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RCH-002

M.Phil. / Ph.D. IN CHEMISTRY (MPHILCHEM / PHDCHEM)

Term-End Examination

00342

December, 2018

RCH-002 : ANALYTICAL TECHNIQUES IN CHEMISTRY - I

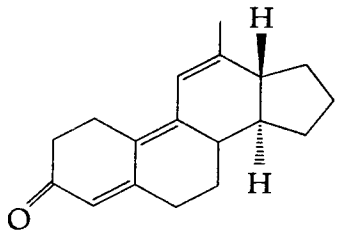
Time : 3 hours *Maximum Marks : 100*

Note : *Answer all the questions.*

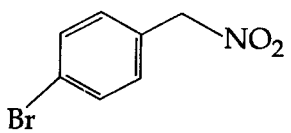
1. Explain the basic principles of ORD and CD. Give their applications in characterisation of organic compounds. 10

2. Distinguish between EIMS and CIMS. Write the advantages and limitations of these techniques. 10

3. (a) Predict the λ_{max} for the following molecule : 5



(b) Predict major peaks observed in the mass spectrum of the following compound (M = 215) : 5



(Atomic masses of $^{12}C = 12$, N = 14, O = 16 $^{79}Br = 79$, $^{81}Br = 81$)

4. Select the compounds that best fill the following IR spectral data : 10

(a) 3080(w), nothing 3000-2800, 2230(s), 1450(s), 760(s), 688(s)

(b) 2955(s), 2850(s), 1120(s)

(c) 3030(m), 730(s), 690(s)

(d) 3080(w), nothing 3000-2800, 1315(s), 1300(s), 1155(s)

(e) 3350(s), 3060(m), 1635(s)

(s = strong, m = medium, w = weak, b = broad)

Each set refers to the list of just a few important bands for each compound.

(i) Benzamide

(ii) Benzoic acid

(iii) Benzonitrile

(iv) Biphenyl

(v) Dioxane

(vi) Diphenyl sulfone

(vii) Formic acid

(viii) Isobutylamine

(ix) 1-Nitropropane

5. Match the following compounds with their IR spectra. **10**

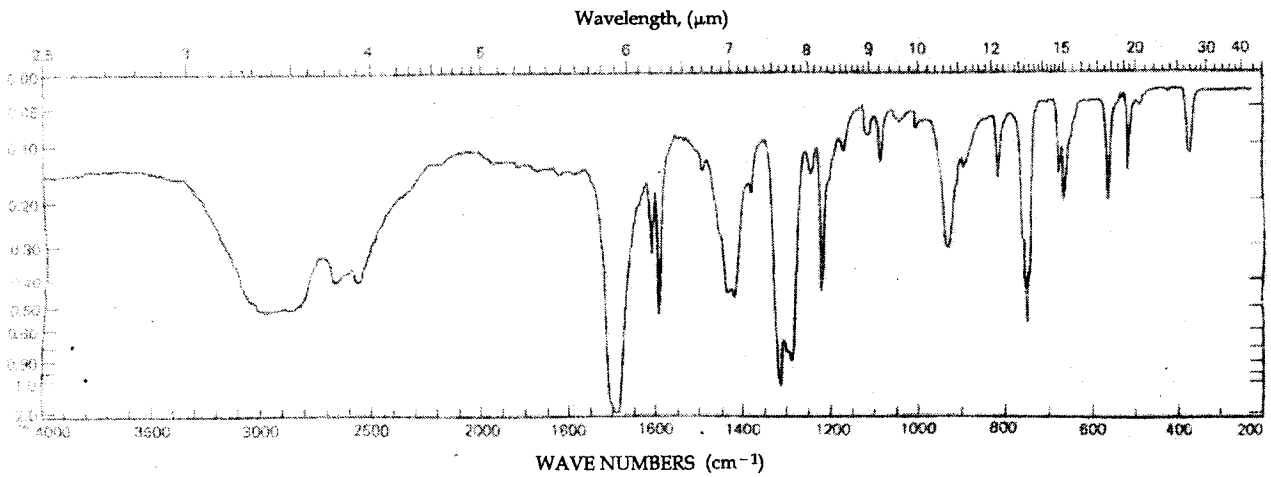
(a) Allyl phenyl ether

(b) Benzaldehyde

(c) *o*-Cresol

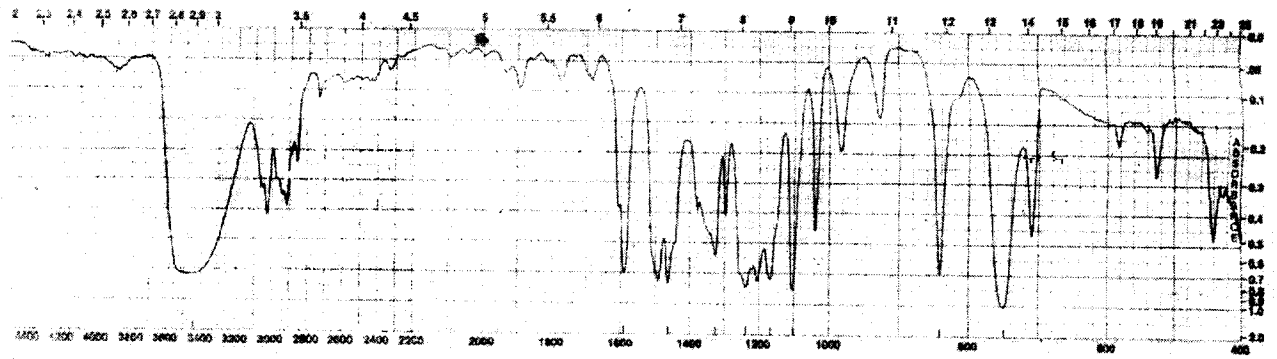
(d) *m*-Toluic acid

SPECTRUM - A



SPECTRUM - B

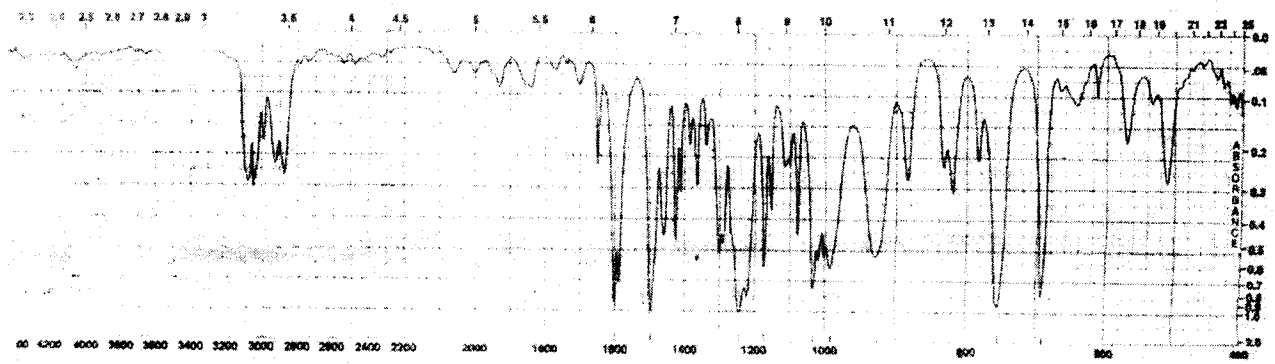
Wavelength, (μm)



WAVE NUMBERS (cm^{-1})

SPECTRUM - C

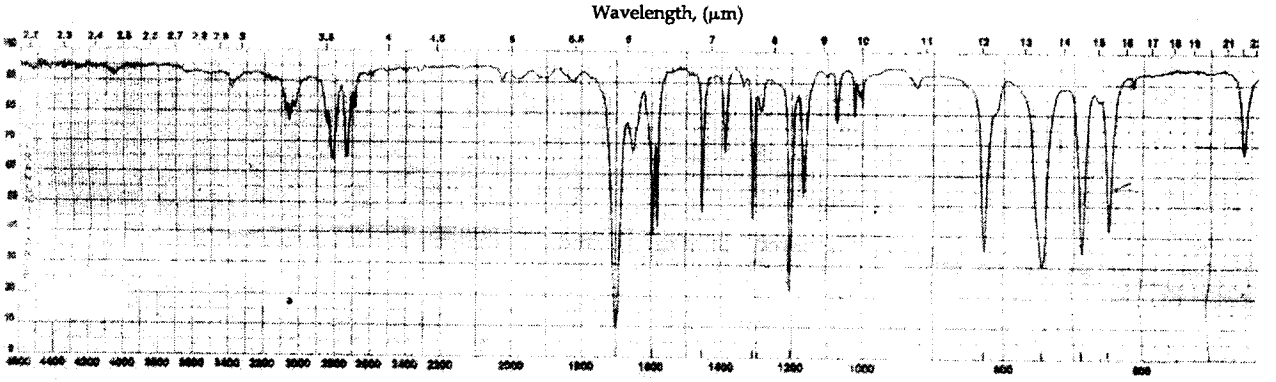
Wavelength, (μm)



WAVE NUMBERS (cm^{-1})

SPECTRUM - D

Wavelength, (μm)

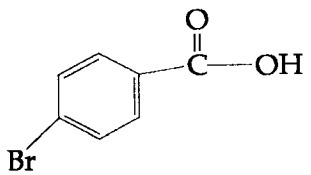


WAVE NUMBERS (cm^{-1})

6. (a) Predict the number of peaks that you would expect in the proton-decoupled ^{13}C spectrum of each of the following compounds. 5

(i) $CH_3-\overset{\overset{O}{\|}}{C}-O-CH_2-CH_3$

(ii)



(b) A compound having molecular formula C_2H_7NO showed the following spectral data : 5

Mass spectrum : (m/z) 61, 30

IR spectrum (cm^{-1}) : 3100 - 3400,

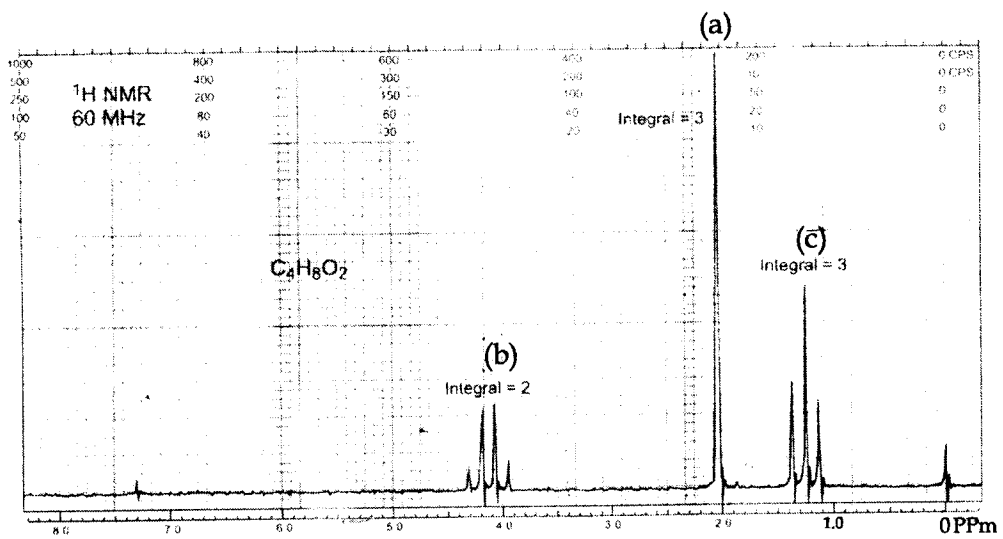
2920, 2850

NMR spectrum : (δ)2.4 (m, 3H)

2.9 (t, 2H), 3.7 (t, 2H)

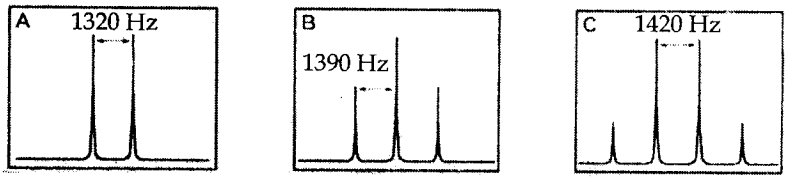
Predict the structure of the compound using the above spectral data.

7. The compound with the formula $C_4H_8O_2$ shows the following ^1H-NMR spectrum. Determine its structure and assign the chemical shift values to various structural units present. 10



8. (a) Draw and explain with proper justification the ^{1}H-NMR of 1, 3 - dichloropropane and *p* - chloroaniline. **10**

(b) Give reasons while matching the ^{31}P NMR spectra below with the appropriate molecule.



(i) PCl_5 (ii) PCl_3

(iii) $PFCl_2$ (iv) PF_2Cl

(v) PF_3 (vi) PF_5

9. (a) A compound ($C_9H_{10}O_2$) shows a molecular ion at $m/z = 150$ and a base peak at $m/z = 135$. Its IR spectrum shows a strong band at 1680 cm^{-1}. Its ^{1}H-NMR spectrum shows three signals at 82.3 (3H, singlet), 83.6(3H, singlet) and at 86.4-7.5 (4H, a pair of doublets J = 8Hz). Assign the structure to this compound. **5**

(b) Predict the structure of the compound having molecular formula $C_{15}H_{14}O$ from the following spectral data : **5**

^{1}H-NMR $\delta = 2.20$ (singlet), 5.08 (singlet), 7.25 (multiplet) with Integration ratio, respectively 3 : 1 : 10.

IR spectrum = 1720 cm^{-1}

10. What is meant by diamagnetic anisotropy in NMR spectroscopy ? Give two examples. **10**