

Select the correct answer :-

Q. (1). (i) Which of the following is an acceptable wave function-

- (a)  $\psi = x$  (b)  $\psi = x^2$  (c)  $\psi = \sin x$  (d)  $\psi = e^x$

(ii) A wave function is given as  $\psi = \sin x$ , then  
(a)  $\psi$  is normalised (b)  $\psi$  is not normalised (c)  $\psi$  is orthogonal (d) none of these.

(iii) The function  $f_1(x) = N_1(a^2 - x^2)$  in the interval  $x = -a$  &  $x = +a$ , the normalisation constant  $N_1$  is

- (a)  $\left(\frac{15}{16a^5}\right)^{1/2}$  (b)  $\left(\frac{15}{16a^4}\right)^{1/2}$  (c)  $\left(\frac{105}{16a^7}\right)^{1/2}$  (d)  $\left(\frac{45}{64a^9}\right)^{1/2}$

(iv) If the operators  $\hat{U} = \sqrt{\quad}$ ,  $\hat{V} = 4$  & function  $f(x) = x^2$

- (a)  $\hat{U}$  &  $\hat{V}$  commute (b)  $\hat{U}$  &  $\hat{V}$  do not commute (c)  $\hat{U}$  &  $\hat{V}$  are linear operator (d) none of the above.

(v) Which of the following is a linear operator

- (a) taking logarithm (b) taking differential (c) taking Sq. root (d) all of the above.

(vi) If two Hermitian operators  $\hat{A}$  &  $\hat{B}$  commute, then

- (a) they must have a common eigenfunction (b) Common eigenfunction is not necessary (c) their eigenfunction values will be same (d) none of these.

(vii) Which of the following is incorrect

- (a)  $[\hat{A}, \hat{B}] = -[\hat{B}, \hat{A}]$  (b)  $[\hat{A}^2, \hat{B}] = \hat{A}[\hat{A}, \hat{B}] + [\hat{A}, \hat{B}]\hat{A}$   
(c)  $[\hat{A}, [\hat{B}, \hat{C}]] = [[\hat{A}, \hat{B}]\hat{C}] + [\hat{B}[\hat{A}, \hat{C}]]$   
(d) None of these.

(viii) Which of the following is an eigenfunction of the operator  $d^2/dx^2$ .  
 (a)  $\psi = x$  (b)  $\psi = x^2$  (c)  $\psi = \sin 2x$  (d) none of the above

(ix) Which of the following is incorrect  
 (a) The vibrational energies are equally spaced ( $h\nu$ ) for harmonic oscillator  
 (b) The lowest value i.e. zero point energy for harmonic oscillator is zero.  
 (c) The energy of the harmonic oscillator is quantised.  
 (d) zero point energy is  $\frac{1}{2} h\nu$ .

(x) Which of the following MO is not normalised  
 (a)  $\psi_1 = \frac{1}{\sqrt{2}} (\phi_1 + \phi_2)$  (b)  $\psi_2 = \frac{1}{\sqrt{3}} (\phi_1 + \phi_2 + \phi_3)$   
 (c)  $\psi_3 = \frac{1}{2} (\phi_1 - 2\phi_2 + \phi_3)$   
 (d) none of the above  
 (Where  $\phi_s$  are the orthonormal atomic orbitals)

(xi) Bonding MO (BMO) and antibonding (ABMO) for  $H_2$  molecule are  
 (a) orthogonal (b) not orthogonal (c) eigenfunction  
 (d) none of the above.

(xii) In the Hamiltonian for  $H_2^+$ , the term  $\frac{1}{r_{AB}}$  represents  
 (a) Kinetic energy operator of the single electron  
 (b) Coulombic attraction of electron with nuclei A & B.  
 (c) Coulombic repulsion between two nuclei A & B.  
 (d) electronic repulsion potential energy.

(xiii) The eigenvalue for the eigenfunction  $\psi = \sin 2x$  of the operator  $d^2/dx^2$  is:

- (a) 4    (b) -4    (c) 2    (d) -2

(xiv) The time-dependent Schrodinger equation is given

by

(a)  $\hat{H}\psi = \frac{i\hbar}{2\pi} \frac{\partial \psi}{\partial t}$     (b)  $\hat{H}\psi = -\frac{i\hbar}{2\pi} \frac{\partial \psi}{\partial t}$

(c)  $\hat{H}\psi = \frac{i\hbar}{4\pi} \frac{\partial \psi}{\partial t}$     (d)  $\hat{H}\psi = -\frac{i\hbar}{4\pi} \frac{\partial \psi}{\partial t}$

(xv) If the operator  $\hat{U} = \left(\frac{\partial}{\partial x}\right)_y$

&  $\hat{V} = \left(\frac{\partial}{\partial y}\right)_x$

then,

- (a) operators  $\hat{U}$  &  $\hat{V}$  commute    (b) they cannot commute  
 (c) they are Hermitian operators    (d) None of the above.

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