{dx} + x\right)^2$ equals to
(A) $\frac{d^2}{dx^2} + 2x\frac{d}{dx} + x^2 + 1$ (B) $\frac{d^2}{dx^2} + 2x\frac{d}{dx} + x^2$
(C) $\frac{d^2}{dx^2} + x\frac{d}{dx} + x^2 + 1$ (D) $\frac{d^2}{dx^2} + x^2$
[WBSET 2020]

219. Brillouin theorem is related to
(A) the physical significance of Hartree-Fock (HF).
(B) failure of HF theory in reproducing ionization spectra.
(C) consideration of electronic relaxation effect in excitation spectra.
(D) configuration interaction between HF determinant and single excited determinant.
[WBSET 2020]

220. If quantum-mechanical operator's P and Q are such that [P, Q] = 1, then [P^2, Q^2] equals to
(A) PQ (B) 2PQ + 2QP
(C) 4PQ (D) 4QP
[WBSET 2020]

221. Paschen-Back effect is related to
(A) perturbation in atomic spectra due to electric field.
(B) anharmonicity in molecular vibration.
(C) effect of high magnetic field on atomic spectra.
(D) L-S coupling in atomic spectra
[WBSET 2020]

222. Due to space quantization, nuclear angular momentum can have discrete orientations about the applied magnetic field and its values (I_z) along the field axis are I_z = SmI, where mI can have values
(A) I, I–1, I–2, ... –I. (B) I, I–1, I–2, ... 2, 1, 0.
(C) I, I–1, I–2, ... 2, 1. (D) I, I–1, I–2, ... –2, –1.

G SET

223. Mathematical expression for Hamiltonian operator, $\hat{H}$ is

(A) $+\frac{h^2}{2m}\nabla^2 - V$ (B) $+\frac{h^2}{2m}\nabla^2 + V$

(C) $-\frac{h^2}{2m}\nabla^2 - V$ (D) $-\frac{h^2}{2m}\nabla^2 + V$

224. The magnitude of the angular momentum $(\vec{L})$ of an electron that couples the 3d orbital is

(A) $\sqrt{2}\frac{h}{2\pi}$ (B) $3\sqrt{2}\frac{h}{2\pi}$

(C) $\sqrt{6}\frac{h}{2\pi}$ (D) $\frac{h}{2\pi}$

225. According to the huckel's theory for conjugated $\pi -$ electron system, the lowest $\pi -$ M.O. energy value for cyclobutenyl system is

(A) $\alpha - 2\beta$ (B) $\alpha + 2\beta$

(C) $\alpha + \beta$ (D) $\alpha - \beta$

226. The lowest energy molecular orbital for the allyl system is

(A) $\frac{1}{\sqrt{2}}\chi_1 - \frac{1}{2}\chi_2 - \frac{1}{\sqrt{2}}\chi_3$

(B) $\frac{1}{\sqrt{2}}\chi_1 - \frac{1}{\sqrt{3}}\chi_1 + \frac{1}{\sqrt{2}}\chi_1$

(C) $\frac{1}{\sqrt{3}}\chi_1 - \frac{1}{3}\chi_2 + \frac{1}{\sqrt{3}}\chi_3$

(D) $\frac{1}{\sqrt{3}}\chi_1 + \frac{1}{\sqrt{3}}\chi_2 + \frac{1}{\sqrt{3}}\chi_3$

ANSWER KEY									
1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
D	D	A	A	C	A	D	C	C	C
11	**12**	**13**	**14**	**15**	**16**	**17**	**18**	**19**	**20**
A	D	D	A	B	C	D	C	D	B
21	**22**	**23**	**24**	**25**	**26**	**27**	**28**	**29**	**30**
B	C	A	D	C	A	B	A	C	B
31	**32**	**33**	**34**	**35**	**36**	**37**	**38**	**39**	**40**
A	D	C	B	D	B	D	B	A	C
41	**42**	**43**	**44**	**45**	**46**	**47**	**48**	**49**	**50**
A	C	C	D	B	B	B	B	A	B
51	**52**	**53**	**54**	**55**	**56**	**57**	**58**	**59**	**60**
A	C	D	C	A	C	C	A	C	A
61	**62**	**63**	**64**	**65**	**66**	**67**	**68**	**69**	**70**
C	B	A	A	B	D	A	C	D	A
71	**72**	**73**	**74**	**75**	**76**	**77**	**78**	**79**	**80**
B	A	C	C	A	A	D	B	B	D
81	**82**	**83**	**84**	**85**	**86**	**87**	**88**	**89**	**90**
A	D	A	B	B	A	A	C	D	A
91	**92**	**93**	**94**	**95**	**96**	**97**	**98**	**99**	**100**
D	C	C	D	B	C	A	C	A	A
101	**102**	**103**	**104**	**105**	**106**	**107**	**108**	**109**	**110**
C	B	D	A	B	C	A	C	D	B
111	**112**	**113**	**114**	**115**	**116**	**117**	**118**	**119**	**120**
B	A	B	B	C	B	D	C	C	B
121	**122**	**123**	**124**	**125**	**126**	**127**	**128**	**129**	**130**
B	B	A	B	A	C	D	D	B	D
131	**132**	**133**	**134**	**135**	**136**	**137**	**138**	**139**	**140**
C	D	A	C	D	B	C	B	D	B
141	**142**	**143**	**144**	**145**	**146**	**147**	**148**	**149**	**150**
C	C	A	C	D	D	A	B	A	B
151	**152**	**153**	**154**	**155**	**156**	**157**	**158**	**159**	**160**
C	D	D	A	A	D	A	B	B	C
161	**162**	**163**	**164**	**165**	**166**	**167**	**168**	**169**	**170**
C	C	B	A	A	B	D	B	B	B
171	**172**	**173**	**174**	**175**	**176**	**177**	**178**	**179**	**180**
A	B	A	C	A	B	A	B	B	A
181	**182**	**183**	**184**	**185**	**186**	**187**	**188**	**189**	**190**
D	A	B	D	C	A	D	D	A	C
191	**192**	**193**	**194**	**195**	**196**	**197**	**198**	**199**	**200**
A	D	C	B	C	A	C	D	D	B
201	**202**	**203**	**204**	**205**	**206**	**207**	**208**	**209**	**210**
B	C	A	D	B	C	A	A	A	B
211	**212**	**213**	**214**	**215**	**216**	**217**	**218**	**219**	**220**
D	C	A	A	C	A	C	A	A	B
221	**222**	**223**	**224**	**225**	**226**				
C	**A**	**D**	**C**	**B**	**D**				

QUANTUM CHEMISTRY SOLUTION

HP SET

1. **Solution: (D)**

Condition for well behaved (Acceptable) wave function: -

* φ must be finite

* φ must be single valued

* φ must be continuous

Sin^{-1} is not a single valued function. Sin^{-1} is not acceptable wave function.

Option (d) is correct.

2. **Solution: (D)**

$[\hat{x}\,, \hat{p}_x^2]$ Trick $[\hat{x}\,, \hat{p}_x^n] = i\hbar n\hat{p}_x^{n-1}$

$$px^2 = \left(-i\hbar\left(\frac{d}{dx}\right)\right)^2 = -\frac{\hbar^2 d^2}{dx^2}$$

$$[x\,, px^2]\varphi = \left[x\left(-\frac{\hbar^2 d^2}{dx^2}\right) - \left(-\frac{\hbar^2 d^2}{dx^2}\right)x\right]\varphi$$

$$= \left[-x \times \frac{\hbar^2 d^2\varphi}{dx^2} + \frac{\hbar^2 d^2(x\varphi)}{dx^2}\right]$$

$$= \left[-x \times \frac{\hbar^2 d^2\varphi}{dx^2} + x \times \frac{\hbar^2 d^2\varphi}{dx^2} + 2\frac{\hbar^2 d\,\varphi}{dx}\right] = 2\frac{\hbar^2 d\,\varphi}{dx}$$

$$[x\,, px^2]\varphi = 2\frac{\hbar^2 d\,\varphi}{dx}$$

$$[x\,, px^2] = 2\frac{\hbar^2 d}{dx}$$

$$2\frac{\hbar^2 d}{dx} = 2i\hbar p_x = 2i\hbar\left(-\frac{i\hbar d}{dx}\right) = 2\frac{\hbar^2 d}{dx}$$

Option (d) is correct

3. **Solution: (A)**

First order correction to energy= ΔE

$$\Delta E = \int_0^l \psi^{o^*}\Delta H\,\psi^o dx$$

$$\Delta H = \lambda x \qquad \psi = \sqrt{\frac{2}{l}}\sin\left(\frac{n\pi x}{l}\right)$$

$$\Delta E =$$

$$\int_o^l \sqrt{\frac{2}{l}}\sin\left(\frac{n\pi x}{l}\right).\lambda x.\sqrt{\frac{2}{l}}\sin\left(\frac{n\pi x}{l}\right)dx$$

$$\Delta E =$$

$$\lambda\int_o^l \sqrt{\frac{2}{l}}\sin\left(\frac{n\pi x}{l}\right).x.\sqrt{\frac{2}{l}}\sin\left(\frac{n\pi x}{l}\right)dx$$

$$\Delta E = \lambda \times \frac{2}{l}\int_o^l x\sin^2\left(\frac{n\pi x}{l}\right)dx$$

$$\Delta E = \lambda \times \frac{2}{l}\int_o^l \frac{x\left(1 - Cos\left(\frac{2n\pi x}{l}\right)\right)}{2}dx$$

on solving integration

$$\Delta E = \frac{\lambda l}{2}$$

Option (a) is correct

4. **Solution: (A)**

The energy levels of cyclopropenyl cation are $\alpha + 2\beta$, $\alpha - \beta$ and $\alpha - \beta$

$$\underline{\quad} \quad \underline{\quad} \quad \alpha - \beta\,,\ \alpha - \beta$$

$$\underline{\uparrow\downarrow} \quad \alpha + 2\beta$$

here one ethylene unit is present in cyclopropenyl cation

Delocalisation energy

$= E_{total} - ethylene\ unit\ energy$

$= 2 \times (\alpha + 2\beta) - (2\alpha + 2\beta) = 2\beta$

Delocalisation energy = 2β

option (a) is correct

5. **Solution: (C)**

Energy of the harmonic oscillator is:-

$$E = \left(n + \frac{1}{2}\right)h\nu = \left(n + \frac{1}{2}\right)h\omega$$

for zero point energy (n=0)

$$E(Z.P.E) = \left(n + \frac{1}{2}\right)h\omega = \left(0 + \frac{1}{2}\right)h\omega = \frac{1}{2}h\omega$$

$$E(Z.P.E) = \frac{1}{2}h\omega$$

option (c) is correct

6. **Solution: (A)**

Energy levels of cyclo-butadiene

$$\underline{\quad} \quad \alpha - 2\beta$$

$$\underline{\uparrow} \quad \underline{\uparrow} \quad \alpha$$

$$\underline{\uparrow\downarrow} \quad \alpha + 2\beta$$

here two ethylene unit is present in cyclobutadiene

Delocalisation energy

$= E_{total} - ethylene\ unit\ energy$

$= 2 \times (\alpha + 2\beta) + 2\alpha - 2(2\alpha + 2\beta) = 0$

So Delocalisation energy in cyclobutadiene = 0

option (a) is correct

7. Solution: (D)

Uncertainty principle also called Heisenberg uncertainty principle. According to Heisenberg uncertainty principle the position and the velocity of an object cannot both be measured exactly, at the same time.

According to uncertainty principle: $\Delta x.\Delta p \geq \frac{\hbar}{2}$

Δx= change in position

$\Delta p = m\Delta v$ = change in momentum

option (d) is correct

8. **Solution: (C)**

When hydrogen atom is placed in an electric field along the y-axis, the orbital that mixes most with the ground state 1s orbital is $2p_y$. On the y-axis $2p_y$ orbital is present so hydrogen orbital mix with $2p_y$

option (c) is correct

9. **Solution: (C)**

Energy for one dimensional box is: -

$$E_n = \frac{n^2h^2}{8ma^2} \qquad ------(i)$$

$$E_{n+1} = \frac{(n+1)^2h^2}{8ma^2} \qquad ------(ii)$$

for separation between energy levels (ii) – (i)

$$E_{n+1} - E_n = \frac{(n+1)^2h^2}{8ma^2} - \frac{n^2h^2}{8ma^2} = \frac{h^2}{8ma^2}(n^2 + 1 + 2n - n^2) = (2n+1)\frac{n^2h^2}{8ma^2}$$

separation between energy levels is $= (2n+1)\frac{n^2h^2}{8ma^2}$

option (c) is correct

10. **Solution: (C)**

Energy $= \frac{hc}{\lambda}$

h = planks constant=$6.626 \times 10^{-34} Js$

$c = velocity\ of\ light = 3 \times 10^8\ ms^{-1}$

$\lambda = wavelength\ (in\ meters)$

wavelength given $= 200nm = 200 \times 10^{-9}m$

$$E = \frac{hc}{\lambda} = \frac{(6.626 \times 10^{-34} Js)(3 \times 10^8\ ms^{-1})}{200 \times 10^{-9}m}$$
$$= 9.9 \times 10^{-19}\ joules$$

energy of photon is $9.9 \times 10^{-19}\ J$

option (c) is correct

11. **Solution: (A)**

Eigen value and Eigen function

$\hat{A}\psi = a\psi$ a= Eigen value ψ =Eigen function=e^{ax}

$\hat{A} = operator$

for $\hat{A} = \frac{d}{dx}$ $\hat{A}\psi = \frac{de^{ax}}{dx} = ae^{ax}$ Eigen value = a

for $\hat{A} = \frac{d^2}{dx^2}$ $\hat{A}\psi = \frac{d^2e^{ax}}{dx^2} = a^2e^{ax}$ Eigen value = a^2

for $\hat{A} = \frac{d^3}{dx^3}$ $\hat{A}\psi = \frac{d^3e^{ax}}{dx^3} = a^3e^{ax}$ Eigen value = a^3

for $\hat{A} = \frac{d^n}{dx^n}$ $\hat{A}\psi = \frac{d^ne^{ax}}{dx^n} = a^ne^{ax}$ Eigen value = a^n

So eigen value for this function is a^n

option (a) is correct.

12. **Solution: (D)**

According to uncertainty principle: $\Delta x.\Delta p \geq \frac{\hbar}{2}$

Δx= change in position

$\Delta p = m\Delta v$ = change in momentum (mass in kg)

$$\Delta x.m.\Delta v = \frac{h}{4\pi}$$

$$\Delta x \times 0.001kg \times 1 \times 10^{-6} ms^{-1} = \frac{6.626 \times 10^{-34} Js}{4 \times 3.14}$$

$$\Delta x = 4.77 \times 10^{-26} m$$

$$\Delta x \approx 5 \times 10^{-26} m$$

minimum uncertainty in its position is $5 \times 10^{-26} m$

option (d) is correct

KERALA SET

13. **Solution: (D)**

According to debroglie light can behave as particle and wave so

$Energy = \frac{hc}{\lambda}\ for\ wave$ --(i)

c is velocity of light

$Energy = mc^2\ for\ light$ –(ii)

(i) and (ii) both will be equal

$$\frac{hc}{\lambda} = mc^2$$

$\lambda = \frac{h}{mc} = \frac{h}{mv} = \frac{h}{p}$ --(iii)

p is momentum =mv

from (iii) equation we can say wavelength is inversely proportional to its momentum

option (d) is correct

14. **Solution: (A)**

According to de-Broglie hypothesis

$\lambda = \frac{h}{mv} = \frac{h}{p}$

Electron is the lightest among all the particle, so the momentum least for an electron

$\lambda = \frac{h}{p}$

So the longest wavelength is of an electron So electron have maximum wavelength So maximum wave character

option (a) is correct

15. **Solution: (B)**

The energy of a particle in a one-dimensional box is given by:-

$$Energy = \frac{n^2h^2}{8ma^2}$$

n = principle quantum number

h = planks constant

m = mass

a = length of the box

option (b) is correct

16. **Solution: (C)**

Number of Radial nodes $= n - l - 1$

n = principle quantum number

l = Azimuthal quantum number

for 3s orbital principle quantum number is 3 and azimuthal quantum number is 0

So number of radial nodes will be $= n - l - 1 = 3 - 0 - 1 = 2$

so number of radial nodes comes out to be 2

option (c) is correct

17. **Solution: (D)**

A fermion is a particle that follows Fermi-Dirac statistics and generally has half -odd integer spin:-

Spin=1/2 , 3/2

Helium-3 with two protons and one neutron has an odd number of nuclei so that atom is a fermion but Helium-4 with two protons and two neutrons has an even nuclei so that atom is not a fermion.

Option (d) is correct

18. **Solution: (C)**

Energy $= \frac{hc}{\lambda}$

h = planks constant=$6.626 \times 10^{-34} Js$

$c = velocity\ of\ light = 3 \times 10^{8}\ ms^{-1}$

$\lambda = wavelength\ (in\ meters)$

wavelength given $= 3.313A = 3.313 \times 10^{-10} m$

$$E = \frac{hc}{\lambda} = \frac{(6.626 \times 10^{-34} Js)(3 \times 10^{8}\ ms^{-1})}{3.313 \times 10^{-10} m}$$
$$= 6 \times 10^{-1}\ J$$

Energy of the photon having a wavelength 3.313 A˚ is $6 \times 10^{-16} J$

option (c) is correct

19. **Solution: (D)**

Number of nodes = n-1

So for 3 nodes n=4

for 2 nodes n=3

Energy for level having 3 nodes

$= E_4 = \frac{n^2 h^2}{8ma^2} = 16 \times \frac{h^2}{8ma^2}$ ------1

Energy for level having 2 nodes

$= E_3 = \frac{n^2 h^2}{8ma^2} = 9 \times \frac{h^2}{8ma^2}$ ---2

for energy difference 1 – 2

$$\Delta E = \frac{h^2}{8ma^2}(16 - 9) = 7 \times \frac{h^2}{8ma^2}$$

in units of $\frac{h^2}{8ma^2}$ energy difference is 7

option (d) is correct

20. **Solution: (B)**

Energy of photon $= h\nu = 6.626 \times 10^{-34} Js \times 5 \times 10^{20} s^{-1} = 3.313 \times 10^{-13} J$

Energy $E = \frac{hc}{\lambda}$

$$\lambda = \frac{hc}{E} = (6.626 \times 10^{-34} Js) \times \frac{(3 \times 10^{8}\ ms^{-1})}{3.313 \times 10^{-1}\ J}$$
$$= 6 \times 10^{-13} m$$

According to de-Broglie hypothesis

$\lambda = \frac{h}{mv} = \frac{h}{p}$

$p = \frac{h}{\lambda} = \frac{(6.626 \times 10^{-34} Js)}{6 \times 10^{-13} m} = 1.1 \times 10^{-21} kgms^{-1}$

$p(momentum) = 1.1 \times 10^{-2}\ kgms^{-1}$

option (b) is correct

21. **Solution: (B)**

Einstein's photoelectric equation state

$$h\nu = w_o + k.E$$

where ν is the frequency of incident light, W_o is the work potential of the metal, and KE is the maximum kinetics energy of released electron.

kinetic energy $= \frac{1}{2}mv^2$

$$h\nu = w + \frac{1}{2}mv^2$$
$$\frac{1}{2}mv^2 = h\nu - w$$

option (b) is correct

22. **Solution: (C)**

$wave\ number = \frac{1}{\lambda} = R_H \left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right] z^2$

For balmer series $n_1 = 2\ , n_2 = 3$

helium atomic number is 2

$wave\ number = \frac{1}{\lambda} = R_H \left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right] z^2 = R_H \left[\frac{1}{2^2} - \frac{1}{3^2}\right] 2^2 = R_H \left[\frac{1}{4} - \frac{1}{9}\right] 4 = \frac{5}{9} R_H$

So wavenumber is $\frac{5}{9} R_H$

option (c) is correct

23. **Solution: (A)**

For Eigen function

$\hat{A}\psi = a\psi$ a= Eigen value $\psi = e^{ikx}$ $\hat{A} = operator$

here operator is $\hat{p}x = -i\hbar \frac{d}{dx}$

for option (a) $\psi = e^{ikx}$

$\hat{A}\psi = -i\hbar \frac{de^{ikx}}{dx} = -i\hbar(ik)e^{ikx} = \hbar k e^{ikx}$

$\hbar k$ both is a constant value comes out to be so it is a eigen function and eigen value is $\hbar k$

So option (a) is correct

24. **Solution: (D)**

The angular momentum of an electron is given by: -

$$= \sqrt{l(l+1)}\hbar$$

l = Azimuthal quantum number (for S =0, p=1, d=2, f=3)

$\hbar = \frac{h}{2\pi}$

for 4d orbital l=2

$$Angular\ momentum = \sqrt{l(l+1)}\hbar = \frac{\sqrt{2(2+1)}h}{2\pi}$$

$$= \frac{\sqrt{6}h}{2\pi}$$

Option (d) is correct

25. **Solution: (C)**

$$< x > = \int_{-\infty}^{\infty} \psi^* \hat{x} \psi \, d\tau$$

$< r >$

$$= \int_{-\infty}^{\infty} \frac{1}{\sqrt{\pi}} \left(\frac{1}{a_o^{3/2}}\right) e^{-r/a_o} . r . \frac{1}{\sqrt{\pi}} \left(\frac{1}{a_o^{3/2}}\right) e^{-r/a_o} d\tau$$

in case of hydrogen atom $\psi = \frac{1}{\sqrt{\pi}} \left(\frac{1}{a_o^{3/2}}\right) e^{-r/a_o}$ $\quad and\ d\tau = r^2 dr sin\theta d\theta d\phi$

$$< r > = \frac{1}{\pi a_o^3} \int_0^{\infty} r^3 e^{-2r/a_o} dr \int_0^{\pi} sin\theta d\theta \int_0^{2\pi} d\phi$$

$= \frac{1}{\pi a_o^3} \left(\frac{3!}{(2/a_o)^{3+1}}\right) [-cos\theta]_0^{\pi} [2\pi] = \frac{4\pi}{\pi a_o^3} \times \frac{3\times 2\times 1 a_o^4}{2^4} =$ $1.5a_o$

So average radius is $1.5a_o$

OR

Direct formula to find out average radius

Average radius $= \frac{a_o}{2}[3n^2 - l(l+1)]$

So for 1s orbital l is 0 and n=1 if we put it we get average radius is $1.5a_o$

option (c) is correct

26. **Solution: (A)**

Number of Radial nodes $= n - l - 1$

n = principle quantum number

l = Azimuthal quantum number

for 4f orbital n=4 and l=3

Number of Radial nodes $= n - l - 1 = 4 - 3 - 1 = 0$

So radial nodes is zero

option (a) is correct

27 **Solution: (B)**

Variational principle: -

* Hit and trial method

* Used for large deviations

* Average energy is calculated

According to variational principle:- The calculated average energy is always greater than exact/true energy.

Option (b) is correct

28. **Solution: (A)**

According to MO theory the ground state wave function including spin of H_2 molecule is represented as:

$$\frac{1}{\sqrt{2}} \begin{vmatrix} \sigma_g 1s(1)\alpha(1) & \sigma_g 1s(1)\beta(1) \\ \sigma_g 1s(2)\alpha(2) & \sigma_g 1s(2)\beta(2) \end{vmatrix}$$

option (a) is correct

29. **Solution: (C)**

The angle between two hybrid orbital is:

$$Cos\theta = \frac{\psi_1 . \psi_2}{|\psi_1||\psi_2|}$$

$\psi_1 . \psi_2 =$ dot product of wave function

$|\psi| = \sqrt{a^2 + b^2 + c^2}$

$a\ , b\ and\ c\ are\ coefficient\ (coefficient\ of\ S - orbital\ does\ not\ participate$

$\psi_1 = \frac{1}{\sqrt{3}} 2s - \frac{1}{\sqrt{6}} 2p_x + \frac{1}{\sqrt{2}} 2p_y$

$\psi_2 = \frac{1}{\sqrt{3}} 2s - \frac{1}{\sqrt{6}} 2p_x - \frac{1}{\sqrt{2}} 2p_y$

$$cos\theta = \frac{\left(\frac{1}{\sqrt{6}} 2p_x + \frac{1}{\sqrt{2}} 2p_y\right)\left(-\frac{1}{\sqrt{6}} 2p_x - \frac{1}{\sqrt{2}} 2p_y\right)}{\sqrt{\left(\frac{1}{6}\right) + \left(\frac{1}{2}\right)} \times \sqrt{\left(\frac{1}{6}\right) + \left(\frac{1}{2}\right)}}$$

$$= \frac{\frac{1}{6} - \frac{1}{2}}{0.66} = -0.5$$

$\theta = \cos^{-1} 0.5 = 120^o$

So angle is 120^o

option (c) is correct

30. **Solution: (B)**

Condition for linear operator is: -

$$f(x+y) = f(x) + f(y)$$

$$\sqrt{x+y} \neq \sqrt{x} + \sqrt{y}$$

so square root is not a linear operator

Option (b) is correct

31. **Solution: (A)**

$$\text{probability of finding electron} = \int_0^{a/2} \psi^{o^*} \psi^o dx$$

$\Delta H = \lambda x$ $\qquad \psi = \sqrt{\frac{2}{l}} \sin\left(\frac{n\pi x}{l}\right)$

$$= \int_o^{a/2} \sqrt{\frac{2}{l}} \sin\left(\frac{n\pi x}{l}\right) \sqrt{\frac{2}{l}} \sin\left(\frac{n\pi x}{l}\right) dx$$

$$= \int_o^{a/2} \sqrt{\frac{2}{l}} \sin\left(\frac{n\pi x}{l}\right) \sqrt{\frac{2}{l}} \sin\left(\frac{n\pi x}{l}\right) dx$$

$$= \frac{2}{l} \int_o^{a/2} \sin^2\left(\frac{n\pi x}{l}\right) dx$$

probability$= \frac{2}{l} \int_o^{a/2} \frac{\left(1 - Cos\left(\frac{2n\pi x}{l}\right)\right)}{2} dx$

on solving integration

$$Probability = \frac{1}{a} \times \frac{a}{2} = \frac{1}{2}$$

So probability is 0.5

option (a) is correct

32. **Solution: (D)**

The angular momentum of an electron is given by: -

$= \sqrt{l(l+1)}\hbar$

l = Azimuthal quantum number (for S =0, p=1, d=2, f=3)

$$\hbar = \frac{h}{2\pi}$$

for f orbital l=3

$$Angular\ momentum = \sqrt{l(l+1)}\hbar = \frac{\sqrt{3(3+1)}h}{2\pi}$$

$$= \frac{\sqrt{12}h}{2\pi}$$

option(d) is correct

33. **Solution: (C)**

According to Born-Oppenheimer approximation Nucleus to nucleus relative motion may be neglected

option (c) is correct

34. **Solution: (B)**

For hydrogen molecule in the excited state $\sigma_g^1\sigma_u^1$, the spin part of the triplet state with $m_s = 0$ is proportional to $\alpha(1)\beta(2) + \beta(1)\alpha(2)$

Option (b) is correct

35. **Solution: (D)**

For term symbol valence electron and orbital in which electron is present

here it is $3\sigma_g^1$ for σ L= 0 so term symbol is $\sum$

value of 2S+1 = 2(because it contain only one electron) also it contain (+ sign)

it is $3\sigma_g$ so grade also comes term symbol is $^2\Sigma_g^+$

option (d) is correct

36. **Solution: (B)**

Energy levels for butadiene

$\alpha - 1.62\beta$ ——

$\alpha - 0.62\beta$ ——

$\alpha + 0.62\beta$ ↑↓

$\alpha + 1.62\beta$ ↑↓

Delocalisation energy $= E_{total} - ethylene\ unit\ energy$

$E_{total} = 2 \times (\alpha + 1.62\beta) + 2 \times (\alpha + 0.62\beta)$

$= 4\alpha + 4.48\beta$

Here 2 ethylene unit is present so energy of 2 ethylene unit is $= 2 \times (2\alpha + 2\beta) = 4\alpha + 4\beta$

Delocalisation energy $= E_{total} - ethylene\ unit\ energy = 4\alpha + 4.48\beta - 4\alpha + 4\beta = 0.48\beta$

Delocalisation energy$= 0.48\beta$

option (b) is correct

37. **Solution: (D)**

For a well behaved function it should follow boundary condition.

At boundary probability of finding the electron will approx. zero.

(A) $y = \exp(a x^2)$ ∞ at boundary if $x = \infty$

(B) $y = ax + b$ ∞ at boundary if $x = \infty$

(C) $y = ax^2$ ∞ at boundary if $x = \infty$

(D) $y = \exp(-a x^2)$ zero at boundary if $x = \infty$

It is a well behaved function

option (d) is correct

38. **Solution: (B)**

The time independent Schrodinger equation is

$$\frac{i\hbar d\psi_{x,t}}{dt} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{x,t}\right]$$

$$\frac{i\hbar d\psi_{x,t}}{dt} = [-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V_{x,t}\psi_{x,t}]$$

$$\frac{i\hbar d\psi_{x,t}}{dt} = [-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_{x,t}]\psi_{x,t}$$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_{x,t}\right] = \hat{H}$$

$$\frac{i\hbar d\psi_{x,t}}{dt} = \hat{H}\psi_{x,t}$$

Option (b) is correct

39. **Solution: (A)**

Energy for 3d box$= \frac{(n_x^2+n_y^2+n_z^2)\,h^2}{8ma^2}$ a= L

Given energy is $\frac{3h^2}{8mL^2}$

if we compare both $\left(n_x^2 + n_y^2 + n_z^2\right) = 3$

$n_x, n_y, n_z\ can'tbe\ zero$

so $n_x, n_y, n_z = 1\ for\ ground\ state$

for first excited state n_x, n_y, n_z any can equal to 2. Three degeneracy

energy of first excited state is $\frac{(n_x^2+n_y^2+n_z^2)\,h^2}{8ma^2} = \frac{(1^2+1^2+2^2)\,h^2}{8ma^2} = \frac{6h^2}{8mL^2}$

$\Delta E = \frac{6h^2}{8mL^2} - \frac{3h^2}{8mL^2} = \frac{3h^2}{8mL^2}$

Energy required for the excitation of the particle into the next higher energy level is $\frac{3h^2}{8mL^2}$

Option (a) is correct

40. **Solution: (C)**

Number of Radial nodes $= n - l - 1$

Angular nodes $= l$

For 4f orbital n= 4 l = 3

So angular nodes = l=3

Radial nodes = 4 – 3 -1 =0

So 0 radial nodes and 3 angular nodes

Option (c) is correct

41. **Solution: (A)**

For Eigen function

$\hat{A}\psi = a\psi$ a= Eigen value $\psi = e^{ikx}$ $\hat{A} = operator$

here operator is $\hat{p}x = -i\hbar\frac{d}{dx}$

for option (a) $\psi = e^{ikx}$

$$\hat{A}\psi = -i\hbar\frac{de^{ikx}}{dx} = -i\hbar(ik)e^{ikx} = \hbar k e^{ikx}$$

$\hbar k$ both is a constant value comes out to be so it is a eigen function and eigen value is $\hbar k$

So option (a) is correct

42. **Solution: (C)**

Energy for 3d box= $\frac{(n_x^2+n_y^2+n_z^2)\,h^2}{8ma^2}$

Given energy is $\frac{14\ ^2}{8mL^2}$

if we compare both $\left(n_x^2 + n_y^2 + n_z^2\right) = 14$

possible n_x, n_y, n_z values is (3,2,1), (3,1,2), (1,2,3), (1,3,2), (2,3,1), (2,1,3) all will give equal value of energy so degeneracy is 6.

So option (c) is correct

43. **Solution: (C)**

Variational principle: -

* Hit and trial method

* Used for large deviations

* Average energy is calculated

According to variational principle: - The calculated average energy is always greater than exact/true energy. So $E \geq E_0$. E_0 is true energy

Option (c) is correct

44. **Solution: (D)**

first Hermite polynomial – 1

Second Hermite polynomial- 2ξ

third Hermite polynomial - $4\xi^2$-2

option (d) is correct

45. **Solution:**

Energy levels for benzene molecule

____		$\alpha - 2\beta$
___	____	$\alpha - \beta$
↑↓	↑↓	$\alpha + \beta$

↑↓	$\alpha + 2\beta$

Delocalisation Energy

$= 2 \times (\alpha + 2\beta) + 4 \times (\alpha + \beta) - 3 \times (2\alpha + 2\beta)$

$= 6\alpha + 8\beta - 6\alpha - 6\beta = 2\beta$

Delocalisation Energy$= 2\beta$

option (b) is correct

46. **Solution: (B)**

For 1D box Energy $= \frac{n^2h^2}{8ma^2}$

for first energy level n=1 (Ground state)

$E_1 = \frac{h^2}{8ma^2} = 0.6032 \text{ x } 10^{-17}$J(Given)

for second energy level n=2 (first excited state)

$E_2 = \frac{4h^2}{8ma^2}$

$Energy\ gap = \Delta E = \frac{4h^2}{8ma^2} - \frac{h^2}{8ma^2} = \frac{3h^2}{8ma^2}$

Energy gap is the three times of the Ground state energy$= 3 \times G.S.E = 3 \times 0.6032 \text{ x } 10^{-17} J$

$\Delta E = 1.8095\text{x}10^{-17}$ J

option (b) is correct

47. **Solution: (B)**

$\left[\hat{L}_x.\hat{L}_y\right] = i\hbar\hat{L}_z$

$\left[\hat{L}_y.\hat{L}_z\right] = i\hbar\hat{L}_x$

$\left[\hat{L}_z.\hat{L}_x\right] = -ih\hat{L}_y$

$\left[\hat{L}_y, \hat{L}_x\right] = -i\hbar\hat{L}_z$

Option (B) is correct

48. **Solution: (B)**

Spherical harmonics: -

$$Y_{l,m}(\theta,\phi) = \sqrt{\frac{2l+1\ \ (l+m)!}{4\pi\ (l+m)!}}\ Cos\theta.Cos(m\phi)$$

$Y_{1,0}(\theta,\phi)\ here\ in\ this\ function\ l = 1\ and\ m\ is\ 0$

Put values of l and m in spherical harmonics

$Y_{l,m}(\theta,\phi)$

$$= \sqrt{\frac{2\times 1+1\ \ (1+0)!}{4\pi\ (1+0)!}}\ Cos\theta.Cos(0.\phi)$$

$CosO^o = 1$

$$Y_{1,0}(\theta,\phi) = \sqrt{\frac{3}{4\pi}}cos\theta$$

Option (b) is correct

49. **Solution: (A)**

The Huckel theory secular determinant equation for cyclobutadiene is:-

$$\begin{vmatrix} x & 1 & 0 & 1 \\ 1 & x & 1 & 0 \\ 0 & 1 & x & 1 \\ 1 & 0 & 1 & x \end{vmatrix} = 0$$

Option (a) is correct

50. **Solution: (B)**

Energy levels for benzene molecule

____ $\alpha - 2\beta$

___ ____ $\alpha - \beta$

↑↓ ↑↓ $\alpha + \beta$

↑↓ $\alpha + 2\beta$

Delocalisation Energy

$= 2 \times (\alpha + 2\beta) + 4 \times (\alpha + \beta) - 3 \times (2\alpha + 2\beta)$

$= 6\alpha + 8\beta - 6\alpha - 6\beta = 2\beta$

Delocalisation Energy$= 2\beta$

option (b) is correct

51. **Solution: (A)**

According to uncertainty principle: $\Delta x.\Delta p \geq \frac{\hbar}{2}$

Δx= change in position

$\Delta p = m\Delta v$ = change in momentum (mass in kg)

Here $\Delta p = \Delta x\ (Given)$

So $\Delta p^2 = \frac{h}{4\pi}$

$m.\Delta v.m.\Delta v = \frac{h}{4\pi}$

$m^2\Delta v^2 = \frac{h}{4\pi}$

$\Delta v^2 = \frac{h}{m^2 4\pi}$

$\Delta v = \sqrt{\frac{h}{m^2 4\pi}} = \frac{1}{2m}\sqrt{\frac{h}{\pi}} = \frac{1}{2m}\left(\frac{h}{\pi}\right)^{1/2}$

Option (a) is correct

52. **Solution: (C)**

If two operators commute and consequently have the same set of eigen functions, then the corresponding physical quantities can be evaluated or. Measured exactly simultaneously with no limit on the uncertainty. So if two operators commute, then they have the same Eigen functions.

Option (c) is correct

53. **Solution: (D)**

Energy levels for Allylic radical

____ $\alpha - \sqrt{2}\beta$

____ α

____ $\alpha + \sqrt{2}\beta$

so energy levels correct order is $\alpha + \sqrt{2}\,\beta, \alpha, \alpha - \sqrt{2}\,\beta$

option (d) is correct

54. **Solution: (C)**

Hence, option (c) is correct.

55. **Solution: (A)**

The quantity hm_ec is known as the Compton wavelength of the electron; it is equal to $2.43 \times 10^{-12}m$

The wavelength shift $\lambda' - \lambda$ is at least zero for $\theta = 0$ and at most twice the Compton wavelength of the electron for $\theta = 180^o$ $\Delta\lambda\ at$ corresponding to the scattering angle θ equal to 90^o

option (a) is correct

K SET

56. **Solution: (C)**

The square of the wave function in quantum mechanics represents the Probability density of finding the particle around a specific location in space.

Option (c) is correct

57. **Solution: (C)**

Energy for 1-D box $= \frac{n^2h^2}{8ma^2}$

for zero-point energy put n = 1

Zero-point energy of an electron is equal to

$= \frac{1^2h^2}{8ma^2} == \frac{h^2}{8ma^2}$

option (c) is correct

58. **Solution: (A)**

Condition for well behaved (Acceptable) wave function: -

* φ must be finite

* φ must be single valued

* φ must be continuous

* Square integrable

Option (a) follow these conditions

Option (a) is correct

59. **Solution: (C)**

The square of the wave function in quantum mechanics represents the Probability density of finding the particle around a specific location in space.

Option (c) is correct

60. **Solution: (A)**

$\nabla^2\Psi + \frac{8\pi^2m(E-V)}{h^2}\Psi = 0$

$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$

∇^2 is Laplacian operator

option (a) is correct

61. **Solution: (C)**

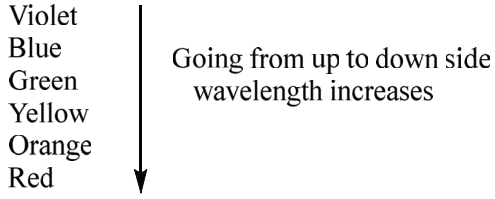
Hamiltonian operator (H) in $H\Psi = E\Psi$

E here is Energy the sum of potential energy and kinetic energy

So Hamiltonian operator (H) in HΨ = EΨ is the operator for the total energy of the system

option (c) is correct

62. **Solution: (A)**



So here wavelength of Red will be maximum and wavelength of violet will lowest i.e (ii)-(d) and (iv)-(a)

option (a) is correct

63. **Solution: (A)**

$< x >= \sum x \times p(x)$

so $< x >= \sum x \times p(x) = 1 \times 0.20 + 3 \times 0.25 + 4 \times 0.55$

$= 0.20 + 0.75 + 2.2 = 3.15$

<x>= 3.15

Option (a) is correct

64. **Solution: (A)**

Condition for linear operator is: -

$f(x+y) = f(x) + f(y)$

$\sqrt{x+y} \neq \sqrt{x} + \sqrt{y}$ $So\ \sqrt{}\ is\ not\ a\ linear\ oprator$

$(x+y)^2 \neq x^2 + y^2$ $so\ x^2\ is\ not\ a\ linear\ operator$

$\frac{d}{dx}(x+y) = \frac{d}{dx}x + \frac{d}{dx}y$ $So\ \frac{d}{dx}\ is\ a\ linear\ opeator$

$\frac{d^2}{dx^2}(x+y) = \frac{d^2}{dx^2}x + \frac{d^2}{dx^2}y$

$So\ \frac{d^2}{dx^2}\ is\ a\ linear\ opeator$

So only $\frac{d}{dx}$ and $\frac{d^2}{dx^2}$ is a linear operator

option (a) is correct

65. **Solution: (B)**

Shape is given by angular node or angular wave function, Radial wave function gives energy So Radial and angular wave function gives Energy, size and shape, orientation of the orbitals respectively

option (b) is correct

66. **Solution: (D)**

Energy for a Particle for 1 dimensional box is $E_n = \frac{n^2h^2}{8ma^2}$

So According to the Schrodinger's wave equation the energy of a particle (E_n) in $1-D$ box $= \frac{n^2h^2}{8ma^2}$

option (d) is correct

67. **Solution: (A)**

Perturbation theory is a method for continuously improving a previously obtained approximate solution to a problem, an it is an important and general method for finding approximate solutions to the Schrodinger equation.

option (a) is correct

68. **Solution: (C)**

S-Orbital are spherical So S-Orbitals are spherically symmetric

A harmonic oscillator obeys Hooke's law

Spin quantum number, S, for an electron $S = \frac{1}{2}$

An azeotrope is a mixture that boils without change of composition

Spin quantum number is incorrect here

Option (c) is correct

69. **Solution: (D)**

Particles with spins that come in half-integer multiple (e.g., $\pm\frac{1}{2}$, $\pm\frac{3}{2}$, $\pm\frac{5}{2}$ etc are known as Fermions

Example: - Proton, Neutron and electron

Deuteron nucleus has Ground sate has spin = 1

thus it is a boson not Fermion

So i, ii and iii are fermions

Option (d) is correct

70. **Solution: (A)**

A Function is called an even function if it's graph is unchanged under reflection in its y-axis. Suppose f(x) is a function such that it is said to be an even function if $f(-x)$ is equal to $f(x)$

ex- $f(x) = x^2$ even function

$f(-x) = (-x)^2 = x^2$ so it is a even function

$f(-x) = -f(x)$ is a odd function

$f(x) = x^3$ odd function

$f(-x) = (-x)^3 = -x^3$ so it is a odd function

property of odd function

* Product of two even functions will be an even function
* Product of two odd functions will be an even function

So statement I, ii and iii is correct

Option (a) is correct

71. **Solution: (B)**

According to de-Broglie hypothesis

$$\lambda = \frac{h}{mv} = \frac{h}{p}$$

$p = \frac{h}{\lambda} = \frac{(6.626\times10^{-34}Js)}{350\times10^{-9}m} = \frac{6.626\times10^{-3}\ kg\ m^2s^{-2}S^1}{350\times10^{-9}m} = 0.0189 \times 10^{-25} kg\ m\ s^{-1}$

linear momentum = $1.89 \times 10^{-27} kg\ m\ s^{-1}$

Option (b) is correct