

INDIAN INSTITUTE OF TECHNOLOGY

Date.....FN/AN Time 2 Hrs. Full Mark 60 No. of Students 43
 Autumn Semester –Mid term.... Department of Chemistry..... Sub. No. CY51003
 2 Yr. M. Sc. Sub. Name: *Spectroscopic Methods of Structure Determination*

Answer all questions. If there is any explanation, always make it brief.

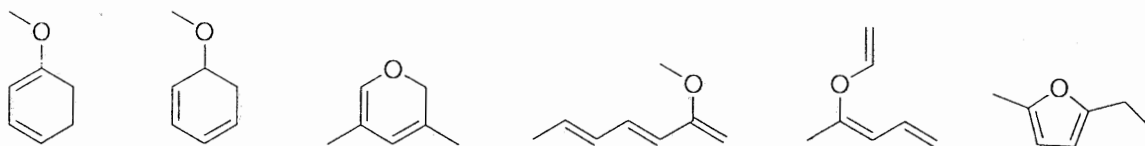
[1.5x6=9]

- a) Predict the relative intensities of the molecular ion peak, M+2, and the M+4 for 2,4-dibromofluorene.
- b) Which will occur at a larger wavenumber the C-N stretch of cyclohexylamine or the C-N stretch of aniline?
- c) Arrange in order of decreasing wavenumber of C=O absorption band of acetaldehyde, acetone and formaldehyde.
- d) Give one absorption band that could be used to distinguish between the following pairs:
 i) CH₃CH₂C=O(OCH₃) & CH₃CH₂C=O(OH); ii) CH₃CH₂C=O(OH) & CH₃CH₂CH₂OH
- e) How do you distinguish *para*- and *ortho*-nitro anilines by UV spectra?
- f) 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.

Questions 2 to 11 each carry 3 marks

Q. 2. Which isomer has the following spectral data?

IR: 3079, 2950, 1625, 1470, 1405, 1100, 810, 715 cm⁻¹; UV/Vis: λ_{max}=268 nm (ε_{max}=11000)



Q. 3. Compound C is composed only of carbon, hydrogen and oxygen, and shows a molecular ion at m/z=180. Carbon accounts for 60% of the molecular mass. Write a plausible **Molecular Formula** for compound C. How many **Rings + Double Bonds** must be present in compound, C?

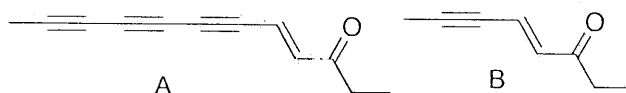
Q. 4. A liquid compound gave a mass spectrum in which the molecular ion appears as a pair of equal intensity peaks at m/e = 122 & m/z = 124. Small fragment ion peaks are seen at m/z = 107 & 109 (equal intensity), and at m/z = 79, 80, 81, & 82 (all roughly the same size). Large fragment ions are seen at m/z = 43 (base peak), 41 & 39. Suggest a name for this compound.

Q. 5. Which of the following molecules would you expect absorb at a longer wavelength in the UV region of the electromagnetic spectrum? Explain your answer.

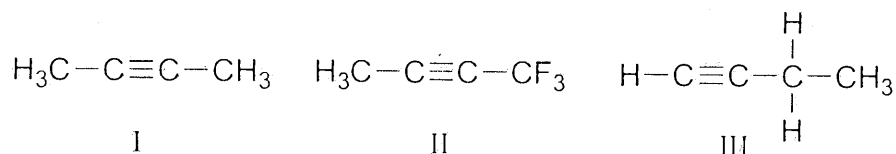


Q. 6. The mass spectrum of an aldehyde gives prominent peaks at $m/z = 59$ (12%, highest value of m/z in the spectrum), 58 (85%), and 29 (100%), as well as others. Propose a structure, and identify the three species whose m/z values were listed.

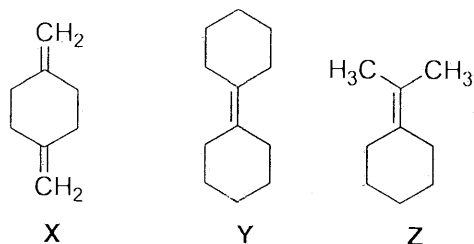
Q. 7. Explain how you could use UV spectroscopy to distinguish between compounds A and B.



Q. 8. Explain how you could use IR spectroscopy to distinguish following compounds.

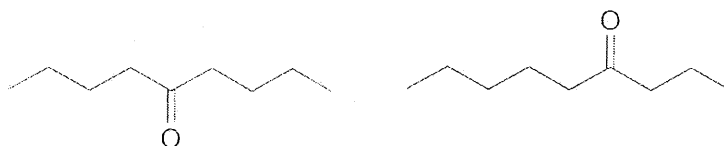


Q. 9. Explain how you could use IR spectroscopy to distinguish following compounds.

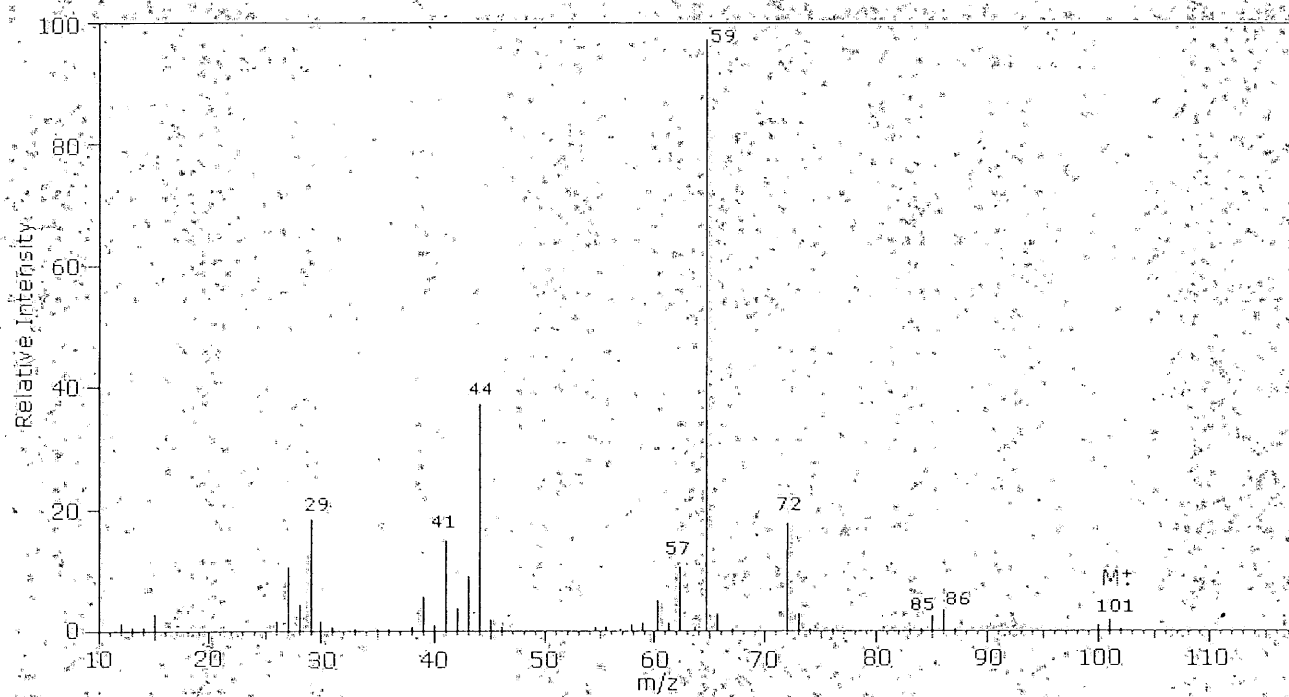
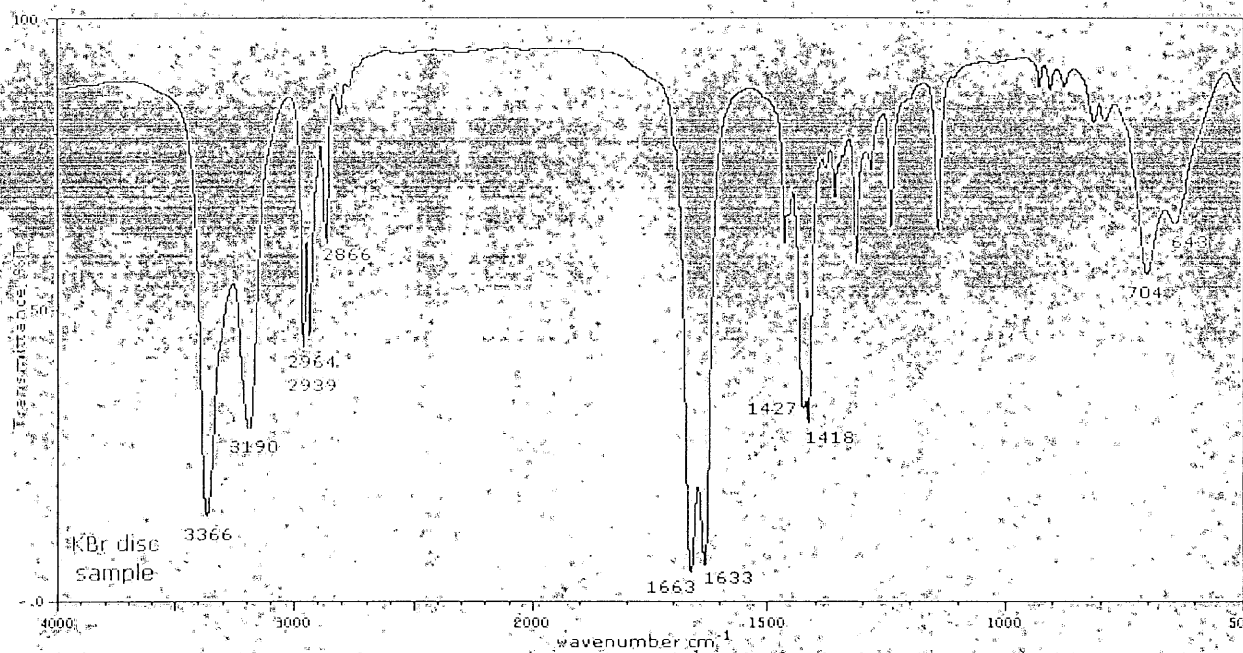


Q. 10. One would expect the mass spectrum of cyclohexanone to show a molecular ion peak at $m/z = 98$. However, the $m/z = 98$ peak in the cyclohexanone spectrum is unusually tall, compared to the molecular ion peaks in the mass spectra of other ketones such as 2-hexanone or 3-hexanone. Explain.

Q. 11. Which analytical technique - IR, UV, or MS - could best be used to distinguish between the two compounds below? Explain.



Q. 12. IR and mass spectra of an oily liquid are given. Identify the compound with justification. [9]



Q. 13. IR and mass spectra of a liquid are given. Identify the compound with justification. [12]

