MCH-018

ASSIGNMENT BOOKLET

M.Sc. in Chemistry/Analytical Chemistry Programme (MSCCHEM/MSCANCHEM)

QUANTUM CHEMISTRY AND GROUP THEORY

(Valid from 1st July 2026 to 30th June 2027)

It is compulsory to submit the assignment before filling in the examination form

School of Sciences
Indira Gandhi National Open University
New Delhi-110068
(2026-2027)

Dear Learner,

Please read the section on assignments in the Programme Guide for M.Sc. in Chemistry that we sent you after your enrolment. A weightage of 30 per cent, as you are aware, has been earmarked for continuous evaluation, which would consist of one tutor-marked assignment for this course. The assignment is in this booklet, and covers both the blocks of the course. The total marks of all the parts are 100, of which 40% are needed to pass it.

Instructions for Formatting Your Assignments

Before attempting the assignment please read the following instructions carefully:

1. On top of the first page of your answer sheet, please write the details exactly in the following format:

ENROLAMENT NO. :…..…….

NAME :……...

ADDRESS :……

COURSE CODE :……..

COURSE TITLE :……..

ASSIGNMENT NO :……..

STUDY CENTRE :…….. DATE :…….

(Name and Code)

PLEASE FOLLOW THE ABOVE FORMAT STRICTLY TO FACILITATE EVALUATION AND TO AVOID DELAY.

2. Use only foolscap size paper (but not of very thin variety) for writing your answers.
3. Leave about 4 cm margin on the left, top and bottom of your assignment response sheet.
4. Your answers should be precise.
5. Submit the complete assignment answer sheets within the due date.
6. The assignment answer sheets are to be submitted to your Study centre within the due date. Answer sheets received after the due date shall not be accepted.
   We strongly suggest that you retain a copy of your answer sheets.
7. This assignment is valid from 1st July, 2026 to 30th June, 2027. If you have failed in this assignment or fail to submit it by June 2027, then you need to get the assignment for the year 2027-2028, and submit it as per the instructions given in the Programme Guide.
8. You cannot fill the examination form for this course until you have submitted the assignment.

Wishing you good luck

Tutor Marked Assignment
Quantum Theory and Group Theory (MCH-018)

Course Code: MCH-018
Assignment Code: MCH-018/TMA/26-27
Maximum Marks: 100

Note: Attempt all questions. The marks for each question are indicated against it.

You may use the following whenever required:
$h = 6.626 \times 10^{-34}\, Js$; $m_e = 9.11 \times 10^{-31}\, Kg$; $c = 3.0 \times 10^{8}\, ms^{-1}$

1. Answer ***any five*** of the following in brief: **(2 × 5)**

(a) State Heisenberg's Uncertainty Principle and provide its mathematical expression for position and momentum.

(b) Calculate the de Broglie wavelength for an electron traveling at a velocity of $2.5 \times 10^{6}\ \mathrm{ms}^{-1}$.

(c) Determine the number of radial nodes for a 4p orbital.

(d) Define an "orthonormal" set of wavefunctions using mathematical notation.

(e) What is the significance of the Bohr radius (a_0)? Provide its approximate value in picometers.

(f) Identify the boundary conditions where the wavefunction $\psi(x, y, z)$ must be zero for a particle in a 3D cubic box of length L.

(g) Explain the term "Stationary State" in the context of the Schrödinger amplitude function.

2.

(a) Show that the commutator $[\hat{x}^n, \hat{p}_x] = \frac{inhx^{n-1}}{2\pi}$, where n is a positive integer and $\hat{p}_x$ is the momentum operator. **(5)**

(b) Compare the experimental and mathematical inadequacies of classical mechanics in explaining Blackbody Radiation versus the Photoelectric Effect. Highlight one specific observation for each that contradicts classical wave theory. **(5)**

3.

(a) For a particle in a 3D cubic box of side L, show that the $(3, 3, 3)$ and $(5, 1, 1)$ energy states are degenerate. Calculate the energy of these states in terms of $h^2/8mL^2$. **(5)**

(b) A particle is confined to a 1D box of length L in the $n = 2$ state. Calculate the probability of finding the particle in the region between $x = 0.4\, L$ and $x = 0.6\, L$. **(5)**

4.

(a) Use the Bohr model energy expression to calculate the energy (in Joules and eV) required to remove an electron from the ground state of a He^{+} ion. **(5)**

(b) Apply the following Rodrigue formula

$$H_n(\xi) = (-1)^n e^{\xi^2} \frac{d^n}{d\xi^n} (e^{-\xi^2})$$

to derive the Hermite polynomials $H_0(\xi)$, $H_1(\xi)$ and $H_2(\xi)$. **(5)**

5.

(a) Calculate the expectation value $\langle r \rangle$ for an electron in the 1s orbital of a Hydrogen atom, given the normalized wavefunction

$$\psi_{1s} = \frac{1}{\sqrt{\pi} a_0^{3/2}} \exp\left(-\frac{r}{a_0}\right)$$

(Use the standard integral: $\int_0^\infty r^n e^{-ar} = \frac{n!}{a^{n+1}}$) **(5)**

(b) Demonstrate that the following kinetic energy operator is a Hermitian operator

$$\widehat{T_x} = -\frac{h^2}{8\pi^2 m} \frac{d^2}{dx^2}$$

(5)

6. Answer ***any five*** of the following in brief: **(2 × 5)**

(a) Define Slater-type Orbitals (STOs) and explain why they are preferred over Gaussian-type orbitals for multielectron atoms.

(b) Differentiate between a Symmetry Element and a Symmetry Operation with one example of each.

(c) State the two primary Hückel Molecular Orbital (HMO) assumptions regarding resonance integrals (β).

(d) What is the "Born-Oppenheimer Approximation" and why is it essential for solving molecular Hamiltonians?

(e) Define the Variation Principle in the context of trial wavefunctions.

(f) Briefly explain the concept of "Effective Nuclear Charge" (Z_{eff}) in multielectron atoms.

(g) What is the significance of the "Hückel magic number" ($4n + 2$) in the context of cyclic conjugated systems?

(h) Sketch the shape of the d_{z^2} orbital, clearly indicating the signs of the wave function lobes.

7.

(a) Write the complete Slater Determinant for the ground state of a Beryllium atom (Z=4). **(4)**

(b) Using the Variation Method, consider a trial wavefunction $\psi = \cos(kx)$ for a system. If the expectation energy $\langle E \rangle$ is expressed as a function of k, outline the mathematical steps to find the value of k that minimizes the ground state energy. **(6)**

8.

(a) Formulate the 3×3 matrix representation for a C_3 rotation operation about the z −axis.

(5)

(b) Assign the point groups for the following molecules: (i) CH_2Cl_2, (ii) PCl_5, (iii) NH_3 and (iv) Benzene (C_6H_6).

(5)

9.

(a) Describe the physical significance of the various terms in the Molecular Hamiltonian for the H_2 molecule. Why can this Hamiltonian not be solved exactly? **(5)**

(b) Using Molecular Orbital (MO) theory, determine the bond order and magnetic nature (paramagnetic or diamagnetic) for the O_2^{2-} ion.

(5)

10.

(a) Apply Hückel Molecular Orbital (HMO) theory to the Ethene system. Set up the secular determinant and solve for the energy levels in terms of α and β.

(5)

(b) For the allyl radical system, given the MO coefficient for the central atom in the non-bonding orbital is zero ($c_2 = 0$), calculate the π-electron charge density on the central carbon atom.

(5)