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 – April / May – 2017**

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| **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 | Marks |
| 1. | a. | Discuss axial haloketone rule with an example. | CO1 | 8 |
| b. | What are the principles of ORD? | CO1 | 7 |
| c. | Calculate the absorption maximum for the following compound. | CO3 | 5 |
| (OR) | | | | |
| 2. | a. | Discuss the factors influencing the absorption maximum in UV visible spectroscopy. | CO1 | 8 |
| b. | Write the effect of solvents in UV visible spectroscopy. | CO1 | 7 |
| c. | Calculate the absorption maximum for the following compound. | CO3 | 5 |
| 3. | a. | Explain the principle and instrumentation of FTIR spectrophotometer. | CO1 | 15 |
|  | b. | From the IR spectra identify the functional groups present in the compound. Give reasons.Peak details:1458 cm-1, 1728 cm-1, 2715 cm-1, 2862 cm-1, 2924 cm-1  C:\Users\Ananthi\Desktop\irt.png | CO3 | 5 |
| (OR) | | | | |
| 4. | a. | Give the requestie properties of the molecules to undergo IR absorption process. | CO1 | 4 |
|  | b. | Write notes on finger print region in IR spectroscopy. | CO1 | 6 |
|  | c. | From the IR spectra identify the functional groups present in the compound. Give reasons. Peak details: 1455 cm-1, 2882 cm-1, 2936 cm-1, 3036 cm-1, 3329 cm-1.C:\Users\Ananthi\Desktop\Untitled.png | CO3 | 10 |
| 5. | a. | What is meant by off resonance decoupling? How this technique is helping in simplifying the spectrum? Explain with an example. | CO2 | 8 |
|  | b. | What is nuclear overhauser effect? | CO2 | 2 |
|  | c. | Write notes on 19F spectroscopy. | CO2 | 5 |
|  | d. | Identify the strucutre of the compound using the following 1H, 13C NMR and DEPT spectral details. Formula of the compound: C6H12O  1H NMR (δ) ppm: 0.98 (t, 3H); 1.31 (t, 3H); 1.79 (sextet, 2H);  2.34 (t, 2H); 4.14 (q, 2H);13C NMR (δ) ppm: 9, 14, 26, 36, 44, 211   |  |  | | --- | --- | | Normal carbon | DEPT-135 | | 9 | positive | | 14 | positive | | 26 | negative | | 36 | negative | | 48 | negative | | 211 | No peak | | CO3 | 5 |
| (OR) | | | | |
| 6. | a. | How HETCOR experiments are carried out? How it is useful for simplifying the complex spectra? | CO2 | 10 |
|  | b. | Write short notes on vicinal coupling. | CO2 | 5 |
|  | c. | Identify the strucutre of the compound using the following 1H, 13C NMR and DEPT spectra: Formula of the compound:C5H10O 1H NMR (δ) ppm: 1.1 (d, 6H); 2.14 (s, 3H); 2.59 (septet, 1H)  13C NMR (δ) ppm: 18, 27, 41, 212   |  |  | | --- | --- | | Normal carbon | DEPT-135 | | 18 | positive | | 27 | positive | | 41 | positive | | 212 | No peak | | CO3 | 5 |
| 7. | a. | What is nitrogen rule?. | CO2 | 2 |
|  | b. | How meta stable ions are formed? | CO2 | 3 |
|  | c. | Discuss electro spray ionization technique in mass spectroscopy? | CO2 | 10 |
|  | d. | In the mass spectrum of butyrophenone (C6H5COCH2CH2CH2CH3), peaks are observed at m/z 162, 120, 105 and 85. Interpret these. | CO3 | 5 |
| (OR) | | | | |
| 8. | a. | Write the fragmentationpatteren for aromatic compounds with an example. | CO2 | 5 |
|  | b. | Explain the principle and instrumentation of mass spectrophotometer. | CO2 | 10 |
|  | c. | Identify the compound from the following mass spectra. Formula: C9H12;Peak details m/z: 120, 91 (most abundant) | CO3 | 5 |
|  | | **Compulsory:** |  |  |
| 9. | a. | Discuss isotopic effect in mass spectroscopy with suitable examples. | CO2 | 10 |
|  | b. | Explain the fragmentation patteren of amines and amides with examples. | CO2 | 10 |