BIRLA INSTITUTE OF TECHNOLOGY, MESRA, RANCHI
(END SEMESTER EXAMINATION)

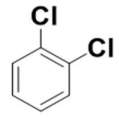
CLASS: MSc/Pre-PhD **SEMESTER : IX/I**
BRANCH: CHEMISTRY **SESSION : MO/2025**

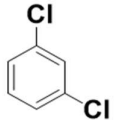
SUBJECT: CH501 SPECTROSCOPIC ELUCIDATION OF MOLECULAR STRUCTURE

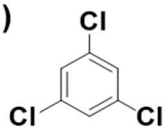
TIME: 3 Hours **FULL MARKS: 50**

INSTRUCTIONS:
1. The question paper contains 5 questions each of 10 marks and total 50 marks.
2. Attempt all questions.
3. The missing data, if any, may be assumed suitably.
***4*. Before attempting the question paper, be sure that you have got the correct question paper.**
5. Tables/Data hand book/Graph paper etc. to be supplied to the candidates in the examination hall.

			CO	BL
Q.1(a)	What will be the effect of isotopic substitution on stretching vibration of IR spectrum? How one can follow the progress of acid chloride to amide conversion reaction through IR spectroscopy?	[5]	1	3
Q.1(b)	Discuss the various reasons of deviations of Beer-Lambert's law. With a suitable example, demonstrate how Auxochrome causes 'red shrift' of a chromophore.	[5]	1	3
Q.2(a)	(i) Draw a clean diagram for the ^{1}H-NMR spectrum of $CH_3CH_2CH_2Br$ mention the multiplicities of different signals. (ii) Explain the multiplicities based on Spin-spin coupling. (iii) Draw a COSY NMR spectrum for the above-mentioned compound. (iv) And correlate with ^{1}H NMR spectra.	[2+1+1+1]	2	3
Q.2(b)	(i) How can you distinguish the following molecules by ^{1}H NMR spectroscopy?	[2+1+2]	2	3

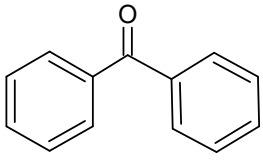
(i) 

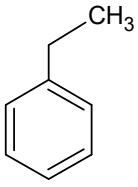
(ii) 

(iii) 

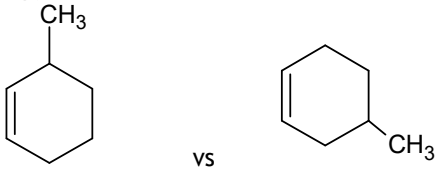
(ii) In the 400 MHz ^{1}H NMR spectrum, organic compounds exhibited a doublet. The two lines of the doublet are at δ 2.375 and 2.396 ppm. The coupling constant (J) value is
(iii)Arrange the following compounds in order of increasing chemical shifts (δ-value) of the α -protons with explanation.
(a)C_3H_7F, (b) C_3H_7I, (c) C_3H_7Br, (d) C_3H_7Cl

Q.3(a)	Outline the complete MS fragmentation of the following compounds? Also, mark the base peak in each case.	[5]	3	3

(i) 

(ii) 

Q.3(b)	How will you distinguish between the following two isomers through mass spectroscopy?	[5]	3	3



PTO

Q.4(a)	Explain why does ESR spectroscopy operate in GHz whereas NMR spectroscopy in MHz range? Show hyperfine splitting pattern of $^{\cdot}CHF_2$ free radical where a^H =22 G and a^F= 84 G.	[5]	4	2
Q.4(b)	What do you mean by 'chemical shrift' in Mossbauer spectroscopy? Illustrate with an example how 'chemical shrift' can be used to determine the metal oxidation state in an organometallic compound.	[5]	4	2,3
Q.5(a)	(i) An organic compound ($C_9H_{10}O_4$) exhibited the following spectral data: 1H-NMR (400 MHz, DMSO-d6) data of a compound: δ in ppm: 3.85 (s, 6H), 6.73 (t, *J* = 2.2 Hz, 1H), 7.1 (d, *J* = 2.2 Hz, 2H), and 13.05 (brs, 1H). Identify the compound with detailed explanation. (ii) An organic compound ($C_9H_{11}NO_2$)exhibited the following spectral data: ^{1}H NMR: δ,7.9 (d, *J* = 8 Hz, 2H), 6.6 (d, *J* = 8 Hz, 2H), 4.3 (q, *J* = 6 Hz, 2H), 4.0 (br s, 2H, D2O exchangeable), 1.4 (t, *J* = 6 Hz, 3H) Mass: m/z 165, 137, 120, 92, Identify the compound with details explanation.	[2+4]	5	3
Q.5(b)	An organic compound ($C_9H_{10}O_3$) exhibited the following spectral data: IR: 3400, 1680 cm $^{-1}$; 1H NMR: δ 7.8 (1H, d, *J* = 8 Hz), 7.0 (1 H, d, *J* = 8Hz), 6.5 (1 H, s), 5.8 (1 H, s, D_2O exchangeable), 3.9 (3H, s), 2.3 (3 H, s). Identify the compound with detailed explanation.	[4]	5	3

::::::19/11/2025::::::E