

C 83711

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Name.....

Reg. No.....

SECOND SEMESTER M.Sc. DEGREE EXAMINATION, JUNE 2015

(CUCSS)

Chemistry

CH 2C 04—THEORETICAL CHEMISTRY—II

(2010 Admissions)

Time : Three Hours

Maximum : 36 Weightage

Section A

Answer all questions.

Each question carries a weightage of 1.

1. Explain with examples :

(a) Abelian group.

(b) Cyclic group.

2. Generate matrices for :

(a) C_3 .

(b) σ_{xy} .

3. Distinguish between degenerate and non-degenerate representation with examples.

4. Explain with example 'projection operator'.

5. Which of the following vanish on integration ? Illustrate :

(a) $\int_0^a x^2 dx$.

(b) $\int_0^a x^3 dx$.

6. Define normal mode of vibration.

7. State Laporte selection rules for centrosymmetric systems.

8. Which of the following molecules give microwave spectrum ? Why ?

(a) CO_2 .

(b) CH_3Cl .

(c) C_2H_4 .

(d) CH_2Cl_2 .

9. Calculate the Doppler shift in frequency when radiation of frequency 10^{12} MHz is absorbed by a sample moving with a velocity of $1 \text{ cm} \cdot 5^{-1}$.

10. Account for the decrease in spacing of lines in the pure rotation spectrum of HCl as J increases.

Turn over

11. Find the number of vibrational quantum states in the ground electronic level of HCl. The anharmonic constant is 0.017.
12. Explain terms 'isotropic polarizability' and 'Anisotropic polarizability'.
13. Define gyromagnetic ratio. Explain its significance.
14. What do you mean by 'COSY'. Explain.

(14 × 1 = 14 weightage)

Section B

*Answer any seven questions.
Each question carries a weightage of 2.*

15. Set up group multiplication table for C_{3v} point group.
16. Derive c_{3u} character table.
17. Find IR and Raman active vibrations of H_2O which belongs to C_{2v} point group

C_{2v}	E	C_{2z}	σ_{vzx}	$\sigma_{v'yz}$		
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

18. Find molecular Orbitals in H_2O use C_{2v} character table in question No. 17.
19. How would you determine the bond lengths in COS using microwave spectroscopy? Explain.
20. State and explain the selection rules for rotational Raman spectrum of polyatomic molecules.
21. What is 'Fortrat diagram'? Explain its significance.
22. Briefly explain the principle of AES.
23. H atom shows EPR spectrum with a coupling constant of 50mT. Use McConnell equation to find the electron density around C atom in methyl radical which shows a coupling constant of 2.3 mT.
24. Briefly explain 'quadrupole relaxation'.

(7 × 2 = 14 weightage)

Section C

Answer any **two** questions.

Each question carries a weightage of 4.

25. Predict allowed electronic transitions in CH_2O . Use C_{2v} character table in question No. 17.
26. Find π molecular orbitals in (C_3H_3^+) . Use C_3 Character table :

C_3	E	C_3	C_3^2
A	1	1	1
E	$\begin{cases} 1 \\ 1 \end{cases}$	$\begin{matrix} \epsilon \\ \epsilon^* \end{matrix}$	$\begin{matrix} \epsilon^* \\ \epsilon \end{matrix}$

$$\epsilon = e^{i2\pi/3}$$

27. How would you predict Raman activity using polarizability ellipsoid ? Discuss.
28. What are the drawbacks of field sweep method in NMR spectroscopy ? How are they overcome in FT NMR ? Discuss.

(2 × 4 = 8 weightage)