K24P 0836

Reg. No. : .....

Name : .....

Second Semester M.Sc. Degree (CBSS – Supple. (One Time Mercy Chance)/Imp.) Examination, April 2024
(2014 to 2022 Admissions)
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. Prove that the numbers from $-\alpha$ to $+\alpha$ form a mathematical group under addition operation.
2. By using the 3×3 matrix prove that C_3 rotation axis is not its own inverse.
3. Find out the point group of a) Ethane (staggered) b) $CH_2 = C = C = C = CH_2$.
4. How Raman spectroscopy is different from other spectroscopic techniques ?
5. What are the two different types of selection rules in spectroscopy ?
6. Sketch the energy level diagram of nucleus with spin I = 1 in a magnetic field.
7. What are the different factors that contribute to the width of spectral lines ?
8. State Frank-Condon principle. **(8×1=8)**

SECTION – B

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

9. What are conjugate elements ? Give an example.
10. All cyclic groups are abelian, but the reverse is not true. Rationalise this statement.

P.T.O.

11. The three reflection planes of ammonia are included in the same class. Why ?

12. Explain the reason for applying the RF radiation perpendicular to the magnetic field in NMR spectroscopy.

13. In a given organic compound two kinds of protons exhibit signals at 100 Hz, 400 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. Differentiate between point group and space group.

15. Explain the relevance of population of energy levels and intensity of spectral lines.

16. Sketch the NMR spectrum of AMX pattern.

17. Classify the molecules based on the moment of inertia along three mutually perpendicular directions.

18. Comment on the differences between the scales in ^{1}H and ^{13}C NMR spectroscopy.

19. What are combination bands in IR spectrum ?

20. Define normal modes of vibrations. **(8×2=16)**

SECTION – C

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

21. Explain the determination force constant of linear diatomic molecules.

22. Stoke lines are more intense than Anti stoke lines in Raman spectroscopy. Why ?

23. Explain the different factors contributing to the chemical shift of protons in NMR spectroscopy.

24. What are the different types of relaxation methods in NMR ?

25. What are the different conditions for selecting the principle rotation axis for molecules ?

26. Using C_{3v} character table find out E⊗E and reduce it.

C_{3v}	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)	($x^2 – y^2$, xy), (xz, yz)

27. Explain the different rules for forming a mathematical group.

28. Generate a 3×3 matrix for C_2 and S_2 rotation axis. What is the equivalent symmetry operation of S_2. **(4×3=12)**

SECTION – D

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

29. A) Find out the IR and Raman active vibrational modes of NH_3 using group theory.

OR

B) Using group theory find out the hybrid orbitals of CH_4.

30. A) Explain the FT NMR spectroscopy. What are the advantages of this technique over CW NMR.

OR

B) Explain the calculation of heat of dissociation of molecules using electronic spectroscopy.

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

OR

B) What is rule of mutual exclusion principle ? Sketch the polarizability ellipsoid of various vibrational modes of CO_2. Which of these are Raman active ?

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

Character table for point group T_d

T_d	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$	Linear functions, rotations	Quadratic functions
A_1	+ 1	+ 1	+ 1	+ 1	+ 1	–	$x^2 + y^2 + z^2$
A_2	+ 1	+ 1	+ 1	– 1	– 1	–	–
E	+ 2	– 1	+ 2	0	0	–	$(2z^2 – x^2 – y^2, x^2 – y^2)$
T_1	+ 3	0	– 1	+ 1	– 1	(R_x, R_y, R_z)	–
T_2	+ 3	0	– 1	– 1	+ 1	(x, y, z)	(xy, xz, yz)

(4×6=24)