K25P 1861

Reg. No. : .....

Name : .....

II Semester M.Sc. Degree (CBCSS – OBE – Reg./Supple./Imp.) Examination, April 2025

(2023 & 2024 Admissions)

CHEMISTRY/CHEMISTRY WITH DRUG CHEMISTRY SPECIALISATION PROGRAMME

MSCHD02C08/MSCHE02C08 : Theoretical Chemistry – II

Time : 3 Hours Max. Marks : 60

SECTION – A

Short answer questions. Answer **any five** questions. **Each** question carries **three** marks.

1. Show that σ_{xz} and σ_{yz} in C_{2v} point group form separate classes.
2. Reduce the following representation using reduction formula. Use C_{3v} character table.

C_{3v}	E	$2C_3$	$3\sigma_v$
Γ	5	2	– 1

3. What is the effect of isotopic substitution in MW spectra ? What are its applications ?
4. State and explain mutual exclusion principle.
5. What is predissociation ? How it occur in electronic spectra ?
6. Describe natural line width and broadening. **(5×3=15)**

P.T.O.

SECTION – B

Paragraph questions. Answer **any three** questions. **Each** question carries **six** marks.

7. Construct the group multiplication table of C_{3v} point group. Show that all the vertical planes in C_{3v} point group forms a single class.

8. Write GOT and explain the terms. Discuss briefly the rules derived from GOT.

9. Discuss the principle of rotational Raman spectra. Derive the wave number expressions for stokes lines and antistokes lines.

10. What is chemical shift ? How it is measured ? What are the factors influencing chemical shift ?

11. How will you calculate the dissociation energy of a molecule ? **(3×6=18)**

SECTION – C

Essay type questions. Answer **any three** questions. **Each** question carries **nine** marks.

12. a) What are abelian and non abelian groups ? Illustrate using examples. 3

    b) Write the symmetry operations generated by S_4. 3

    c) Illustrate using suitable example, explain the difference between order and class of a point group. 3

13. Construct the character table for C_{2h} point group.

14. Identify the IR and Raman active vibrational modes in H_2O molecule.

15. a) What is Morse function of an anharmonic oscillator ? 2

    b) Discuss in detail the IR spectra of an anharmonic oscillator. 7

16. a) What is spin-spin coupling ? Write notes on coupling constant J and discuss the factors influencing J. . **5**

b) Write notes on Fortrat diagram. **2**

c) Discuss the shielding mechanism in NMR spectra. **2**

C_{3v} (3m)	E	$2C_3$	$3\sigma_v$		
A_1	1	1	1	z	$x^2 + y^2$, z^2
A_2	1	1	– 1	R_z	
E	2	– 1	0	(x, y) (R_x, R_y)	($x^2 - y^2$, 2xy) (xz, yz)

C_{2v} (2mm)	E	C_2	σ_v(xz)	σ'_v(yz)		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	– 1	– 1	R_z	xy
B_1	1	– 1	1	– 1	x, R_y	xz
B_2	1	– 1	– 1	1	y, R_x	yz

(3×9=27)