MCH-018

ASSIGNMENT BOOKLET

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

QUANTUM CHEMISTRY AND GROUP THEORY

(Valid from 1st July 2025 to 30th June 2026)

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)

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, 2025 to 30th June, 2026. If you have failed in this assignment or fail to submit it by June 2026, then you need to get the assignment for the year 2027, 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/2026
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. **(2X5)**

(a) State Heisenberg's Uncertainty Principle and write its mathematical expression.

(b) What is meant by an orthonormal set of wavefunctions.

(c) The ground state energy of a particle in a 1-D box cannot be zero? Comment.

(d) Give the boundary conditions where the wavefunction for a particle confined to move in a three-dimensional box must be zero.

(e) Calculate the number of radial nodes for a 3d orbital.

(f) Sketch the wavefunction for the first excited state of a quantum harmonic oscillator.

(g) Give the energy expression for a rigid rotor in three dimensions. What is the significance of J = 0?

2. **(a) (i)** What is the difference between probability density and probability. **(2)**

(ii) Show that the commutator $[\hat{x}^n, \hat{p}_x] = \frac{inhx^{n-1}}{2\pi}$, where n is a positive integer. **(4)**

(b) Outline the important experimental observations on photoelectric effect. How did Einstein's explain the experimental observation of threshold frequency in the context of photoelectric effect? **(4)**

3. **(a)** Show that the (3, 3, 3) and (5, 1, 1) energy states for a particle in three-dimensional box are degenerate. **(2)**

(b) A particle confined to move in a one-dimensional box of length L, is in its ground state. Calculate the probability, p, for finding the particle between x=0.25L and *x* = 0.75L. **(4)**

(c) Calculate the expectation (average) value of the energy of a particle of mass m confined to move in a one-dimensional box of width *a* and infinite height with potential energy zero inside the box. The normalized wave function of the particle is

$$\psi_n(x) = \left(\frac{2}{a}\right)^{1/2} sin\left(\frac{n\pi x}{a}\right)$$

Where, n = 1, 2, 3… **(4)**

4. **(a) (i)** How many quantum numbers emerge as a consequence of solving the Schrodinger's wave equation for hydrogen like ions? **(2)**

(ii) Calculate the most probable distance, r_{mp}, of the electron from the nucleus in the ground state of hydrogen atom, given that the normalized ground state wave function is **(4)**

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

(b) Calculate $H_0(\xi), H_1(\xi), H_2(\xi)$ by using following Rodrigue formula. **(4)**

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

5. (a) (i) Which state of the triply ionized beryllium (Be^{3+}) has the same orbital radius as that of the ground state of hydrogen atom. **(2)**

(ii) Calculate the probability for the electron to be found in the region $r = a_0$ to $r = \infty$ for 1s orbital of H atom. For 1s orbital the normalised wavefunction is defined as **(4)**

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

(b) Show that $\left[\hat{L}^2, \hat{L}_x\right] = \left[\hat{L}^2, \hat{L}_y\right] = \left[\hat{L}^2, \hat{L}_z\right] = 0$ **(4)**

6. Answer ***any five*** of the following in brief. **(2X5)**

(a) Find the energy of n = 2 level of helium ion, He^+ in eV. Assume that its reduced mass is same as that for hydrogen atom.

(b) What are the main differences between the spin and orbital angular momentum?

(c) The expectation energy as determined by the variation method cannot be less than the true ground state energy of the system. Comment.

(d) What are Slater type functions for multielectron atoms? What is their importance?

(e) Which of the perturbation methods used gives a better estimate of the ground state energy of helium atom?

(f) Give the difference between symmetry element and symmetry operation.

(g) What are the factors that determine the energy of molecular orbitals?

(h) What is Hückel's assumption for an exchange integral?

7. (a) (i) Write the Slater determinant for the ground state for lithium atom. **(2)**

(ii) Why the approximation methods are necessary in quantum chemistry? Give the difference between variation method and the Perturbation theory. **(4)**

(b) Consider the following trial wavefunction for a particle of mass m confined to move in a one-dimensional box of length, L.

$$\psi = ax(L - x)^2$$

Determine the corresponding energy by using variation theorem. **(4)**

8. **(a)** Formulate the matrix representation for reflection of a vector through *xy* plane. **(2)**
(b) Deduce the point group of all the isomers of difluoroethane. **(4)**
(c) Define mathematical groups and outline their characteristics. **(4)**

9. **(a) (i)** Write the complete Hamiltonian for the Hydrogen Molecule and specify different terms involved . **(3)**
(b) Draw a schematic diagram of the variation of E^+ and E^- for hydrogen molecule as a function of internuclear distance. **(3)**
(c) Formulate the spatial wavefunction for hydrogen molecule using the ground state wavefunction of hydrogen molecule ion. **(4)**

10. **(a) (i)** Write down the molecular orbital configuration of B_2^+ ion. **(2)**
(ii) Wite down the wave function for the nonbonding molecular orbital for a heteronuclear diatomic molecule AB assuming that the electron on an average spend 90% of its time on nucleus A and 10% of its time on nucleus B. **(3)**

(b) One of the three HMO molecular orbitals (MOs) for allyl radical is given below:

$$\psi = \frac{1}{2}\chi_1 - \frac{1}{\sqrt{2}}\chi_2 + \frac{1}{2}\chi_3$$

Find out all three MOs of allyl radical and arrange them in order of increasing energy. Justify your answer. **(5)**