

Dr Parvinder Arora

2/12/2022

2/12/2022 (89)
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National Institute of Technology, Hamirpur, H.P

M.Sc Final Examination

Department of Chemistry

Year 2nd semester 3rd

Course: Interpretive molecular spectroscopy

Course code: CY-632

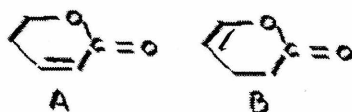
Dated 2-12-2022

Time 9.30am-12.30pm

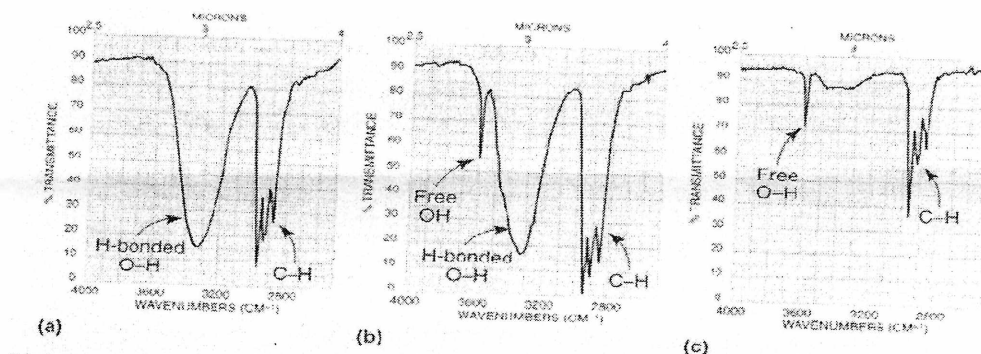
Total marks 50

Q. 1. 2+2+3+3=10

- Vibrational frequency for carbonyl group is 1810 cm^{-1} in anhydrides whereas 1715 cm^{-1} in keton. why? 2
- N,N-Dimethylacetamide absorbs at 1647 cm^{-1} in dioxane and 1615 cm^{-1} in methanol. How? 2
- "-C=O" group in molecule "A" exhibiting absorption at 1720 cm^{-1} and "B" at 1760 cm^{-1} . Why? 3



d) Explain the spectra- 3



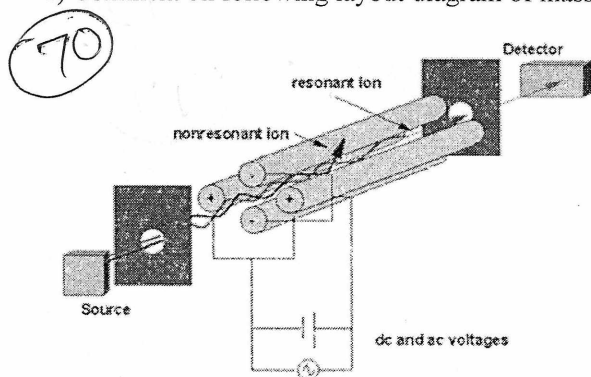
Q.2. 2.5×4=10

- Discuss the Woodward-Fieser rules for dienes. 2.5
- "n- π^* transitions are forbidden. Pronounced hypsochromic effect is observed in case of amides, acids and esters". Comment 2.5
- 3-Buten-2-one showing $\pi-\pi^*$ transition at $213\text{ m}\mu$ ($\epsilon=7100$) while n- π^* transition at $320\text{ m}\mu$ ($\epsilon=27$). why? 2.5
- Draw the schematic diagram of double beam uv-visible spectrophotometer. 2.5

Q.3. 2.5×4=10

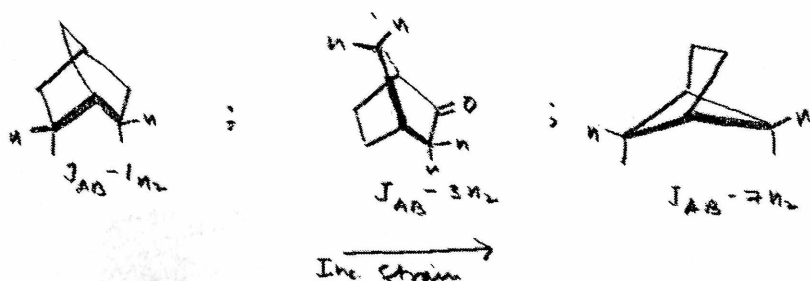
- Write down the ESI-MS fragmentation pattern for aldehyde. 2.5
- Following data is obtained for benzyl alcohol on ESI-MS spectrometer. Write down the structure of various fragments and also discuss the mechanism of mode of fragmentation. 2.5
- i) $m/z=108$; ii) $m/z=107$; iii) $m/z=79$ and iv) $m/z=77$
- Write down the fragmentation pattern of Acetal. 2.5

d) Comment on following layout diagram of mass spectrometer 2.5

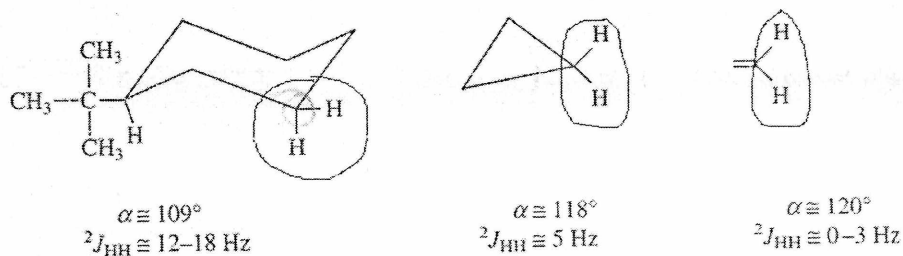


Q. 4. 3+2+3+2=10

a) Comment. 3

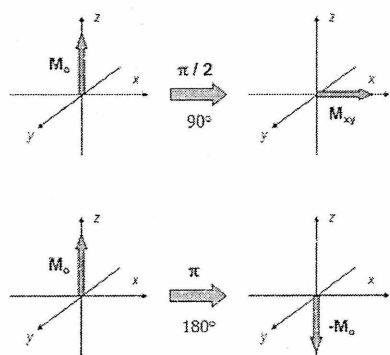


b) With the variation in angle, 2J changes. How? 2



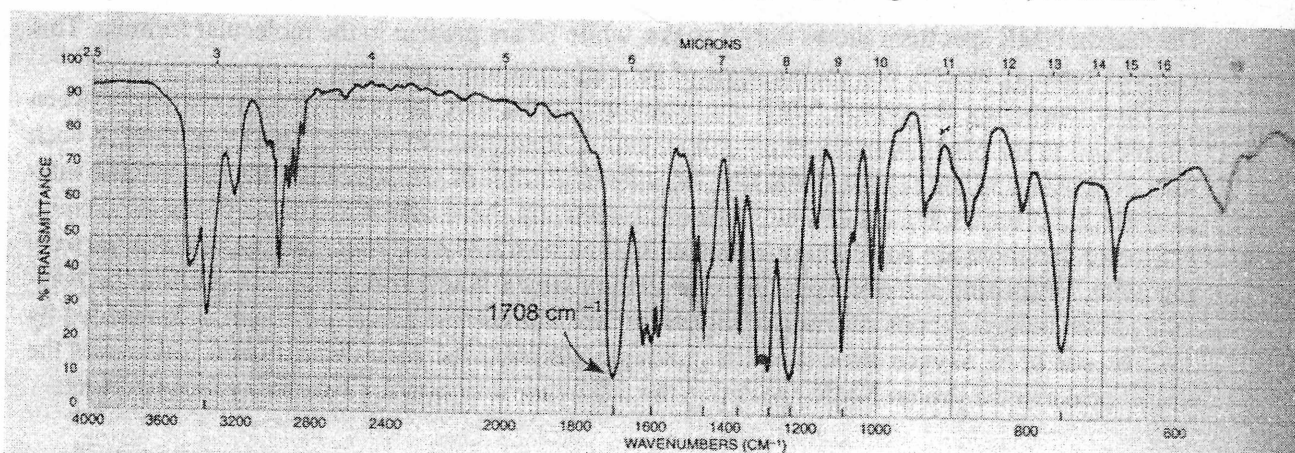
c) What is first and second order NMR spectra. Explain A_2 , AB and AX system. 3

d) What do you understand by following - 2.

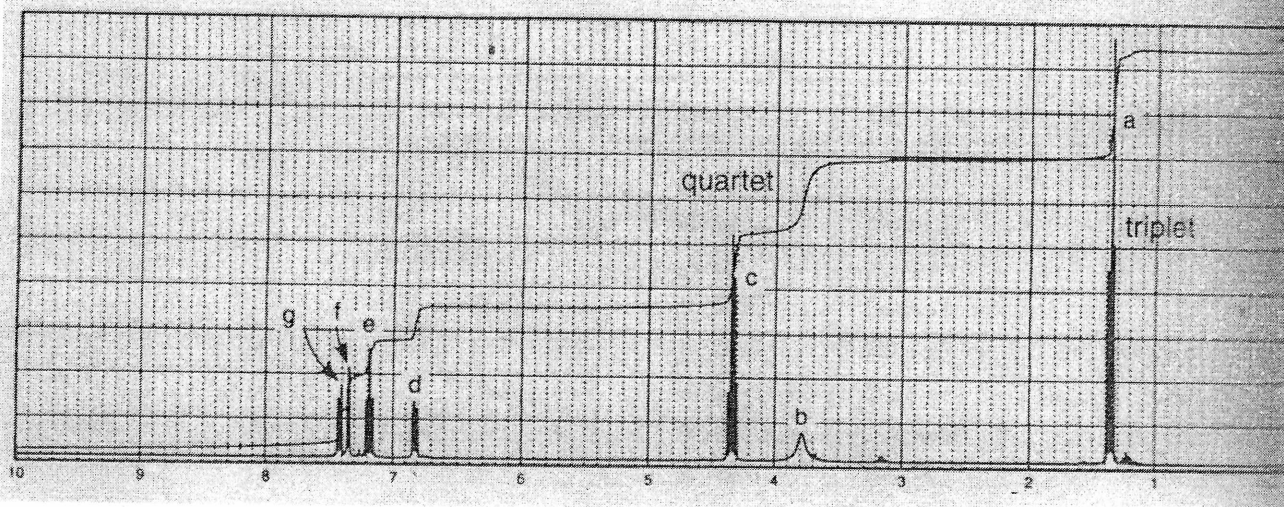


Q.5. (5+5=10)

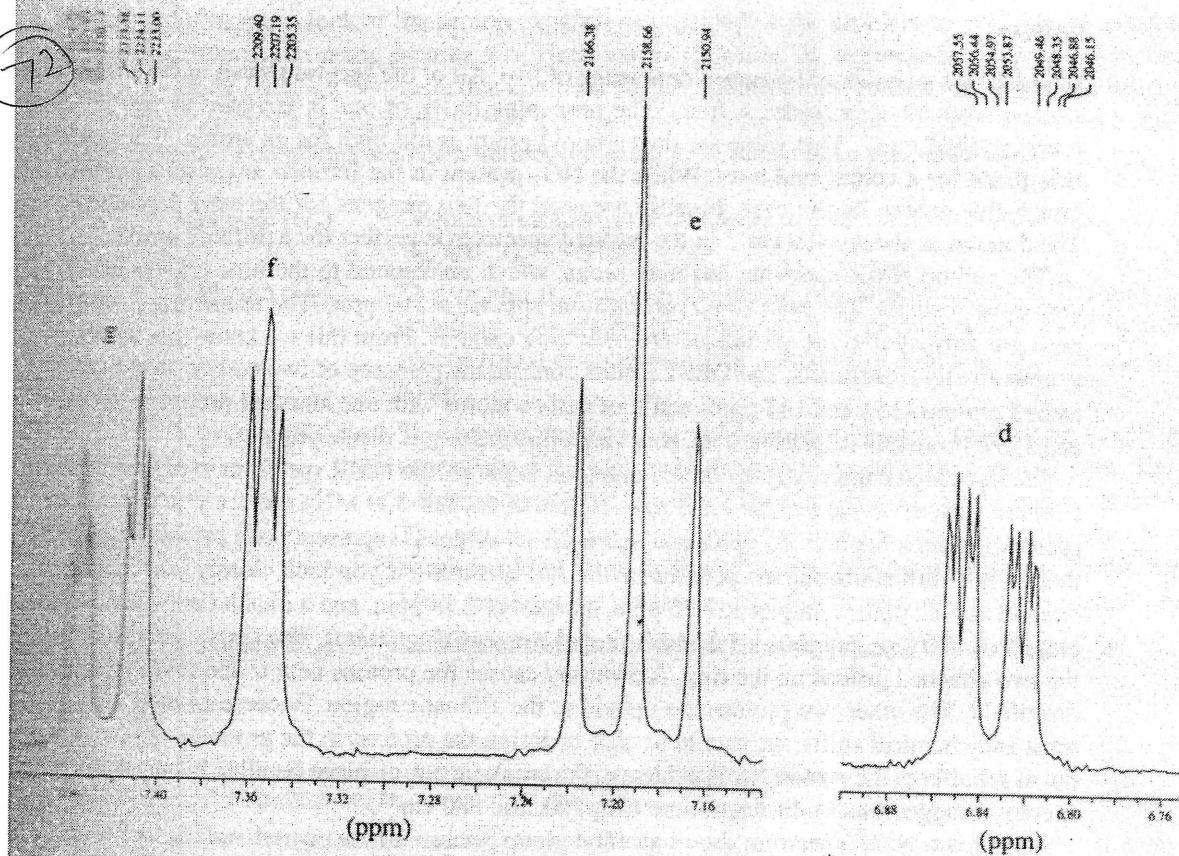
a) Deduce the structure of compound with molecular formulae $C_9H_{11}NO_2$ from given FT-IR, NMR data - 5



| Normal Carbon | DEPT-135 | DEPT-90 |
|---------------|----------|----------|
| 14 ppm | Positive | No peak |
| 61 | Negative | No peak |
| 116 | Positive | Positive |
| 119 | Positive | Positive |
| 120 | Positive | Positive |
| 129 | Positive | Positive |
| 131 | No peak | No peak |
| 147 | No peak | No peak |
| 167 | No peak | No peak |



72



b) What do you understand by two dimensional COY spectroscopy techniques? Following is the COSY spectra of 2-nitropropane. Explain it? 5

