EASTERN UNIVERSITY, SRI LANKA
SECOND EXAMINATION IN SCIENCE FIRST SEMESTER (2004) (Repeat)
CH 203 SPECTROSCOPIC METHODS

Time: 01 Hour

Answer all questions

1.

(a) Three isomeric compounds **A**, **B** and **C** having the molecular formula $C_4H_8O_3$ give the following ^1H NMR spectra. Deduce the possible structures of these compounds.

Compound **A** (δ): 1.3 (3H, t, J=7Hz), 3.6 (2H, q, J=7Hz), 4.15 (2H, s) and 12.1 (1H, s).

Compound **B** (δ): 1.2 (3H, d, J=7Hz) 2.35 (2H, d, J=7Hz) and 4.15 (1H, sextet, J=7Hz). The spectrum is run in D_2O.

Compound **C** (δ): 3.5 (3H, s), 3.8 (3H, s) and 4.05 (2H, s).

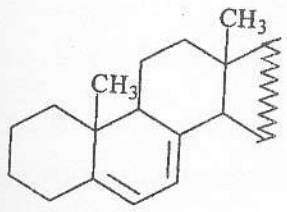
(b) Explain the following observation

One molar solution of cyclohexanol in CCl_4 shows IR absorption band at 3640 (weak) and 3320 (strong) cm^{-1}. But 0.03 molar solution shows only one absorption band at 3640 cm^{-1} (strong).

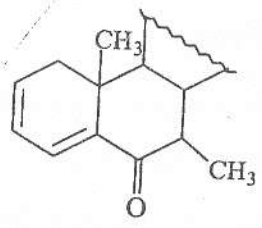
2.

(a) Using Woodward- Fieser- Scott rule, calculate the λ_{max} values of the following compounds in their UV spectra.

(i)

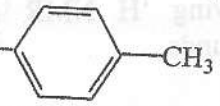


(ii)



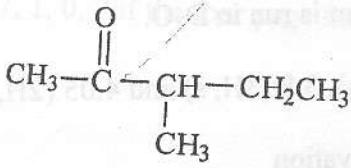
(b) A solution of 1.03 mg of benzonitrile (PhCN) in ethanol (100 ml) had absorbance of 1.20 at 224 nm, when measured in a 2 cm cell. What is t molar absorptivity (molar extinction co-efficient) of this band?

(c) Sketch out the proton NMR spectrum, including multiple patte expected for the following compounds with TMS as standard. Predict t approximate chemical shift values in your spectrum.

(i) 

(ii) $CH_3-CD_2-CH_3$

(d) The mass spectrum of 3-methyl-pentan-2-one shows prominent peaks the following m/z values: 100, 85, 72, 57 and 43. How would you acco these peaks?



3-methyl-pentan-2-one