M.Sc.Examination, 2018

Semester-III

Chemistry

Course: CH-914

Elective-2 (Organic Chemistry)

Time: Three Hours **Full Marks: 40**

Questions are of value as indicated in the margin.

Answer ***any four*** questions.

1. a) What is meant by 'resonance point' relating to NMR spectroscopy? 2

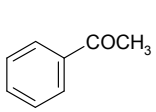
   b) Two isomeric compounds 'A' and 'B' (mf $C_9H_{10}O$) exhibit their ^{1}H-NMR properties as:

   A: δ2.00 (3H, s), 3.50 (2H, s), 6.90 (5H, s)

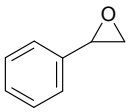
   B: δ2.68 (3H, s), 3.46 (2H, d), 7.15 (4H, s), 8.70 (1H, t)

   Deduce the structures of 'A' and 'B'. 3

   c) The proton-decoupled ^{13}C-NMR spectrum of an unknown compound shows resonances at δ 26.3, 128.2, 128.4, 132.9, 137.1 and 197.6. Which of the following structures is consistent with these data? 2



(I)



(II)

   d) An organic Compound having molecular formule $C_9H_9NO_4$, exhibits the following spectral properties:

   FT-IR: 3120, 2930, 1735 cm^{-1}

   ^{1}H-NMR: δ 8.22(2H, dd, J = 7.2, 2.0 Hz), 7.51(2H, dd, J = 8.8, 2.0 Hz), 5.19(2H, s), 2.15(3H, s) ppm.

   ^{13}C-NMR: δ 170.64, 147.86, 143.34, 128.51, 123.92, 64.89, 20.94 ppm.

   Mass: m/z 195(M^+).

   Deduce the structure of the compound. 3

2. a) An organic compound (mf $C_8H_8O_3$) exhibits the following spectral properties:

   IR: 3250, 3060, 2950, 2840, 1700, 1600, 1580, 1500, 1250, 1040, 870, 840 cm^{-1}

   ^{1}H-NMR: δ 3.75(3H, s), 7.35(1H, d, J = 2 Hz), 7.1(1H, d, J = 8 Hz), 7.4(1H, dd, J = 2, 8 Hz), 8.1(1H, brs), 9.8(1H, s).

   EIMS: m/z 152, 151, 137, 136, 123, 109, 107, 81.

   Deduce the structure of the compound. 6

   b) Assign the structure of a compound, $C_{10}H_{12}O$, whose mass spectrum shows m/z values of 15, 43, 65, 57, 91, 105 and 148. Justify your answer as well. 4

3. a) Define 'coupling constant' in NMR experiment. What is its importance in elucidating structural pattern of an unknown compound? Explain with suitable examples. 1+3

   b) An organic compound (mf $C_6H_{10}O$) showed the following spectral characteristics:

   IR: 3600-3500, 3300, 2800, 2140 cm^{-1}

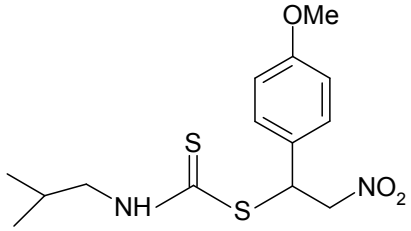
   ^{1}H-NMR: δ 1.0(3H, t), 1.52(2H, q), 1.40(3H, s), 2.48(1H, s), 3.3(1H, brs).

   EIMS: m/z 98(M^+), 83, 82, 69 (base peak)

   Deduce the structure of the compound. 6

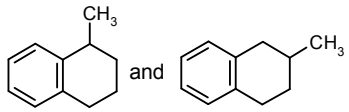
P.T.O.

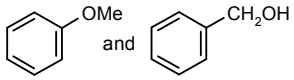
4. a) Predict ^{1}H- and ^{13}C-NMR spectral data for the following molecule.Also assign the respective values: 3+3



b) An organic compound (mf $C_9H_{10}O_2$) bears the following spectral properties:
UV: λ_{max} 270 nm
IR: 1680 cm^{-1}
^{1}H-NMR: δ 7.6(2H, d, J = 8 Hz), 6.9(2H, d, J = 8 Hz), 3.9(3H, s), 2.0(3H, s).
Assign a suitable chemical structure for the compound. 4

5. How would you distinguish the following on the basis of mass spectral analysis: 5x2
a) $CH_3CH{=}CHCH_2CH_2CH_3$ and$CH_2{=}CHCH_2CH_2CH_2CH_3$

b) 

c) 

d) $CH_3COOC_2H_5$ and $C_2H_5COOCH_3$
e) 1-butanol and 2-butanol

6. a) Describe in brief on the instrumental aspects for scanning the mass spectrum of an organic compound. 5
b) Explain briefly –
i) Electron ionisation method
ii) Chemical ionisation method
Mention only advantages and disadvantages in mass spectrometry. 5

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