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

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**End Semester Examination – Nov/Dec – 2018**

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| **Code :** | **17CH3019** | **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. | Explain octant rule and axial haloketone rule with an example. | CO1 | 10 |
| b. | Calculate the absorption maximum for the following compounds using Woodward Fieser rules. | CO2 | 10 |
| (OR) | | | | |
| 2. | a. | Describe the instrumentation of UV Visible spectrophotometer with neat diagram. | CO1 | 10 |
| b. | Calculate the absorption maximum for the following compounds using Woodward Fieser rules. | CO2 | 10 |
|  |  |  |  |  |
| 3. | a. | Discuss the factors influencing the vibrational frequencies in IR spectroscopy. | CO1 | 15 |
| b. | Identify the functional groups present in a compound from the following IR spectral data. Peaks details: 2750, 2850 cm-1,  1300 cm-1, 3400 cm-1, 1650 cm-1, 2150 cm-1, 2250 cm-1. | CO2 | 5 |
| (OR) | | | | |
| 4. | a. | Indicate the importance of finger print region. | CO1 | 10 |
| b. | Explain the concept of combination bands and overtones in IR spectroscopy. | CO1 | 5 |
| c. | Identify the functional groups present in a compound from the following IR spectral data. Peaks details: 1690 cm-1,1714 cm-1, 1760 cm-1, 1800 cm-1, 2998 cm-1. | CO2 | 5 |
|  |  |  |  |  |
| 5. | a. | Describe the instrumentation of NMR spectrophotometer with a neat diagram. | CO3 | 10 |
| b. | Explain the spin-spin coupling in 1H NMR spectroscopy with an example. | CO3 | 5 |
| c. | Elucidate the structure of the compound and assign the chemical shift values from the following 1H NMR spectral data. The molecular formula of the compound is C5H10O  1H NMR (δ) ppm: 0.95 (t, 3H), 1.38 (sextet, 2H), 1.64 (quintet, 2H), 2.45 (t, 2H), 9.78 (s, 1H) | CO3 | 5 |
| (OR) | | | | |
| 6. | a. | Explain the effect of electronegativity and magnetic anisotropy on the chemical shift values in 1H NMR spectroscopy with suitable examples. | CO3 | 15 |
| b. | Elucidate the structure of the compound and assign the chemical shift values from the following 1H NMR spectral data. The molecular formula of the compound is C5H10O  1H NMR (δ) ppm: δ (ppm): 0.97 (3H, t), 1.11 (3H, d), 1.47 (1H, m), 1.77 (1H, m), 2.29 (1H, sextet), 9.64 (1H,s) | CO3 | 5 |
|  |  |  |  |  |
| 7. | a. | Describe Nuclear Overhauser Effect in NMR spectroscopy. | CO5 | 5 |
| b. | Explain HETCOR NMR spectroscopy. | CO5 | 5 |
| c. | Identify the strucutre of the compound using the following 1H, 13C NMR and DEPT spectral data. Molecular formula of the compound is C8H14O3. 1H NMR δ (ppm): 1.5 (s, 3H), 2.3 (s, 2H), 3.3 (s, 9H)   |  |  |  | | --- | --- | --- | | **13C NMR** | **DEPT 135** | **DEPT 90** | | 27.9 | +ve | - | | 30.1 | +ve | - | | 51.5 | -ve | - | | 81.9 | - | - | | 200.1 | - | - | | 202.2 | - | - | | CO6 | 10 |
| (OR) | | | | |
| 8. | a. | Differentiate proton coupled, proton decoupled and off resonance decoupled 13C NMR spectroscopy with an example. | CO5 | 10 |
| b. | Identify the strucutre of the compound using the following 1H, 13C NMR and DEPT spectral data. Molecular formula of the compound is 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)   |  |  |  | | --- | --- | --- | | **Normal carbon** | **DEPT-135** | **DEPT 90** | | 9 | +ve | - | | 14 | +ve | - | | 26 | -ve | - | | 36 | -ve | - | | 48 | -ve | - | | 211 | - | - | | CO6 | 10 |
|  | |  |  |  |
|  | | **Compulsory**: |  |  |
| 9. | a. | Explain the desorption ionization techniques in mass spectroscopy and the requirements of matrix. | CO5 | 10 |
| b. | Explain Mc Lafferty rearrangement of aromatic compounds and esters in mass spectroscopy. | CO5 | 10 |