MASTER OF SCIENCE (CHEMISTRY) (CBCS - 2018 COURSE)
M.Sc. (Chemistry) Sem-III : WINTER :- 2021
SUBJECT: SPECTROSCOPIC METHODS IN STRUCTURE DETERMINATION

Day : Saturday | Time : 02:00 PM-05:00 PM
Date 22-01-2022 | **W-20151-2021** | Max. Marks: 60

N.B:
1) All questions are **COMPULSORY**.
2) Figures to the right indicate **FULL** marks.
3) Answer to both the section should be written in **SEPARATE** answer book.

SECTION-I

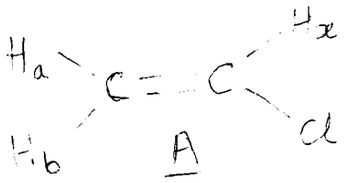
Q.1 Explain **ANY THREE** of the following: **(15)**

a) DMSO $-d_6$ shows seven lines in ^{1}HNMR.

b) Methylene protons of R_1R_2 CH-CH_2 –OH are diastereotopic.

c) Piperizine shows two singlets while N–nitroso piperizine shows four triplets & one singlet.

d) Following coupling constants are seen in the PMR of compound A.

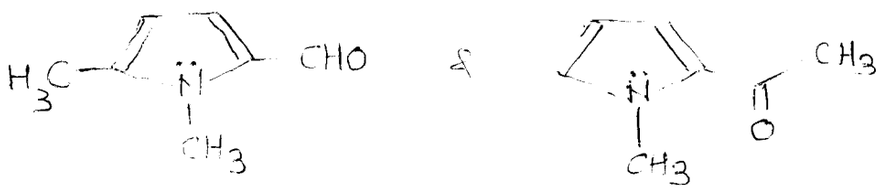


Jab= 1.4Hz; Jax=7.3Hz & Jbx=14.6Hz

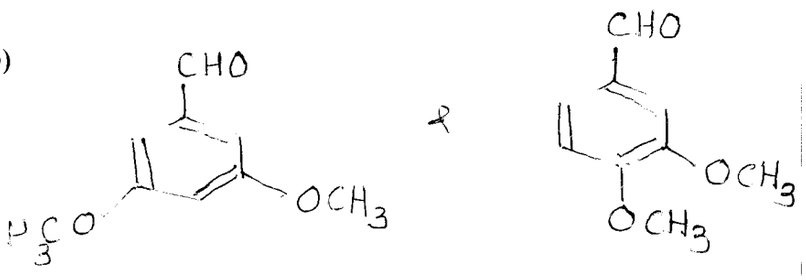
e) CIMS is preferred method for detection of M^+ over EIMS in mass spectrometry.

Q.2 Distinguish between **ANY THREE** of the following by given spectral method. **(15)**

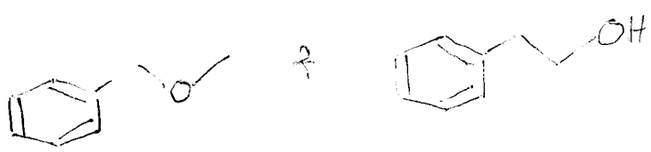
a) ^{1}H NMR



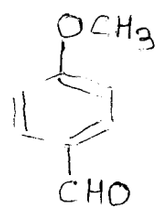
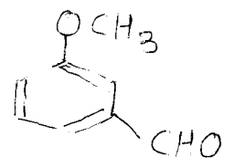
b) ^{1}H NMR

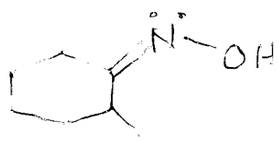
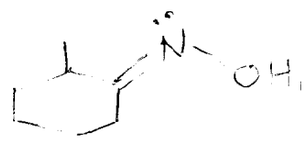


c)



Mass

d)  &  CMR

e)   CMR

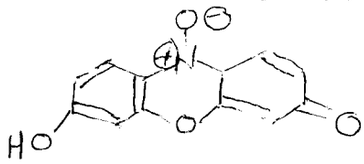
SECTION-II

Q.3 Write notes on **ANY THREE** of the following **(15)**

- **a)** Karplus equation
- **b)** Metastable ion
- **c)** Two methods for simplification of complex ^{1}HNMR spectrum.
- **d)** Off resonance spectroscopy
- **e)** Spin decoupling

Q.4 Attempt **ANY THREE** of the following: **(15)**

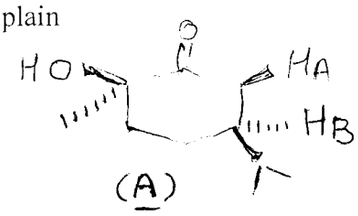
a) Assign ^{13}CNMR signals to various carbons in the following compound. Give reasons and justify your answer.



185(s), 160(s), 154(s), 148(s), 141(s), 129(d), 138(d), 128(d), 121(d), 116(d), 108(d), 104(d)

b) The sodium salt of aspartic acid in D_2O show signals in ^{1}HNMR as: 3.5δ (dd, J = 10 & 4Hz); 2.4δ (dd, J = 15 & 4Hz); 2.2δ (dd, 15 & 10Hz). Explain.

c) The compound (A) when dissolved in benzene it shows J_{AB}=3Hz in methanol it shows J_{AB} = 11 Hz. Explain



d) Deduce the structure based on following data.
M.F.$C_6H_{18}O$; IR : 3360 & 2200cm^{-1}
^{1}HNMR: ($CDCl_3$); 1.0 (d, J = 6Hz, 9mm); 1.02 (d, J = 6Hz, 9mm); 1.82 (eight lines, J = 6Hz, 3mm; 2.47(d, J = 2Hz, 3mm); 2.82 (S, exchangeable, 3mm); 4.18(dd, J = 2 & 6Hz, 3mm);

e) Give the logical fragmentation for the following ions observed in their mass spectrum (any one)

- i) 1-phenyl – 2- propanone : m/z: 134, 119, 91, 43
- ii) 2 – methoxy pentane : m/z : 102, 85, 59, 31

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