Mahindra University Hyderabad
École Centrale School of Engineering
Mid-Term Examination
(2022-Batch)

**Program: B. Tech** **Branch: All** **Year: I** **Semester: I**

**Subject: Chemistry - I (CH 1101)**

**Date: 09/11/2022** **Start Time: 10.00 AM**

**Time Duration: 1.5 Hours** **Max. Marks: 50**

---

**Instructions**

1. Answer any 5 out of 7 questions (only first 5 answers will be evaluated).
2. No clarifications will be entertained during the examination.
3. If any information is missing, make appropriate assumptions and proceed.

---

Table 1: Useful physical constants and conversion factors

| | | |
|---|---|---|
| Speed of light (c) | = | $2.997 \times 10^{8}$ m $s^{-1}$ |
| Mass of electron ($m_e$) | = | $9.109 \times 10^{-31}$ kg |
| Planck constant (h) | = | $6.626 \times 10^{-34}$ J s |
| Boltzmann constant ($k_B$) | = | $1.381 \times 10^{-23}$ J $K^{-1}$ |
| Avogadro number ($N_A$) | = | $6.023 \times 10^{23}$ $mol^{-1}$ |
| Elementary charge (e) | = | $1.602 \times 10^{-19}$ C |
| Mass of proton ($m_p$) | = | $1.672 \times 10^{-27}$ kg |
| Rydberg Constant ($R_H$) | = | 109677 $cm^{-1}$ |
| 1 eV | = | $1.602 \times 10^{-19}$ J |

## Q1. Marks: 10

i) Write True or False for the following statements:

(a) Bohr's fixed-orbit concept agrees with Heisenberg's uncertainty principle.

(b) The larger the work function of a metal the higher the kinetic energy of the ejected photoelectrons.

(c) Particle in one-dimensional box has zero-point energy.

(d) The radius of the first Bohr orbit is often denoted as $a_0$ (1 bohr).

(e) A free particle travels under external forces.

ii) Answer the following questions:

(a) What are the quantum numbers of the wavefunction given below:

$$\Psi_{n,l,m_l}(r,\theta,\phi) = R_{3,2}(r)Y_{2,-1}(\theta,\phi)$$

(b) State boundary conditions for a particle travelling freely in a ring (of radius r) model.

## Q2. Marks: 10

Derive the expression for radius of Bohr orbit of electron revolving around the nucleus from Bohr's model.

## Q3. Marks: 10

i) Write down the expression for Schrödinger equation; explain its each term.

ii) For a single particle moving in three dimensions, the classical kinetic energy is given in Cartesian coordinates as:

$$T = \frac{1}{2}\sum_{i=1}^{3} mv_i^2 = \sum_{i=1}^{3} \frac{p_i^2}{2m}$$

Show that the quantum mechanical kinetic energy operator is

$$\hat{T} = -\frac{\hbar^2}{2m}\nabla^2$$

## Q4. Marks: 10

For a free particle moving in a 1-dimensional box (length $a$) with infinite potential energy walls, what is the probability of finding the particle in region: $a/3 \leq x \leq 2a/3$, if it is in its ground state (n=1)?

## Q5. Marks: 10

The $\Psi_{2s}$ atomic orbital for hydrogen-like atom is given as:

$$\Psi_{2s} = \frac{1}{4\sqrt{2\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\left(2 - \frac{Zr}{a_0}\right)e^{-Zr/2a_0}$$

Find, where the radial node of the wavefunction occurs in terms of $a_0$ for H, $He^+$, $Li^{2+}$ atoms, and comment on your results.

## Q6. Marks: 10

Imagine 6 $\pi$ electrons of benzene freely moving in a circular ring of carbon atoms. The carbon-carbon bond length in benzene is 1.4 Å. Calculate the absorption wavelength for electronic transition to occur from the ground state (highest occupied) to the next excited state (lowest unoccupied).

## Q7.

Marks: 10

A set of molecular orbitals (MOs) is given below. Label each MO as either $\sigma$ or $\pi$, and either $u$ or $g$. Identify whether it is a bonding or an anti-bonding MO. Imagine each MO was formed by the linear combination of a pair of atomic orbitals.