Reg. No. | | | | | | | | | |

ICH 501

III Semester M.Sc. Examination, December 2018
INDUSTRIAL CHEMISTRY
Spectroscopic Techniques

Time : 3 Hours Max. Marks : 70

Note : *Answer **any five** questions from Part – **A** and **any five** questions from Part – **B**.*

PART – A

(5×2=10)

1. a) How to distinguish between spherical, symmetric and asymmetric top molecules ?

   b) The rotational constant for $H^{35}Cl$ is observed at 10.5909 cm^{-1}. What is the value of B for $H^{37}Cl$?

   c) Reason out why symmetric stretching of CO_2 is IR inactive but Raman active.

   d) How you distinguish between $CH_3 - O - CH_3$ and $CH_3 - \overset{O}{\overset{\|}{C}} - CH_3$ using IR spectroscopy ?

   e) What is the significance of blank solution in UV-V is spectroscopy ?

   f) Calculate the chemical shift value of whose frequency of a ^1H nucleus is 1250 Hz on 400 MHz spectrometer. What will its frequency in 60 MHz spectrometer ?

   g) Calculate number ^{13}C of signals for toluene and 2-chlorotoluene.

   h) How to distinguish the presence of chlorine and bromine in a molecule through mass spectrometry ?

PART – B

2. a) Derive an expression for the rotational energy levels of diatomic molecule based upon rigid-rotor model.

   b) Sketch the rotational spectrum for $^{12}C\ ^{16}O$ and $^{13}C\ ^{16}O$ molecules. (6+6)

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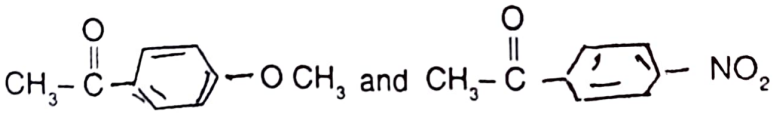
3. a) "Rotational spectrum of OCS molecules enables to calculate bond lengths" Justify the statement.
   b) Derive an expression for the energy levels of anharmonic oscillation.
   c) Sketch vibration-rotation spectrum with an emphasis to PQR branches. (4+4+4)

4. a) Illustrate with examples how to distinguish between amides and esters using IR spectroscopy.
   b) How intermolecular and intramolecular hydrogen bonding can be distinguished by IR spectroscopy ?
   c) How do you distinguish between using IR spectroscopy ?



(4+4+4)

5. a) Discuss different types of electronic transitions and how they affect λmax.
   b) Write a notes on :
      i) Frank – Condon principle
      ii) Wood word Fisher rule. (6+6)

6. a) Discuss about the relaxation processes of a nucleus revert back to α state.
   b) Why TMS used as an internal standard in ^{1}H NMR experiments ?
   c) How FTNMR technique offers itself as a advantage over CWNMR ? (4+4+4)

7. a) "In [18] annulene the peripheral protons appear δ 8.9 ppm where as inner protons at δ – 1.8 ppm" Justify the statement.
   b) Predict the ^{1}HNMR spectrum of following compounds :
      i) Acetaldehyde
      ii) Acetamide
      iii) Ethylacetate
      iv) Benzyl alcohol
   c) Distinguish between AX and AMX spectral patterns with justifications. (4+4+4)

8. a) Discuss how vicinal protons coupling constants vary based on Karplus equation.

   b) Explain the technique and use of spin decoupling.

   c) Distinguish these compounds on the basis of ^{13}C NMR :

      i) $CH_2CH_2OCH_2CH_3$

      ii) $CH_3–O–CH_2CH_2CH_3$

      iii) CH_3OCH < CH_3, CH_3

(4+4+4)

9. a) Illustrate with example how double irradiation technique helps in understanding NOE.

   b) Explain with examples the fragmentation process in mass spectroscopy.

   c) Write the feasible structures for these ions :

      i) 1-Methyl cyclohexanone : m/z, 96, 81, 68, 67

      ii) 4-Heptanone : m/z, 114, 86, 71, 58, 43, 41.

(4+4+4)

10. a) Discuss with examples McLaferty rearrangement.

    b) The organic compound has following spectral data with mol formula $C_9H_{10}O_2$

       IR ν_{max} = 1745 cm^{-1} (S) 1225 cm^{-1} (br-S), 749 cm^{-1}(S), 697 cm^{-1} (s)

       UV = λmax at 268, 264, 262, 257 nm.

       ^1H NMR δ ppm : 1.96 (3H, s); 5.00 (2H, s) 7.22 (5H, s). Deduce the structure of the compound.

    c) An organic compound containing C, H, N and halogen gave following spectral Data UV λmax : 240 nm

       IR ν_{max} = 3400, 3300, 3200 (w), 2900, 1620, 1500, 1380, 880, 820 cm^{-1}

       ^1H NMR δ ppm : 7.20, (1H d, J = 9Hz), 6.50 (1 H, d, J = 3.5 Hz), 6.30 (1 H, dd, J = 9 & 3.5 Hz), 3.5 (2 H, s, D_2O exchangeable), 2.30 (3H, s).

       Mass : m/z (RA) : 187 (90), 185 (90), 160 (20), 158 (10), 106 (100)

       Deduce its structure.

(4+4+4)
