Reg.No. \_\_\_\_\_\_\_\_\_\_\_\_



**UNIVERSITY**

(Karunya Institute of Technology & Sciences)

(Declared as Deemed-to-be University under Sec.3 of the UGC Act, 1956)

**End Semester Examination – Nov/Dec – 2016**

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|  |  | **Semester :** | **2016-17 ODD** |
| **Code :** | **15CH3019** | **Duration :** | **3hrs** |
| **Sub. Name :** | **SPECTROSCOPIC METHODS FOR STRUCTURAL ELUCIDATION** | **Max. marks :** | **100** |

**ANSWER ALL QUESTIONS (5 x 20 = 100 Marks)**

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| Q. No. | Sub Div. | Questions | | Course  Outcome | Mark |
| 1. | a. | What is cotton effect? Explain with an example. | | CO1 | 8 |
| b. | Discuss octant rule with an example. | | CO1 | 7 |
| c. | Calculate the absorption maximum for the following compound. | | CO3 | 5 |
| (OR) | | | | | |
| 2. | a. | Discuss the principle and instrumentation of UV Visible spectrophotometer. | | CO1 | 15 |
| b. | Calculate the absorption maximum for the following compound. | | CO3 | 5 |
| 3. | a. | Explain the factors influencing vibrational frequencies in FTIR spectroscopy. | | CO1 | 15 |
|  | b. | From the following IR spectral data, identify the functional groups present in the compound. Give reasons for the assignment. Peaks details: 1424 cm-1, 1717 cm-1, 2874 cm-1, 2967 cm-1, 3044 cm-1.  C:\Users\Ananthi\Desktop\ir.png | | CO3 | 5 |
| (OR) | | | | | |
| 4. | a. | What are the different modes of stretching and bending vibrationsin the molecules. Explain with examples. | CO1 | | 10 |
|  | b. | Write short notes on combination bands and over tones in IR spectroscopy. | CO1 | | 5 |
|  | c. | From the following IR spectral data, identify the functional groups present in the compound. Give reasons for the assignment. Peaks details: 1422 cm-1,1715 cm-1, 2918 cm-1, 2964 cm-1, 2995 cm-1.  C:\Users\Ananthi\Desktop\Untitled.png | CO3 | | 5 |
| 5. | a. | What is meant by proton decoupling technique? Explain with an example. | CO2 | | 5 |
|  | b. | Discuss spin spin relaxation and spin lattice relaxation in NMR spectroscopy. | CO2 | | 10 |
|  | c. | The 1H NMR spectral data of a compound with the formula C9H12 is given below. Elucidate the structure of the compound and assign the chemical shift values. 1H NMR (δ) ppm: 1.25 (d, 6H); 2.99 (septet, 1H), 7.32 (s, 5H) | CO3 | | 5 |
| (OR) | | | | | |
| 6. | a. | Discuss the factors influencing chemical shift in NMR spectroscopy. | CO2 | | 15 |
|  | b. | A compound with formula C5H10O2 shows bands at 3450 cm-1 and 1713 cm-1 in the infrared spectrum. Its 1H NMR spectral data are as follows. Identify the structure of the compound and give reason.  1H NMR (δ) ppm: 1.35 (s, 6H); 2.25 (s, 3H); 3.85 (s, 1H) | CO3 | | 5 |
| 7. | a. | What are the necessary requirments for McLafferty rearrangement to occur? Explain with two examples. | CO2 | | 10 |
|  | b. | Differentiate base peak and molecular ion peakin mass spectrum with one example. | CO2 | | 5 |
|  | c. | Identify the compoundfrom the following mass spectral data. Write the fragmentation pattern and give reason.  Formula: C5H10O; m/z: 86, 57 (most abundant), 29 | CO3 | | 5 |
| (OR) | | | | | |
| 8. | a. | Explain the MALDI technique in mass spectroscopy. | CO2 | | 10 |
|  | b. | Write short notes on chemical ionization method in mass spectroscopy. | CO2 | | 5 |
|  | c. | Identify the compound from the following mass spectral data. Write the fragmentation pattern and give reason.  Formula: C6H14; m/z: 86, 71, 57 (most abundant), 43, 29. | CO3 | | 5 |
|  | | Compulsory: |  | |  |
| 9. | a. | Explain the fragmentation patternof thiols and thioethers with examples. | CO2 | | 10 |
|  | b. | Explain the fragmentation pattern of alkyl chlorides and alkyl bromides with examples. | CO2 | | 10 |

ALL THE BEST