(f) Give examples of two NMR active and two NMR inactive nuclei and explain why.

(g) What is a proton decoupled spectrum in $^{13}C$ NMR ?

(h) What is the difference between a base peak and a molecular ion peak in Mass spectroscopy ?

(i) What is NMR shift reagent ?

(j) Which reference compound is used for NMR in $D_2O$ ? Write its structure.

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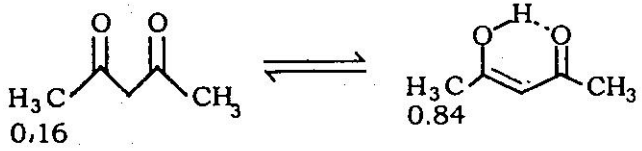
**7.** (a) What is chemical exchange ? 2

(b) Calculate the percentage of keto and enol forms of acetyl acetone from the integral data given below ? 2

(c) A compound $C_9H_{10}O_2$ compound has strong infrared absorption at 1695 $cm^{-1}$.




The $^1H$ NMR spectrum has five sets of line : a triplet at $\delta$1.3 (3H), a quartet at $\delta$ 4.1 (2H), a doublet at $\delta$ 7.0 (2H), a doublet at $\delta$ 7.8 (2H) and a singlet at $\delta$ 9.8 (1H) ppm. Suggest a structure for this compound. 4

**8.** Answr any *eight* of the following: 8×1

(a) What is spin-spin relaxation ?

(b) NMR is an absorption spectroscopy: True or False.

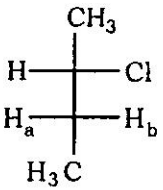
(c) What is spin-spin coupling ?

(d) What are the full forms of HMQC and DEPT ?

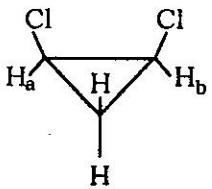
(e) What is the temperature at which the magnet of a high field (e.g., 400 MHz) NMR is kept ?

(c) Write the possible configurations of dimethyl muconate having the general structure $MeO_2C$-CH=CH-CH=CH-$CO_2Me$ and assign their geometries using $^1H$ NMR.

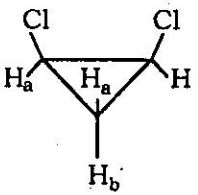
(i)




(i)




(iii)

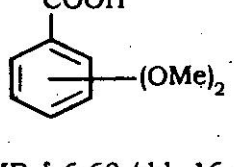


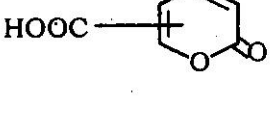

**6.** (a) Two lines of a doublet in 400Mhz $^1H$-NMR spectrum appear at 2.32 and 2.36 ppm. Calculate the coupling constant. 2

(b) What will be the separation (in ppm) between the two lines in 200MHz and 800Mhz $^1H$-NMR ? 1

(c) Show qualitavely how a complex NMR spectrum recorded in a lower magnetic field can be simplified in a higher magnetic field. 2

(d) What are NMR shift reagents ? Give examples and write the mechanism of their activity. 3




NMR-$\delta$ 6.62 (dd, 16 & 7Hz, 1H), 7.41 (d, 1H), 7.49 (m, 5H), 9.66 (d, 1H). 4

**4.** (a) Identify the compound with molecular formula $C_3H_7NO$
IR-$\nu$ 3428, 1681 $cm^{-1}$
NMR-$\delta$ 1.87 (s, 1H), 7.30 (s, 3H), 8.1 (s, 3H) 3

(b) An organic compound with a molecular mass 120 absorbs in UV spectrum at 268nm shows the following data in IR spectrum absorption bands are found at 3068-2907 $cm^{-1}$ and 1608$cm^{-1}$ and 1473$cm^{-1}$. The NMR spectrum 3.21 (9H, s) 7.74 (3H, s). Write down the structure of the compound. 3

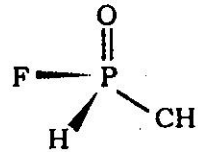
(c) A certain compound has molecular formula $C_2H_3N$, compound exhibit a single peak in its $^1$H-NMR spectrum at $\delta$ 2.15 ppm. Propose the structure of the molecule and explain its chemical shift. 2

**5.** (a) What is Karplus equation ? Give an example. 2

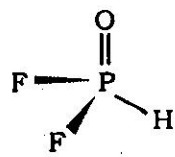
(b) What are the stereochemical relationships between the $H_a$ and $H_b$ of the compounds (i)-(iii) ? 2

2. (a) Proton NMR of $K^+BH_4^-$ consist of four peaks with higher intensity as well as seven peaks consist of lower intensity. Explain. 2

(b) Write down the $^1H$, $^{19}F$ and $^{31}P$ NMR spectra of HOP(O)FH system. 3



(c) Write down the $^1H$, $^{19}F$ and $^{31}P$ NMR spectra of $HP(O)F_2$ system. 3



3. (a) One isomer of dimethoxy benzoic acid (A) has the $^1H$ NMR spectrum: $\delta$ : 3.85 (s, 6H), 6.63 (t, 2Hz, 1H), 7.17 (d, 2Hz, 2H) and one isomer of coumalic acid (B) has the $^1H$ NMR spectrum: $\delta$ 6.14 (d, 10Hz, 1H), 7.82 (dd, 10Hz, 2Hz, 1H), 8.51 (d, 2Hz, 1H). Deduce the structure compounds in each case. 4

(b) Deduce the structure of the compound $C_9H_8O$ which exhibited the following spectral data,
IR-$\nu$ ($cm^{-1}$) 3090, 2820, 2750, 1685, 1610, 970, 745

# 2017

## M.Sc. 4th Semester Examination

## CHEMISTRY

### PAPER—CEM-403

*Full Marks : 40*

*Time : 2 Hours*

*The figures in the margin indicate full marks.*

*Candidates are required to give their answers in their own words as far as practicable.*

*Illustrate the answers wherever necessary.*

Answer Q.No.8 and any *four* questions from the rest

**1.** (a) Explain the $^{31}P$ NMR spectrum for $[H_2P_2O_5]^{2-}$ ion, indicating stick diagram. 3

(b) Two peaks in a proton NMR spectra recorded at 400 MHz occur at 4.1 and 4.2 ppm. What is their separation in Hz ? 2

(c) How can we distinguish among $\alpha P_4S_4$, $\beta P_4S_5$ and $\beta P_4S_4$ by $^{31}P$ NMR spectra ? 3