Combined Spectroscopy Problems

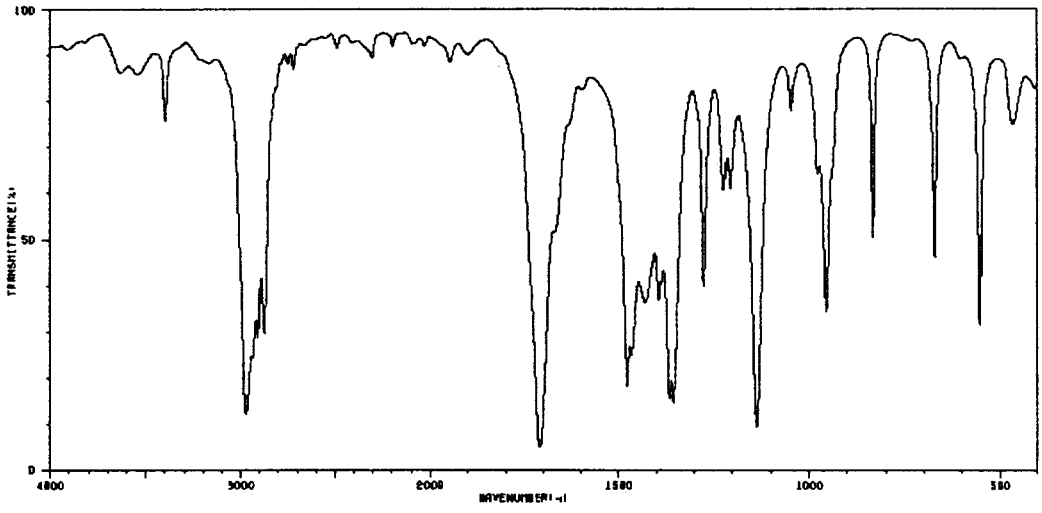
(Remember H atoms bonded to heteroatoms, e.g., N, O, S etc., can often appear as broad peaks, and do not always participate in coupling with protons on adjacent atoms)

Compound A

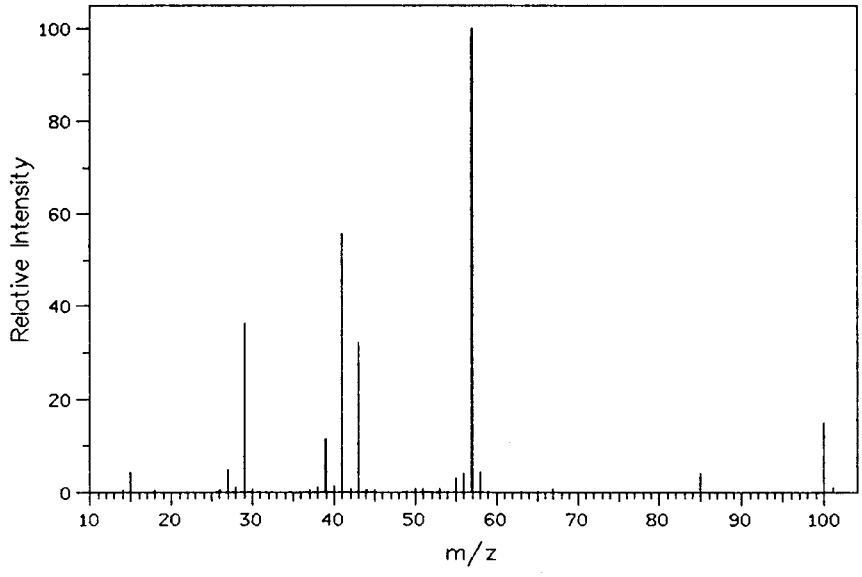
13C–NMR: 4 peaks, δ = 24, 26, 44, 214; [Only two peaks (24, 26) are observed in the 13C–DEPT spectrum, and they both point up (rather than down)]

1H–NMR: 2 peaks, δ = 1.5 (singlet, integration = 3), δ = 2.3 (singlet, integration = 1)

IR Spectrum:



Mass Spectrum: Base Peak (*m*/*z* = 57); Molecular Ion (*m*/*z* = 100; M+1 peak at *m*/*z* = 101 has a relative intensity of 6.9% as compared with the peak at *m*/*z* = 100)

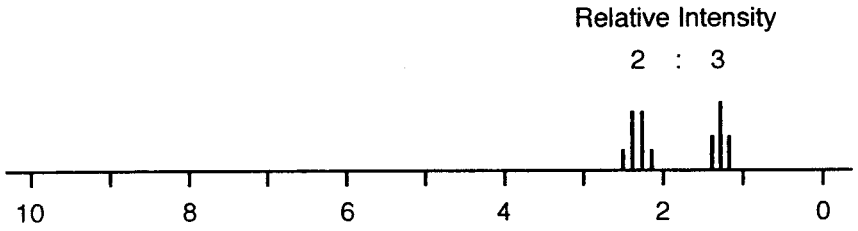


What is the structure of **compound A**, and what fragment gives rise to the base peak (*m*/*z* = 57) in the mass spectrum?

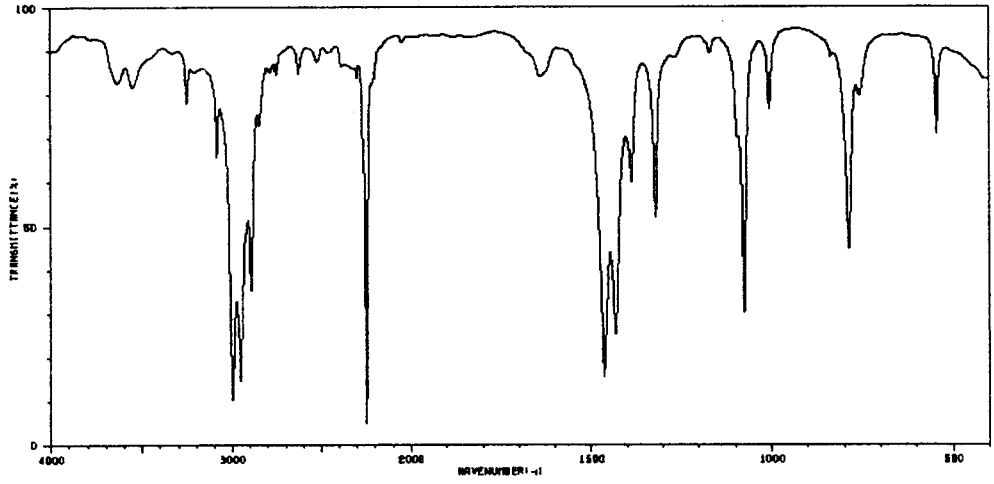
Compound B

13C–NMR: 3 peaks, δ = 10, 11, 121; [Only two peaks (10, 11) are observed in the 13C–DEPT spectrum, and they point in opposite directions, one up, one down]

1H–NMR:



IR Spectrum:



Mass Spectrum: Molecular Ion ($m/z = 55$)

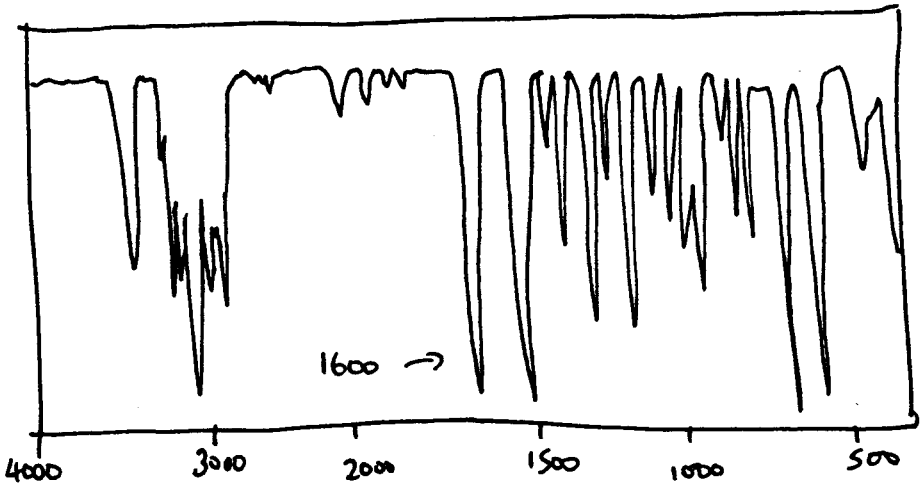
What is the structure of **compound B**?

Compound C

13C–NMR: 6 peaks, δ = 23, 44, 113, 117, 129, 148; [Only five peaks (all except 148) are observed in the 13C–DEPT spectrum, and they all point up (rather than down)]

1H–NMR: 4 peaks, δ = 1.4 (doublet, integration = 6), δ = 2.8 (septet, integration = 1), δ = 3.5 (broad singlet, integration = 1), δ = 6.9–7.4 (multiplet, integration = 5)

IR Spectrum:



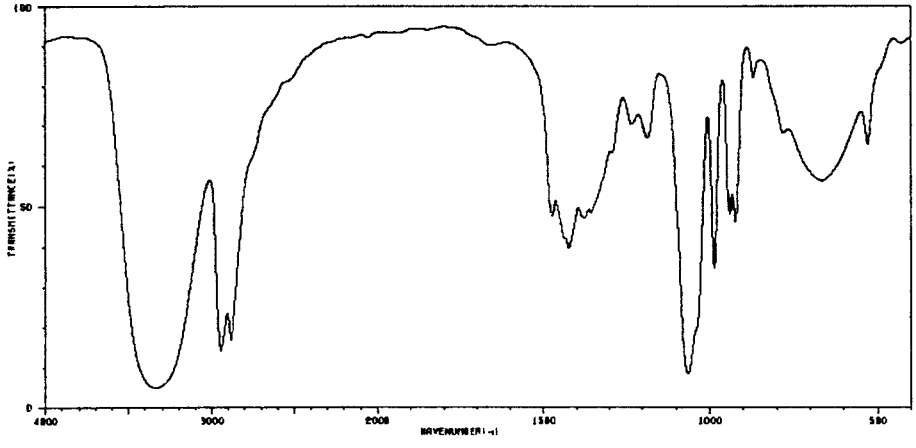
Mass Spectrum: Molecular Ion (*m*/z = 135): What is the structure of **compound C**?

Compound D

13C–NMR: 2 peaks, δ = 34, 62; [Both peaks are observed in the 13C–DEPT spectrum, and they both point down (rather than up)]

1H–NMR: 3 peaks, δ = 1.8 (quintet, integration = 1), δ = 2.6 (slightly broad singlet, integration = 1), δ = 3.8 (triplet, integration = 2)

IR Spectrum:



Mass Spectrum: Molecular Ion (*m*/z = 76; M+1 peak at *m*/z = 77 has a relative intensity of 3.7% as compared with the peak at *m*/z = 76): What is the structure of **compound D**?