

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 – A

Answer **all** questions **each** in **one** word or sentence. **Each** question carries **1** mark.

- Define the reciprocal of an element in a group.
- What is a subgroup ?
- What is the Mulliken symbol for one dimensional representation ?
- What is the result of product $C2(x)C2(y)$?
- Which of the following diatomic molecules don't absorb in the IR region ?
HCl, ClBr, N_2 , H_2 , O_2 .
- 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 $v = 4$.
- Mention any two nuclei having half integer spin.
- Write down the approximate chemical shift value of aldehyde proton. **(8×1=8)**

SECTION – B

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

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

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- What is called an irreducible representation ?
- Differentiate between operator E and Mulliken symbol E.
- Explain with example D_{2h} point group.
- 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 ?
- Explain the significance of transition moment integral.
- Calculate the wave number of IR radiation whose wave length is $2\mu m$.
- State the significance of Franck-Condon principle.
- Why a reference standard is needed in NMR spectroscopy ? Give one example.
- What is chemical shift ? **(8×2=16)**

SECTION – C

Answer **four** questions **each** in **one** paragraph. **Each** question carries **3** marks.

- Prove that in any Abelian group, each element is in a class by itself.
- Derive the matrix representation of symmetry operations, proper rotation and improper rotation.
- State and explain Great Orthogonality Theorem.
- 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
- Discuss the vibrational coarse structure or progressions.
- Describe quantum theory of Raman spectra.
- Illustrate dissociation and predissociation with diagrams.
- Explain the spin-spin coupling involved in the NMR spectra of AMX type molecule. **(4×3=12)**

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SECTION – D

Answer either **A** or **B** of **each** question. **Each** question carries **6** marks.

- Assign the point groups to following molecules and justify : N_2 , CO, NH_3 , BF_3 .
 - Explain with examples improper axis and improper rotation. What are the different kinds of operations generated by S_n ($n = \text{odd and even}$) operation ?

OR

 - Construct the reducible representation for SO_2 molecule from the Cartesian coordinates of atoms.
- Derive the character table for C_{2h} .

OR

 - Determine the hybridization in BF_3 using the D_{3h} character table given below.
- Compare and contrast IR and Raman spectroscopy.

OR

 - Explain in detail various factors that influence the intensity of spectral lines.
- Explain shielding effects in NMR spectrum.

OR

 - 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		$x^2 + y^2, z^2$
A_2'	1	1	-1	1	1	-1	R_z	
E'	2	-1	0	2	-1	0	(x, y)	$(x^2 - y^2, xy)$
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)	(xz, yz)

(4×6=24)