

Reg. No. :

Name :

II Semester M.Sc. Degree (CBSS – Reg./Suppl. (Including Mercy Chance)/Imp.)
Examination, April 2021
(2014 Admission Onwards)
CHEMISTRY
CHE 2C.05 : Theoretical Chemistry – II

Time : 3 Hours

Max. Marks : 60

SECTION – AAnswer **all** questions **each** in **one** word or sentence. **Each** question carries **1** mark.

1. Define the reciprocal of an element in a group.
2. What is a subgroup ?
3. What is the Mulliken symbol for one dimensional representation ?
4. What is the result of product $C_2(x)C_2(y)$?
5. Which of the following diatomic molecules don't absorb in the IR region ?
HCl, CIBr, N_2 , H_2 , O_2 .
6. Which of the following vibrational transitions will be observed for a diatomic molecule (treated as harmonic oscillator) ?
 $v = 1$ to $v = 3$; $v = 2$ to $v = 3$; $v = 5$ to $v = 4$.
7. Mention any two nuclei having half integer spin.
8. Write down the approximate chemical shift value of aldehyde proton. **(8×1=8)**

SECTION – BAnswer **eight** questions. Answer may be in **two** or **three** sentences. **Each** question carries **2** marks.

9. Define similarity transformation.
10. Prove that if element, A is conjugate with B, then B is conjugate with A.
11. Distinguish between horizontal and vertical plane with diagrams.

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12. What is called an irreducible representation ?
13. Differentiate between operator E and Mulliken symbol E.
14. Explain with example D_{2h} point group.
15. What information about the molecular geometry of N_2O can be determined from knowing that a pure rotational absorption spectrum is observed for this molecule ?
16. Explain the significance of transition moment integral.
17. Calculate the wave number of IR radiation whose wave length is $2\mu m$.
18. State the significance of Franck-Condon principle.
19. Why a reference standard is needed in NMR spectroscopy ? Give one example.
20. What is chemical shift ? **(8×2=16)**

SECTION – CAnswer **four** questions **each** in **one** paragraph. **Each** question carries **3** marks.

21. Prove that in any Abelian group, each element is in a class by itself.
22. Derive the matrix representation of symmetry operations, proper rotation and improper rotation.
23. State and explain Great Orthogonality Theorem.
24. Write down the C_{2v} character table and reduce the following C_{2v} representations :

C_{2v}	E	C_2	$\sigma(XZ)$	$\sigma(YZ)$
Γ_1	3	-1	1	1
Γ_2	2	0	0	2

25. Discuss the vibrational coarse structure or progressions.
26. Describe quantum theory of Raman spectra.
27. Illustrate dissociation and predissociation with diagrams.
28. Explain the spin-spin coupling involved in the NMR spectra of AMX type molecule. **(4×3=12)**

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SECTION – DAnswer either **A** or **B** of **each** question. **Each** question carries **6** marks.

29. A) i) Assign the point groups to following molecules and justify : N_2 , CO, NH_3 , BF_3 .
 ii) Explain with examples improper axis and improper rotation. What are the different kinds of operations generated by S_n (n = odd and even) operation ?
 OR
 B) Construct the reducible representation for SO_2 molecule from the Cartesian coordinates of atoms.

30. A) Derive the character table for C_{2h} .
 OR
 B) Determine the hybridization in BF_3 using the D_{3h} character table given below.

31. A) Compare and contrast IR and Raman spectroscopy.
 OR
 B) Explain in detail various factors that influence the intensity of spectral lines.

32. A) Explain shielding effects in NMR spectrum.
 OR
 B) What is Fortrat Parabola ? Obtain the expression for the band head in terms of B' and B'' .

D_{3h}	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$		
A_1'	1	1	1	1	1	1	R_z (x, y)	$x^2 + y^2, z^2$
A_2'	1	1	-1	1	1	-1		$(x^2 - y^2, xy)$
E'	2	-1	0	2	-1	0		
A_1''	1	1	1	-1	-1	-1	z (R_x, R_y)	(xz, yz)
A_2''	1	1	-1	-1	-1	1		
E''	2	-1	0	-2	1	0		

(4×6=24)