K23P 0461

Reg. No. : .....

Name : .....

II Semester M.Sc. Degree (CBSS – Reg./Supple./Imp.) Examination, April 2023
(2019 Admission Onwards)
CHEMISTRY
CHE. 2C.05 : Theoretical Chemistry – II

Time : 3 Hours Max. Marks : 60

SECTION – A

Answer **all** questions in **one** word or **one** sentence. **Each** question carries **one** mark.

1. What is the resulting point group by combining inversion to C_{2v} point group ?
2. By using the 3 × 3 matrix prove that C_2 rotation axis is its own inverse.
3. Find out the point group of
   a) Ethane (eclipsed)
   b) $CH_2 = C = C = CH_2$.
4. What is the difference between the rigid and non-rigid rotator model ?
5. What are the two different types of selection rules in spectroscopy ?
6. Which region of electromagnetic spectrum is used in NMR spectroscopy ?
7. What are the different factors that contribute to the intensity of spectral lines ?
8. Define normal mode of vibration. **(8×1=8)**

P.T.O.

SECTION – B

Answer **any eight** questions. Answer may be in **two** or **three** sentences. **Each** question carries **two** marks.

9. What are Abelian groups ? Give an example.
10. Define cyclic group. Give an example.
11. By using the 3 × 3 matrix for C_n and C_n^{-1} prove $C_n \times C_n^{-1} = E$ (identity operation).
12. Explain the reason for applying the external magnetic field in magnetic resonance spectroscopy.
13. In a given organic compound two kinds of protons exhibit signals at 50 Hz, 200 Hz using a 60 MHz instrument. What will be their relative position using 90 MHz instrument ? Also convert the position of signals into delta scale.
14. Sketch the vibrational modes of H_2O molecule.
15. Explain the relevance of Heisenberg's uncertainty principle in predicting the line width of spectrum.
16. How many NMR energy levels are possible for nucleus with a spin I=3/2 ?
17. Show that all cyclic groups are abelian.
18. How IR spectroscopy is used in identifying the nitro and cyano groups ?
19. What are overtone bands in IR spectrum ?
20. How do you calculate the fundamental vibrational modes of poly atomic molecules ? **(8×2=16)**

SECTION – C

Answer **any four** questions. **Each** question carries **three** marks.

21. Explain Predissociation.
22. The rotational spectrum of $^{79}Br^{19}F$ shows a series of equidistant lines separated by 0.71433 cm^{-1}. Calculate the rotational constant, moment of inertia and Br-F bond length.

23. Discuss the classical theory of Raman effect.
24. Explain the rule of mutual exclusion principle. Rationalize this using group theory.
25. Write down the group multiplication table for C_{2v} point group.
26. Taking the Px orbital on each carbon atom of the Cis- butadiene generate a reducible representation and reduce it.
27. Generate a 3 × 3 matrix for C_3 and S_4 rotation axis.
28. Explain the difficulties involved in recording ^{13}C NMR spectra. **(4×3=12)**

SECTION – D

Essay type questions. Answer **any four** questions. **Each** question carries **6** marks.

29. A) Find out the IR and Raman active vibrational modes of H_2O using group theory.

    OR

    B) Using group theory, explain the MO diagram of water molecule.

30. A) Explain the different types of measurement techniques in NMR spectroscopy.

    OR

    B) Explain the different types of electronic transitions in molecules and Fortrat diagram.

31. A) How microwave spectroscopy can be used in determining the bond length of linear diatomic molecules.

    OR

    B) How IR and Raman spectroscopies can be used in determining the structure of molecules ?

32. A) State and explain Great Orthogonality Theorem. Using this derive the C_{2v} character table.

    OR

    B) Generate a 3 × 3 matrix for C_n and C_n^{-1} rotation axis using x, y, z co-ordinates of point in three dimensional space. **(4×6=24)**

Character table for C_{2v} point group

	E	$C_2(z)$	$\sigma_v(xz)$	$\sigma_v'(yz)$	Linear, rotations	Quadratic
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