MCH-020

# ASSIGNMENT BOOKLET

## M.Sc. in Chemistry Programme
## (MSCCHEM)

## ATOMIC AND MOLECULAR SPECTROSCOPY

(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
# Atomic and Molecular Spectroscopy (MCH-020)

**Course Code: MCH-020**
**Assignment Code: MCH-020/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 questions in brief: **(2X5)**

**(a)** Explain the origin of atomic spectrum.

**(b)** What is meant by anisotropy of chemical bond? Give an example.

**(c)** What makes TMS a molecule of choice to act as a reference in the NMR spectrometry?

**(d)** What is meant by polarizability of a molecule?

**(e)** In what way is NMR spectrometry different from other molecular spectroscopic methods?

**f)** What is the importance of $^{13}$C-NMR spectroscopy in structure determination?

**(g)** What is the requirement of the vibrational mode of a molecule to be Raman active?

**(h)** What is the photoelectric effect? Write the equation of Einstein's photoelectric law.

**2.** **(a) (i)** 5G services in India are provided at a frequency of 3300 MHz. Calculate the wavelength of the radiation. **(2)**

**(ii)** Explain why the atomic spectra are line spectra whereas the molecular spectra are band spectra. **(3)**

**(b)** A photon of visible light has a wavelength of 550 nm. Calculate its **(5)**

(i) wavenumber

(ii) frequency

(iii) energy per mol

**3.** **(a)** What is meant by the Balmer series of hydrogen? What will be the wave number of the longest wavelength in the Balmer series? **(5)**

**(b)** A photoelectron spectrum of a compound containing nitrogen (N), aluminium (Al), and fluorine (F) shows three strong peaks at the following binding energies:

- Peak X: ~686 eV
- Peak Y: ~399 eV
- Peak Z: ~73 eV

Find the best option from the choices given below that best explains the relative positioning of these peaks in terms of binding energy.

(i) Peak X corresponds to F 1s electrons, which have the highest binding energy because fluorine's high electronegativity and small size give its 1s electrons a large effective nuclear attraction. Peak Y is N 1s and Peak Z is Al 2p.

(ii) Nitrogen has more valence electrons than fluorine or aluminium, therefore its peak appears at the highest binding energy.

(iii) The spectrum shows more aluminium atoms than nitrogen or fluorine, so its peak appears at the lowest binding energy due to dilution.

(iv) Aluminium has the highest nuclear charge, so its 2p peak should have the largest binding energy, but shielding effects reverse this trend.

Justify your answer. **(5)**

**4.** **(a) (i)** What information about the molecule can be obtained from a rotation spectrum? **(2)**

**(ii)** What is meant by a selection rule? Give the selection rule for a rotating diatomic molecule modelled as a rigid rotator. **(3)**

**(b)** Assuming that the force constants of H-Cl and D-Cl are the same, calculate the fundamental vibration frequency of D-Cl if that of H-Cl is 2890 $cm^{-1}$. **(5)**

**5.** **(a)** In Raman spectra, the Stokes line are more intense than the anti-Stokes lines. Why? **(2)**

**(b)** The rotational Raman spectrum of a diatomic molecule has the first line of a series of Stokes and anti-Stokes lines at 346 $cm^{-1}$, relative of the $\overline{\nu}$ of incident light. What would be its bond length. **(4)**

**(c)** $CN^+$ has bond length 129 pm. Calculate the wavenumbers of the first four lines in its microwave spectrum. **(4)**

[Given: mass of C=12.000 u and mass of N=14.007 u]

**6.** **(a) (i)** Calculate the number of vibrational modes for a molecule of methane. **(2)**

**(ii)** The frequencies of the first and second overtones respectively are exactly double and triple of the fundamental vibration frequency. Comment. **(3)**

**(b)** Raman rotational spectra of $H_2$ was observed with Hg light with Rayleigh line at 2294 $cm^{-1}$. Stokes lines were observed at 22581, 22337, 22094, 21851 $cm^{-1}$. Draw the rotational energy level diagram with Stokes and anti Stokes lines. **(5)**

**7.** **(a) (i)** Electronic transitions are called vertical transitions. Comment. **(2)**

**(ii)** A light source of wavelength $\lambda$ illuminates a metal surface and electron are ejected with the maximum kinetic energy 2 eV. If the same surface is illuminated by a light source of wavelength $\lambda/3$, then calculate the maximum kinetic energy of the ejected electron. (Work function of metal is 1 eV) **(3)**

**(b) (i)** How does the rule of Mutual Exclusion help in predicting the symmetry in case of $H_2O$ and $CO_2$ molecules? **(2)**

**(ii)** The molecule $X_2Y$ has 3 fundamental vibrational frequencies. One is Raman active and two are IR active. Identify the structure of the molecule. **(3)**

**8. (a) (i)** Explain why the $^{13}C$-$^{13}C$ spin splitting is not observed in $^{13}C$-NMR spectrum? **(2)**

**(ii)** Predict the number of signal and multiplicity of peaks in the $^{13}C$ spectrum of the following compounds: **(4)**

a) 2,5-Dimethylhexane

b) Cyclohexanol

**(b) (i)** What is meant by AX spin system in NMR? Draw a schematic energy level diagram for this system and show the allowed transitions. **(2+2)**

**9. (a) (i)** Calculate the ESR frequency of an unpaired electron in a magnetic field of 3000 G (0.3 T). **(2)**

[Given: g = 2.0023; $\mu_B = 9.2741 \times 10^{-24}\ JT^{-1}$; and h = $6.626\times10^{-34}\ Js$]

**(ii)** Which of the following systems will show electron spin resonance (ESR) spectrum? (i) H (ii) $H_2$ (iii) $Na^+$ (iv) $Cl^-$ (v) $^{\bullet}CH_3$ (vi) $NO_2$ **(3)**

**(b)** What are different mechanisms that contribute to the relaxation of nuclear spins in the excited state? Explain any one of them. **(5)**

**10. (a) (i)** What is Mossbauer effect? **(2)**

**(ii)** The lifetime of $^{57}Fe$ (excited state) is 1.52 x $10^7$ s. If the excited state is 14.3 keV above the ground state determine the linewidth $\tau$ and ratio $\tau$ /E. **(4)**

**(b)** Write short notes on the following. **(4)**

(a) Isomer shift (b) Spin-Spin splitting