ISLAMIC UNIVERSITYOF SCIENCE & TECHNOLOGY
DEPARMENT OF CHEMISTRY

M Sc. (1st Semester) (Mid. term) **Max. Marks: 30**
Course Title: Chemical Kinetics and Quantum Chemistry (PCH-CC-103) **Time: 40 min.**
Roll No:

1) Let $\hat{A} = \frac{d}{dx}$ and $f(x) = ax^2$,then $\frac{d}{dx} f(x) =$
   a) 2ax
   b) 2x
   c) $2x^2$
   d) $4ax^2$
2) If $\hat{A} = \frac{d}{dx}$, $\hat{B} = \frac{d^2}{dx^2}$ and $f(x) = Sinx$ then
   a) $\hat{A}$ *and* $\hat{B}$ commute
   b) $\hat{A}$ *and* $\hat{B}$ do not commute
   c) $\hat{A}$ *and* $\hat{B}$ may or may not commute
   d) None of the above
3) If the function $f = e^{-ax}$ is acted upon by operator $\frac{d}{dx}$, then its Eigen value is:
   a) a
   b) –a
   c) –ax
   d) e^{-ax}
4) Characteristic of Hermitian operator is/are:
   a) The eigen values are real
   b) Eigen functions corresponding to different eigen values are orthogonal to each other
   c) Eigen values are not real
   d) Both a) and b)
5) An operator is said to be Hermitian if it satisfies the following condition:
   a) $\int \psi_i^* \hat{A} \psi_j dx = \int \psi_j (\hat{A}\psi_j)^* dx$
   b) $\int \psi_i^* \hat{A} \psi_j dx = \int \hat{A} \psi_j \psi_j dx$
   c) $\int \psi_i^* \psi_j dx = 1$
   d) None
6) The acceptable wavefunction must satisfy the condition that it is:
   a) Single valued
   b) Continuous
   c) Finite
   d) All of the above
7) Suppose ψ is Eigen function of $\hat{A}$ and suppose a is corresponding Eigen-value, then:
   a) $\frac{\int \psi^* a \psi \ dx}{\int \psi \ \psi \ d\tau} = a \frac{\int \psi^* \psi \ d\tau}{\int \psi^* \psi \ d\tau}$
   b) $< \hat{A} >= a$
   c) Both a) and b)
   d) Only b) is correct
8) The state function which obeys the time dependent Schrodinger equation is:
   a) $i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi$
   b) $i \frac{h}{2\pi} \frac{\partial \psi}{\partial t} = \hat{H}\psi$
   c) $\sqrt{-1}\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi$
   d) All of the above
9) For one dimensional system, then:
   a) $i\hbar \frac{\partial \psi(x,t)}{\partial t} = \left[\frac{-\hbar}{2m} \frac{\partial}{\partial x^2} + V(x,t) \right] \psi(x,t)$
   b) $i\hbar \frac{\partial \psi(x,t)}{\partial t} = \hat{H} \psi(x,t)$
   c) Both a) and b)
   d) None
10) If $\lambda = 9$, $j = 4$ then a_6 is given by:
   a) Zero
   b) Starting from a_6 all are zero
   c) Both a) and b)
   d) Not equal to zero
11) Which of the following is a generating function?
   a) $S(r,\xi) = e^{-s^2 + 2s\xi}$
   b) $S(r,\xi) = e^{-\xi^2 + 2s\xi}$
   c) $S(r,\xi) = e^{-s\xi^2 + 2s}$
   d) None
12) Hermite polynomial of degree 2 for harmonic oscillator is given by:

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a) $H(\xi) = 4\xi^2 - 2$
b) $H(\xi) = 2\xi^2 - 2$
c) $H(\xi) = 2\xi^2 - 4$
d) None

13) If $\psi = 0$ at $x = 0$ for a particle in 1-D box, then
   a) $\psi = BSinkx$
   b) $\psi = 0$
   c) $A = 0$
   d) Both a) and c)

14) The normalized wave-function ψ of a particle in a 1-D box is:
   a) $\psi = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$
   b) $\psi = \sqrt{\frac{a}{2}} \sin \frac{n\pi x}{a}$
   c) $\psi = \sqrt{\frac{2}{a}} \sin \frac{a}{n\pi x}$
   d) $\psi = \sqrt{\frac{a}{2}} \sin \frac{a}{n\pi x}$

15) If $n = 4$, then E of 1-D box calculated is:
   a) $\frac{4^2 h^2}{8ma^2}$
   b) $\frac{4\hbar^2}{8ma^2}$
   c) $\frac{4h^2}{4ma^2}$
   d) $\frac{4\hbar^2}{4ma^2}$

16) The dimensions of 1-D box in terms of wavelength is given by:
   a) $a = \frac{n\lambda}{2}$
   b) $a = \frac{2\lambda}{n}$
   c) $a = \frac{\lambda}{2}$
   d) None

17) The total energy (E) of a particle in 3-D box is given by:
   a) $\frac{\hbar^2 \pi^2}{2m} \left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2} \right)$
   b) $\frac{\hbar^2 \pi^2}{2m} \left(\frac{n_x^2 + n_y^2 + n_z^2}{a^2} \right)$ for a cube
   c) Both a) and b)
   d) None

18) If $a = b = c$, then 211, 121, and 112 states in a 3-D box are:
   a) Degenerate
   b) Non-degenerate
   c) Have accidental degeneracy
   d) None

19) For 123 states, the energy and degeneracy of a cubic system is given by:
   a) $14\frac{h^2}{8ma^2};6$
   b) $12\frac{h^2}{8ma^2};3$
   c) $6\frac{h^2}{8ma^2};1$
   d) None

20) Inside the 3-D box, the Hamiltonian is given by:
   a) $\frac{-\hbar^2}{2m}\nabla^2 + V$
   b) $\frac{-\hbar^2}{2m}\nabla^2$
   c) $\frac{-\hbar^2}{2m}\nabla^2 - V$
   d) None

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