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Name.....33

Reg. No.....

SECOND SEMESTER M.Sc. DEGREE EXAMINATION, JUNE 2014

(CUCSS)

Chemistry

CH 2C 04—THEORETICAL CHEMISTRY—II

(2010 Admissions)

Three Hours

Maximum : 36 Weightage

Section A

Answer all questions.

Each question carries a weightage of 1.

1. Explain with example "similarity transformation".
2. Write Schoenflies symbol of point groups for the following :—
(a) CH_2Cl_2 ; (b) POCl_3 .
3. State and explain rearrangement theorem.
4. State rules for assigning Mulliken's symbol for irreducible representation.
5. What do you mean by direct product of irreducible representation ?
6. Taking the $2p_x$ atomic orbitals perpendicular to the plane of cis-butadiene on basis, find the reducible representation.
7. Radio frequency radiation is employed in nmr while microwave radiation is employed in esr spectroscopy. Why ?
8. Find the rotational quantum number corresponding to the maximum intensity in the microwave spectrum of HCl $B = 10.7 \text{ cm}^{-1}$
9. Stoke's lines are more intense than antistoke's lines in the vibrational Raman spectrum. Why ?
10. What do you mean by Resonance Raman ?
11. How would you distinguish XPS peaks from AES peaks in the spectrum ? Explain.
12. State and explain Birge-Sponer approximation.
13. How many lines do you expect in the EPR spectrum of naphthalene negative ion ? Explain.
14. State and explain Karplus relationship.

(14 × 1 = 14 weightage)

Section B

Answer any seven questions.

Each question carries a weightage of 2.

15. Explain the importance of group multiplication table in group theory.

Turn over

16. State "Great orthogonality theorem". What are the consequences of the theorem ?
 17. State mutual exclusion principle. Rationalise using group theory.
 18. Find allowed electronic transitions in $>C=O$. Use C_{2v} character table :

C_{2v}	E	C_{2z}	σ_{xz}	σ_{yz}
	1	1	1	1
	1	1	-1	-1
	1	-1	1	-1
	1	-1	-1	1

19. Briefly discuss rotation spectrum of symmetric top molecules.
 20. Discuss briefly atomic spectrum of H atom.
 21. State Franck-Condon principle. Discuss its importance in understanding electronic spectra of diatomic molecule.
 22. Briefly explain the principle of 2d-NMR spectroscopy.
 23. Write Mc Connell equation. Discuss its importance.
 24. What is the significance of 'g' value in EPR spectrum. Distinguish between $g_{||}$ (parallel) and g_{\perp} (perpendicular). (7 × 2 = 14 weight)

Section C

Answer any two questions.

Each question carries a weightage of 4.

25. Find hybridized orbitals of C atom in CH_4 . Use T_d character table.
 26. Find π molecular orbitals of $(C_3H_3^+)$. Use C_3 character table.
 27. What are the drawbacks of field sweep method in NMR spectroscopy? How are they overcome in FTNMR? Discuss.
 28. Discuss the applications of Mössbauer spectroscopy in structural elucidation :

T_d	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
E	2	-1	2	0	0
T_1	3	0	-1	1	-1
T_2	3	0	-1	-1	1

C_3	E	C_3	C_3^2
A_1	1	1	1
E	{	ϵ	ϵ^*
	1	ϵ^*	ϵ

$$\epsilon = e^{i(2\pi/3)}$$

(2 × 4 = 8 weight)