UNIVERSITY WITH A PURPOSE

UNIVERSITY OF PETROLEUM AND ENERGY STUDIES
Examination, July 2020

Programme: M.Sc. Chemistry | **Semester : II**
Course Name: Quantum Chemistry | **Max. Marks : 100**
Course Code: CHEM7010 | **Attempt Duration : 3 Hrs.**
End Semester Examination July 2020

Note:

1. Read the instruction carefully before attempting.
2. This question paper has two section, Section A and Section B.
3. There are total of six questions in this question paper. **One** in **Section A** and **five** in **Section B**
4. **Section A** consist of multiple choice based questions and has the total weightage of 60%.
5. **Section B** consist of long answer based questions and has the total weightage of 40%.
6. The maximum time allocated to **Section A** is 90 minutes.
7. **Section B** to be submitted within 24 hrs from the scheduled time i.e. if the examination starts at 10:00 AM, the long answers must be submitted by 09:59:59 AM next day. Similarly, if the examination starts at 2:00 PM it must be submitted by 01:59:59 PM next day. (*Exceptional provision due extraordinary circumstance due to COVID-19 and due to internet connectivity issues in the far-flung areas*)**.**
8. No submission of **Section B** shall be entertained after 24 Hrs.
9. **Section B** should be attempted after **Section A**
10. **The section B** should be attempted in blank white sheets (hand written) with all the details like programme, semester, course name, course code, name of the student, Sapid at the top (as in the format) and signature at the bottom (right hand side bottom corner)
11. Both section A & B should have questions from entire syllabus.
12. The COs mapping, internal choices within a section is same as earlier

Section A

1. CO3
   The concept of matter wave was suggested by 1 marks

(a) Heisenberg

(b) de Broglie

(c) Schrodinger

(d) Laplace

2. CO1
   The normalized wave function must have _____ norm 2 marks

(a) infinite

(b) zero

(c) finite

(d) complex

3. CO1
   For normalized wave function $\psi \rightarrow 0$ as $r \rightarrow$ ___ 2 marks

(a) 0

(b)1

(c) α

(d) -1

4. CO1
   The operator $\nabla.\nabla$ is called _____ operator 2 marks

(a) Hamiltonian

(b) Laplacian

(c) Poisson

(d) vector

5. CO1
   Which of the following is an eigen function of the operator $\hat{p}r = -i\bar{h}r^{-1} (\partial/\partial r)\, r$ 2 marks

(A) exp(*ikr*)

(B) sin(*kr*)

(C) $r^{-1} \exp(ikr)$

(D) $r \exp(ikr)$

6. CO3
   Which of the following is known as the Schr¨odinger equation 2 marks

(A) $E = h\nu$

(B) $E = mc2$

(C) $\lambda = h/p$

(D) $H\psi\hat{} = E\psi$

7. CO3
   The wave function of the particle lies in which region? 2 marks
   a) $x > 0$
   b) $x < 0$
   c) $0 < X < L$
   d) $x > L$

8. CO1
   The Energy of the particle is proportional to _____ 2 marks
   a) n
   b) n^{-1}
   c) n^2
   d) n^{-2}

9. CO1
   The Eigen value of a particle in a box is _____ 3 marks
   a) L/2
   b) 2/L
   c) $\sqrt{L/2}$
   d) $\sqrt{2/L}$

10. CO3
    What is the minimum Energy possessed by the particle in a box? 3 marks
    a) Zero
    b) $\pi^2\hbar^2/2mL^2$

c) $\pi^2\hbar^2/2mL$
d) $\pi^2\hbar^2/mL$

11. CO2
How many values does the spin quantum number have? 2 marks
a) 2
b) 2l
c) 2n
d) $2m_e$

12. CO3
If Ψ is the wave function, the probability density function is given by _____ 2 marks
a) $|\Psi|$
b) $|\Psi|^2$
c) $|\Psi|^3$
d) $|\Psi|^4$

13. CO1
Calculate the minimum uncertainty in the momentum of a 4He atom confined to 0.40 nm. 3 marks
a) 2.02 X 10^{-25} kg m/s
b) 2.53 X 10^{-25} kg m/s
c) 2.64 X 10^{-25} kg m/s
d) 2.89 X 10^{-25} kg m/s

14. CO2
Molecular orbitals are formed in such a way that: 3 marks
a. total number of Atomic Orbitals combine equals to total number of Molecular Orbitals formed
b. total number of Atomic Orbitals combine are less than total number of Molecular Orbitals formed
c. total number of Atomic Orbitals combine are greater than total number of Molecular Orbitals formed
d. all three possibilities will be there

15. CO2
Antibonding molecular orbitals are formed by 2 marks

a. Constructive interference
b. Destructive interference
c. Diffraction
d. Scattering of radiation

16. CO2
Selection rule for pure vibrational spectra is: 3 marks

a. $\Delta J = \pm 1$
b. $\Delta J = \pm 2$
c. $\Delta n = \pm 1$
d. $\Delta n = \pm 2$

17. CO1

A cricket ball weighing 100 g is to be located within 0.1 A^o. The uncertainty in its velocity will be:

(Mass of electron = 9.1×10^{-31} kg and Plank's constant = 6.626×10^{-34} Js) 3 marks

a. 0.527×10^{-22} m s^{-1}
b. 0.200×10^{-22} m s^{-1}
c. 0.725×10^{-22} m s^{-1}
d. 0.444×10^{-22} m s^{-1}

18. CO1

The function *cos ax* is an eigen function of the operator: 3 marks

a. d/dx
b. d^2/dx^2
c. Both of these
d. None of these

19. CO3

For a particle in 3-dimensional box, the number of all possible energy levels below $15h^2/8ma^2$ are: 3 marks

a. 2

b. 3
c. 4
d. 5

20. CO1
The de-Broglie wavelength of an electron moving with a velocity of 1.20×10^7 cm sec^{-1} will be: 3 marks
a. 40.22 A^0
b. 60.68 A^0
c. 26.86 A^0
d. None of these

21. CO1
The function Ψ = cos ax cos by cos cz is an eigen function of the Laplacian operator. Its corresponding eigen value is: 3 marks
a. abc
b. $a^2b^2c^2$
c. $a^3b^3c^3$
d. All of these

22. CO2
The total energy of a simple harmonic oscillator is given by: 3 marks
a. $E = ½ K_f A^2$
b. $E = 2 K_f A^2$
c. $E = ½ K_f^2 A$
d. $E = 2 K_f^2 A$

23. CO2
For a 3p orbital, what are the total number of nodes? 2 marks
a) 3
b) **2**
c) 1
d) 0

24. CO3
In the Schrodinger equation, $H\Psi=E\Psi$, Ψ represents the 2 marks
a. Momentum operator
b. Wave function of the system
c. Probability density

d. Total energy operator

25. CO3

The principle that all microscopic physical entities have both wave and particle properties is called the wave-particle… 2 marks

a. Singularity
b. Duality
c. Triality
d. Infinality

Section B

1. Apply quantum mechanical principles to calculate the coefficients of atomic orbitals in sp hybrid orbitals and write their wave functions. (CO2)

2. What are the main points of similarities and differences between VBT and MOT? (CO2)

3. For a particle confined to move in a one-dimensional box, find out the solution of wave function (Ψ) for the Schrodinger wave equation and normalize it. (CO3)

4. Set up the Schrodinger wave equation for a Simple harmonic oscillator and solve it by factorization method. (CO1)

5. Discuss Born-Oppenheimer Approximation of molecular energies giving details of vibrational and rotational energies. (CO3)