



K24P 1065

Reg. No. :

Name :

Second Semester M.Sc. Degree (C.B.C.S.S. – OBE – Regular)
Examination, April 2024
(2023 Admission)
CHEMISTRY

MSCHE02C08/MSCHD02C08 : Theoretical Chemistry – II

Time : 3 Hours

Max. Marks : 60

SECTION – A

Short answer questions. Answer **any five** questions. **Each** question carries **three** marks. **(5×3=15)**

1. Construct the group multiplication table of C_{3v} and discuss the generalization made from this table.
2. Write a note on transition moment integral and its application in group theory.
3. Discuss the isotope effect on rotational spectra.
4. Explain Franck Condon principle and its relevance.
5. Assign each molecule below to proper point group
 - a) Trans-1, 3-dibromocyclobutane
 - b) Bromoethane
 - c) Phosphorous oxychloride
6. The rotational constant for $H^{35}Cl$ is observed to be 10.5909 cm^{-1} . What are the values of B for $H^{37}Cl$ and for $^2D^{35}Cl$?

SECTION – B

Paragraph questions. Answer **any three** questions. **Each** question carries **six** marks. **(3×6=18)**

7. Construct matrices for each of the elements in C_{2h} and verify the group theoretical rules using these matrices.

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8. Discuss the great orthogonality theorem and explain the rules derived from the theorem.
9. Find out the atomic orbitals of Carbon taking part in the hybridisation of CH_4 molecule.
10. Using the energy level expression and appropriate selection rules draw an energy level diagram and the spectral transitions for the rotational Raman spectrum of a rigid diatomic rotor. Also show the appearance of the spectrum.
11. Discuss spin spin coupling and coupling constant and describe the high resolution proton NMR spectrum of 1, 1, 2-trichloroethane.

SECTION – C

Essay type questions. Answer **any three** questions. **Each** question carries **9** marks.

(3×9=27)

12. a) Construct the general matrix for C_n and S_n . (3 Marks)
b) Decompose the reducible representation $(\Gamma) 6 0 0$ in the point group C_{3v} into a sum of irreducible representations. Write the product $E \times E$ in this group as a sum of irreducible representation. (6 Marks)
13. Determine the IR and Raman active vibrations of BF_3 and CH_4 molecules.
14. Describe the vibrational-rotational spectrum of a diatomic molecule.
15. Explain the following in electronic transitions
 - a) Dissociation
 - b) Pre-dissociation
 - c) Birge-Sponer plot.(3 Marks each)
16. Discuss the factors influencing the chemical shift and coupling constant in NMR spectroscopy.



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)

T_d ($\bar{4}3m$)	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$	
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	$(2z^2 - x^2 - y^2, \sqrt{3}(x^2 - y^2))$
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)

D_{3h} ($\bar{6}$)m2	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$	
A'_1	1	1	1	1	1	1	$x^2 + y^2, z^2$
A'_2	1	1	-1	1	1	-1	R_z
E'	2	-1	0	2	-1	0	(x, y) ($x^2 - y^2, 2xy$)
A''_1	1	1	1	-1	-1	-1	
A''_2	1	1	-1	-1	-1	1	z
E''	2	-1	0	-2	1	0	(R_x, R_y) (xy, yz)

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