



EASTERN UNIVERSITY, SRI LANKA
SECOND EXAMINATION IN SCIENCE – 2003/2004
SECOND SEMESTER
(June/July-2005)
CH 203 SPECTROSCOPIC METHODS

Answer all questions

Time: 1 Hour

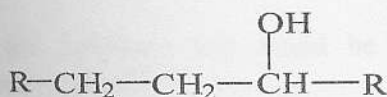
1) a) Calculate the chemical shift in ppm for a proton that has resonance 128 Hz downfield from TMS on a spectrometer that operates at 60 MHz.

(10 marks)

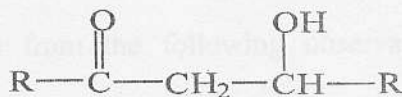
b) Sketch the ^1H NMR spectrum of DCH_2OCH_3 ($I=1$ for D) and compare it to that of FCH_2OCH_3 ($I=1/2$ for F)

(20 marks)

c) In the ^1H NMR spectrum, the chemical shift of the O-H proton of compound A depends on the nature of the solvent and the concentration of the sample, whereas that of compound B is unaffected by change in the solvent and concentration. Give reason for this observation.



A



B

(10 marks)

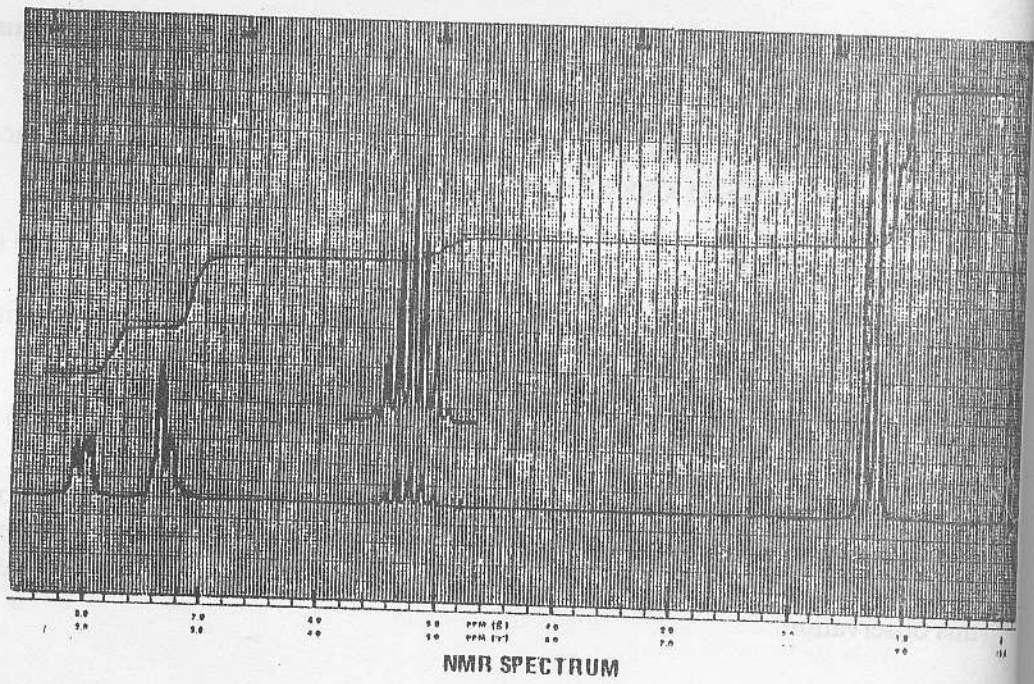
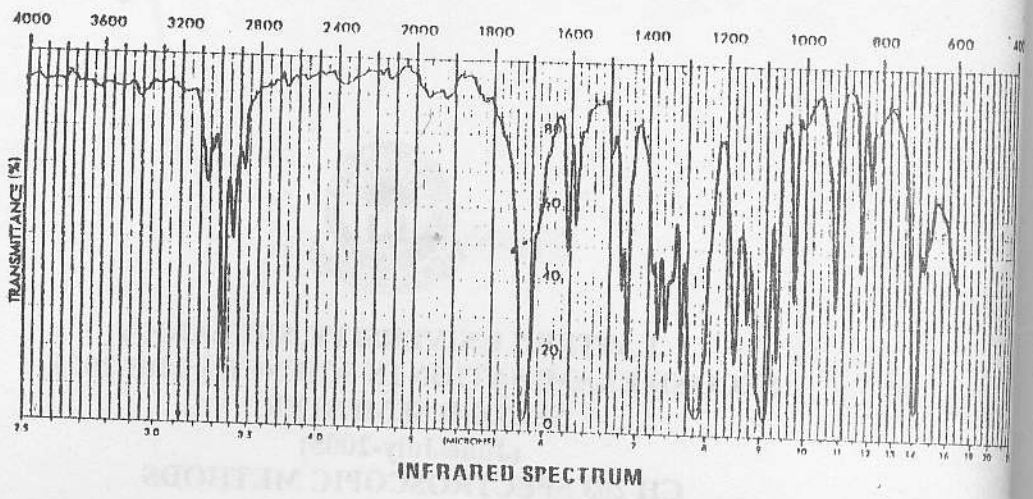
d) The mass spectrum of 2-octanone showed fragmentations at 113, 58 and 43. Give the structures of these ions and indicate the possible pathways for their formations.

(15 marks)

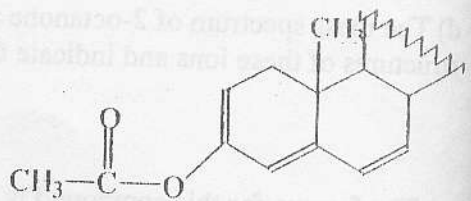
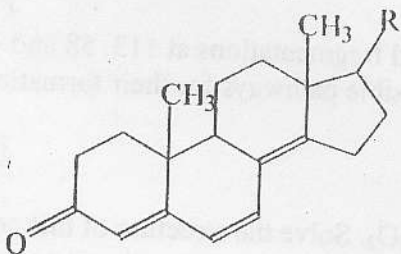
e) The formula for this compound is $\text{C}_{10}\text{H}_{12}\text{O}_2$. Solve the structure of this compound with only the IR and NMR. The IR spectrum is determined on a neat liquid sample.

(45 marks)

Cont...



2) a) Using Woodward-Fieser-Scott rules, predict the λ_{max} value of the UV absorption band of the following compounds.



(20 marks)

b) An unknown substance (contain only C, H and a hetero atom) shows a molecular ion peak at $m/e = 107$ with a relative intensity of 100. Propose a molecular structure for the unknown.

(15 marks)

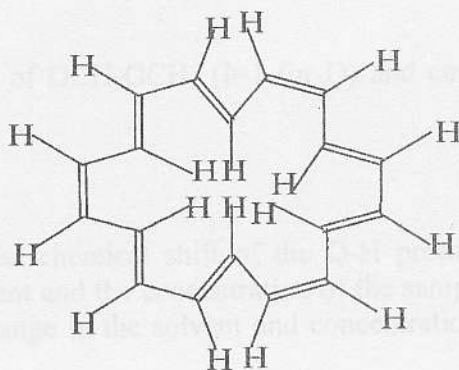
c) The wave length in the observable UV region increases with the increase in conjugation in the compound. Justify this statement.

(15 marks)

d) The ^1H NMR spectrum of a low molecular mass polyethylene $\text{CH}_3(\text{CH}_2)_n\text{CH}_3$ shows the methylene protons at 1.2 ppm and terminal methyl groups at 0.9 ppm. Careful integration gives a ratio of 8.0:1.0 for the methylene to methyl ratio. What would be the average molecular mass of the polyethylene?

(20 marks)

e) Explain why the inner H on the following molecule has resonance at -1.8δ and the outer H has resonance at 8.9δ .



(15 marks)

f) Give the inference that could be made from the following observations. No explanations required.

- 1) The mass spectrum of an organic compound A had peaks of 1:1 intensity at 200, and 198
- 2) One of the signals of the ^1H NMR spectrum of an organic compound B shows a singlet at $\delta 9.5$. This signal disappears on shaking with D_2O .

(15 marks)
