Registration no:

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<u>M.Sc.I</u> FCYC803

(2 x 10)

8th Semester Regular Examination-2017-18 SPECTROSCOPIC IDENTIFICATION OF MOLECULES BRANCH: M.Sc.I(AC) Time: 3 Hours Max Marks: 70 Q.CODE: C257

Answer Question No.1 which is compulsory and any five from the rest. The figures in the right-hand margin indicate marks. Answer all parts of a question at a place.

- **Q1** Answer the following questions:
 - a) On the basis of Woodward rules, calculate the λ_{max} of the following





compound.

- **b)** How the different bands in UV-VIS spectroscopy are designated? Describe each bands.
- c) How can you identify the presence of –OH group in IR and NMR spectroscopy?
- **d)** What is Fermi resonance?
- e) Why TMS is taken as reference in ¹H NMR?
- f) One of the proton(s) shows a nonet in the spectrum of 2-methyl-1-propanol. Identify this proton.
- **g)** How can you distinguish 3-methylcyclohexene from 4-methylcyclohexene on the basis of mass spectroscopy?
- **h)** The mass spectrum of 1-hexanol gives a base peak at m/z=56. How can you account for this?
- i) What is zero field splitting?
- **j)** What is the selection rule for the transition of an electron when it comes under the vicinity of a nucleus with I=1/2?
- **Q2** Draw and discuss the ¹H NMR and COSY spectrum of m-dinitrobenzene? (5+5)
- **Q3 a)** Write the structures of all the isomeric alcohols, $C_4H_{10}O$. How the number and (5) position of ¹³C NMR signals can help in the identification of these isomers?
 - b) The chemical shift, peak multiplicity and integral ratios of an organic compound, (5) C₇H₁₂O₄, in its ¹H NMR spectrum are given below: 1.3, (triplet), 2.94; 3.3 (singlet), 1.01; 4.2 (quartet), 2.05. Identify the compound with proper reason.

Q4		The peaks of mass and IR spectrum of an organic compound, C_7H_8O , is observed at the following positions: m/z in mass spectrum: 108, 107, 79, 77 IR band positions: 697, 735, 1017, 1208, 1453, 1497, 2980, 3100 and 3300cm ⁻¹ . Identify the compound with assigning each peak positions in both the spectrum. Also sketch its ¹ H NMR spectra.	(10)
Q5		 Draw the esr spectrum of the following compound with explanation: (i) p-benzosemiquinone anion (ii) naphthalene anion (iii) triphenyl methyl radical (iv) methyl radical (considering both ¹³C and ¹²C) 	(10)
Q6	a)	The UV spectrum of acetone shows absorption maxima at 166, 189 and 279nm.	(5)
	b)	What is Beer-Lambert Law? Derive an expression for it. The absorbance of a 10 ⁻⁴ M solution through 1cm path length is found to be 1.30. What is its molar absorptivity?	(5)
Q7		Discuss the IR, ¹ H NMR and mass spectra of benzaldehyde	(10)
Q8	a) b) c)	Write notes on Auxochrome McLafferty rearrengement Spin-Lattice relaxation	(2x5)

- c) Spin-Lattice relaxationd) Spin-spin couplinge) Bending vibrations