

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

Time Duration: 1.5 Hours

Start Time: 10.00 AM

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

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:

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

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 Ψ_{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.

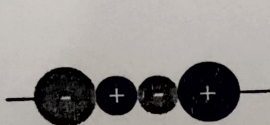
Marks: 10

Imagine 6 π 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).

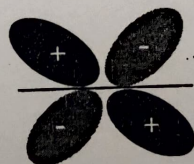
Q7.

Marks: 10

A set of molecular orbitals (MOs) is given below. Label each MO as either σ or π , 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.



(a)



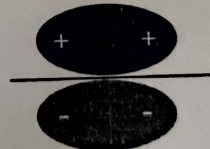
(b)



(c)



(d)



(e)



(f)