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



**End Semester Examination – Nov/Dec – 2017**

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| **Code :** | **15CH3019** | **Duration :** | **3hrs** |
| **Sub. Name :** | **SPECTROSCOPIC METHODS FOR STRUCUTRAL 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 octant rule and axial halo ketone rule with suitable examples. | CO1 | 10 |
| b. | Write short notes on i. chromophore ii. auxochrome iii. red shift iv. blue shift. | CO1 | 5 |
| c. | Calculate the absorption maximum for the following compound. | CO1 | 5 |
| (OR) | | | | |
| 2. | a. | Write the effects of solvents in UV visible spectroscopy. | CO1 | 7 |
| b. | Discuss the applications of UV visible spectroscopy. | CO1 | 8 |
| c. | Calculate the absorption maximum for the following compound. | CO1 | 5 |
|  |  |  |  |  |
| 3. | a. | What are the requisite properties of a molecule to be IR active? | CO1 | 4 |
|  | b. | Write short notes on the concept of combination bands and overtones in IR spectroscopy. | CO1 | 8 |
|  | c. | Write the applications of IR spectroscopy. | CO1 | 3 |
|  | d. | From the following IR spectral data, identify the functional groups present in the compound. Give reasons for the assignment. Peaks details: 1420 cm-1,1714 cm-1, 2917 cm-1, 2962 cm-1, 2998 cm-1. | CO1 | 5 |
| (OR) | | | | |
| 4. | a. | Discuss the factors influencing vibrational frequencies in IR 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: 1420 cm-1,1680 cm-1, 2917 cm-1, 3310 cm-1. | CO1 | 5 |
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| 5. | a. | Explain the nuclear magnetic resonance phenomenon. | CO2 | 5 |
|  | b. | What are the differences between 1H and 13C NMR spectroscopy? | CO2 | 3 |
|  | c. | What is meant by coupling constant? Explain the types of coupling constant. | CO2 | 7 |
|  | 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 | | CO2 | 5 |
| (OR) | | | | |
| 6. | a. | Explain the principle and instrumentation of NMR spectrophotometer with neat diagram. | CO2 | 10 |
|  | b. | Write short notes on i. Nuclear overhauser enhancement effect, ii. Chemical shift | 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 | | CO2 | 5 |
|  |  |  |  |  |
| 7. | a. | Write short notes on metastable ions in mass spectroscopy. | CO3 | 5 |
|  | b. | Explain the fragmentation patteren of aldehydes and ketones with suitable examples. | CO3 | 10 |
|  | c. | Identify the compound from the following mass spectrum. Molecular Formula: C9H12; Peak details m/z: 120, 91 (most abundant) | CO3 | 5 |
| (OR) | | | | |
| 8. | a. | Explain the principle and instrumentation of mass spectrophotometer with neat diagram. | CO3 | 10 |
|  | b. | Explain nitrogen rule and odd even rule in NMR spectroscopy. |  | 5 |
|  | c. | A liquid compound gave a mass spectrum showing a strong molecular ion at m/z = 156. The only fragment ions are seen at m/z = 127 & 29.  Suggest a structure for this compound. | CO3 | 5 |
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|  | | **Compulsory**: |  |  |
| 9. | a. | Discuss the fragmentation pattern of alkyl chlorides and alkyl bromides with examples. | CO3 | 10 |
|  | b. | Explain the fragmentation pattern of thiols and thioethers with examples. | CO3 | 5 |
|  | c. | Write notes on isotopic effect in mass spectroscopy. | CO3 | 5 |

ALL THE BEST