Yet more...
...combined spectroscopy problems

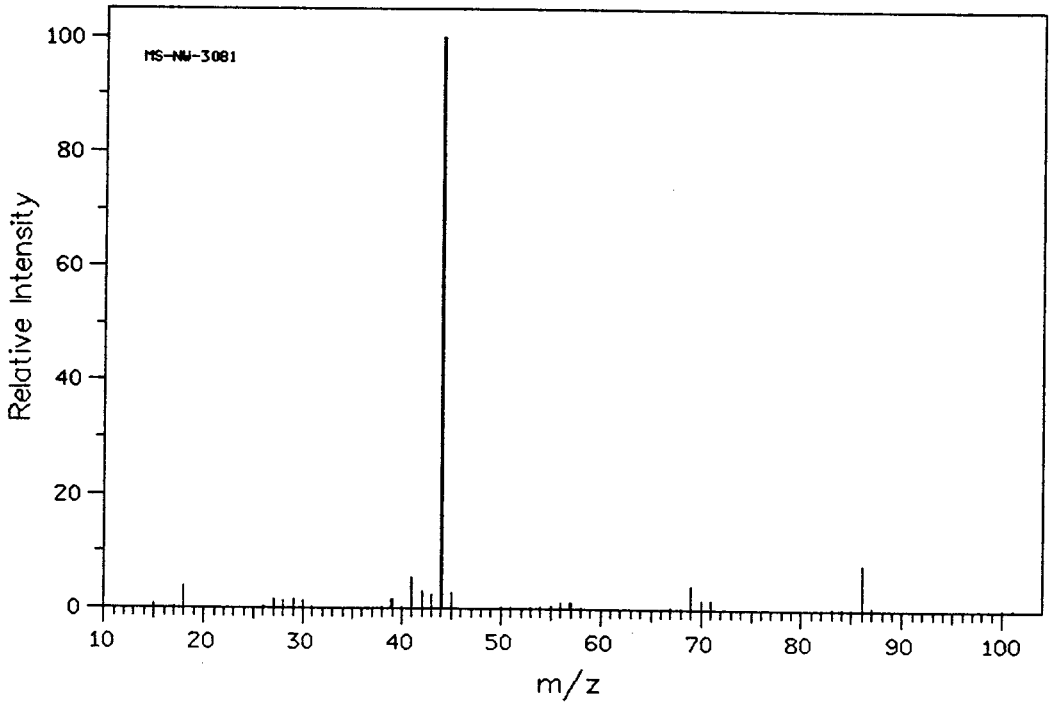
Spring 2004

Chem 30B

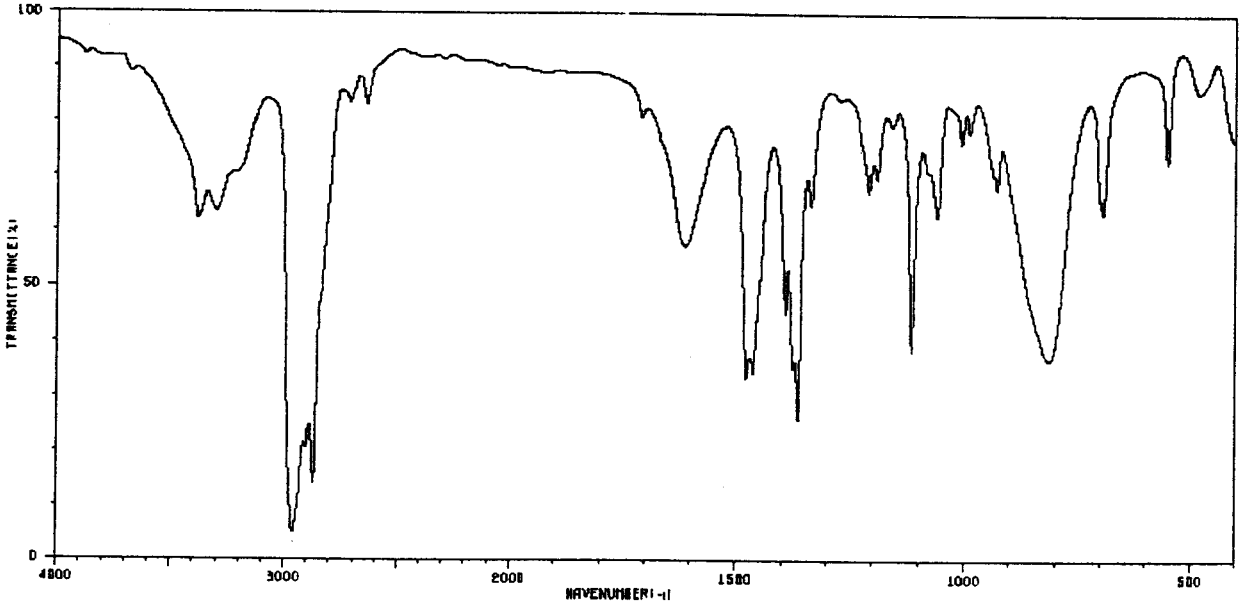
(If you can't figure these out before the final, you may have problems...)

Compound A

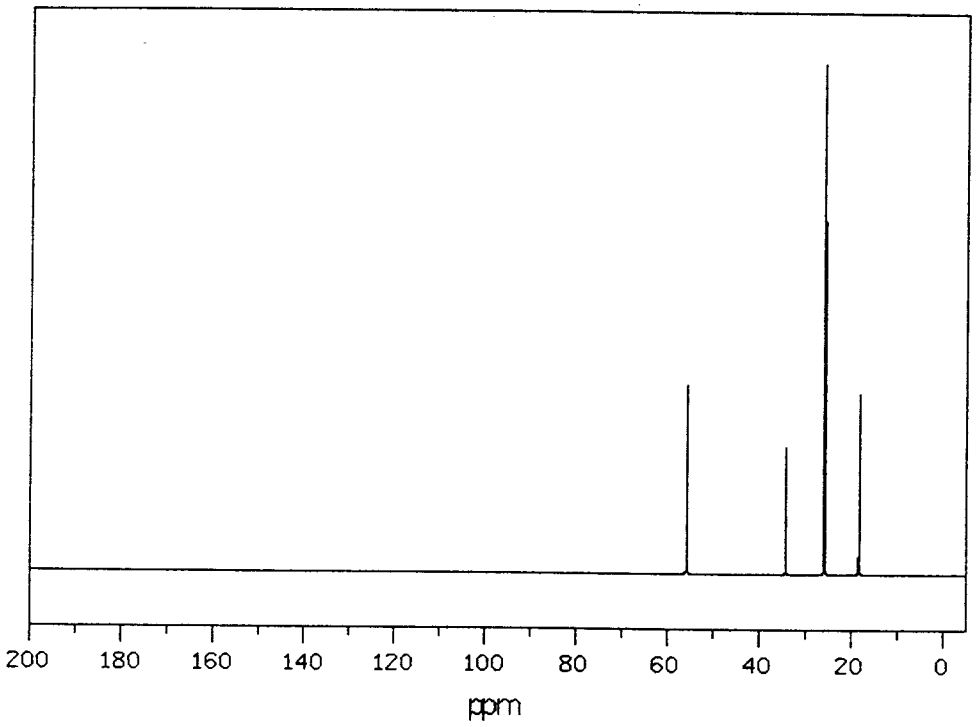
Mass Spectrum (molecular ion peak barely visible, would be at *m*/z =101)



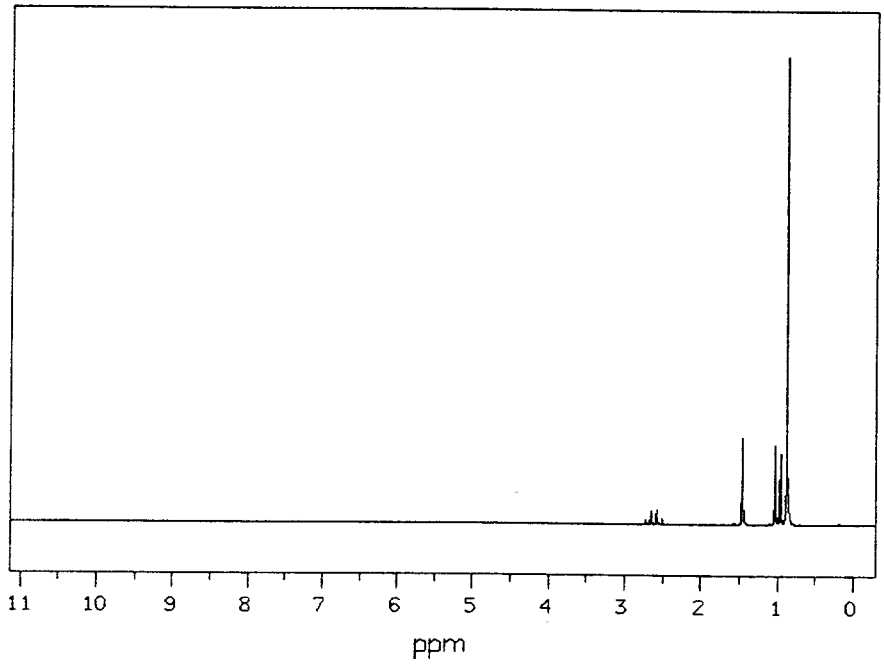
IR Spectrum



13C-NMR Spectrum (4 peaks)



1H-NMR Spectrum

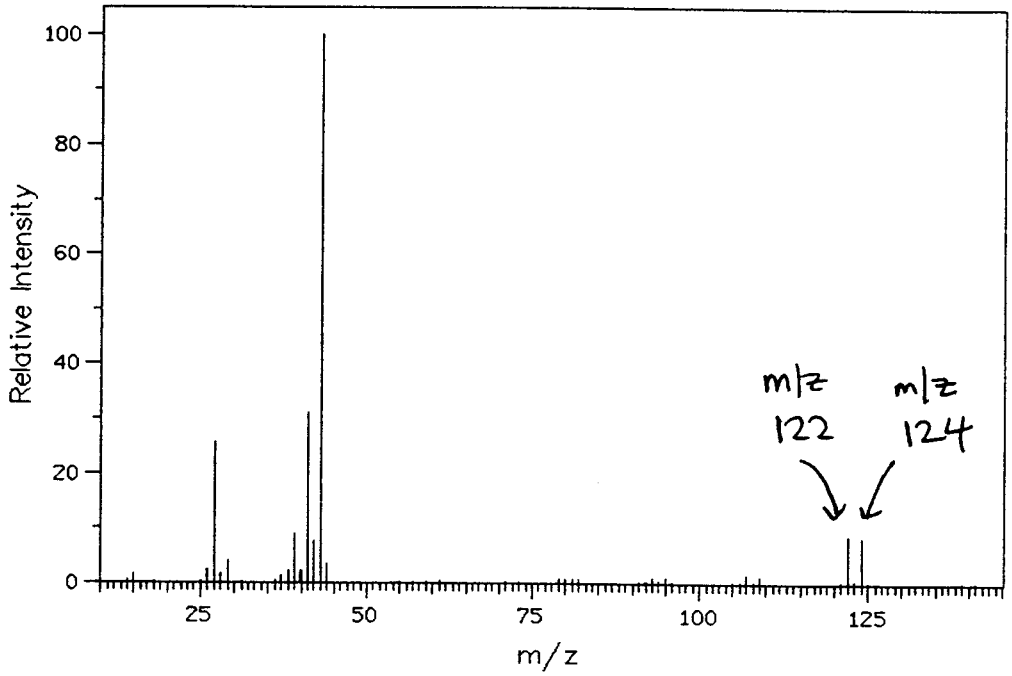


From left to right: quartet (1H), singlet (2H), doublet (3H), singlet (9H)

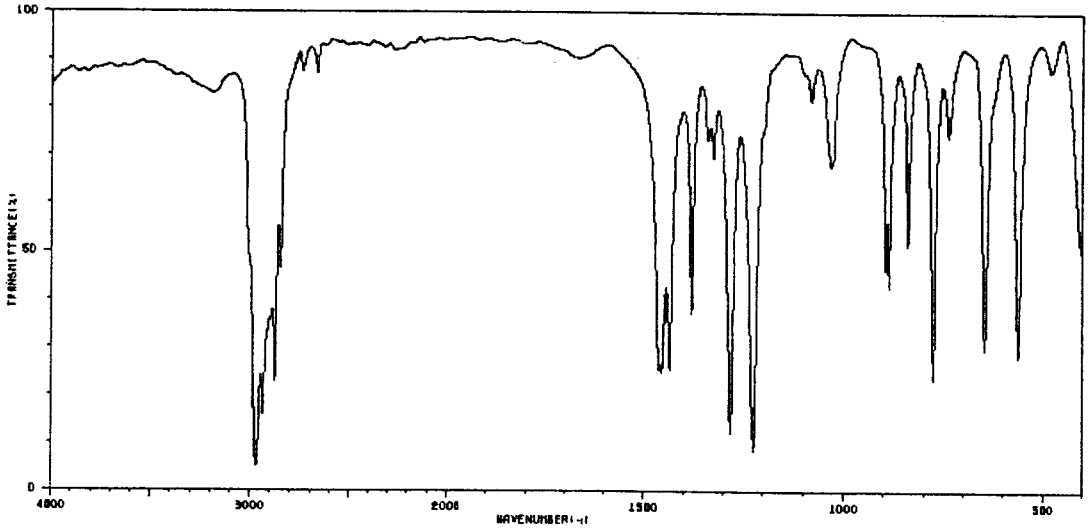
RELATIVE INTEGRATIONS

Compound B

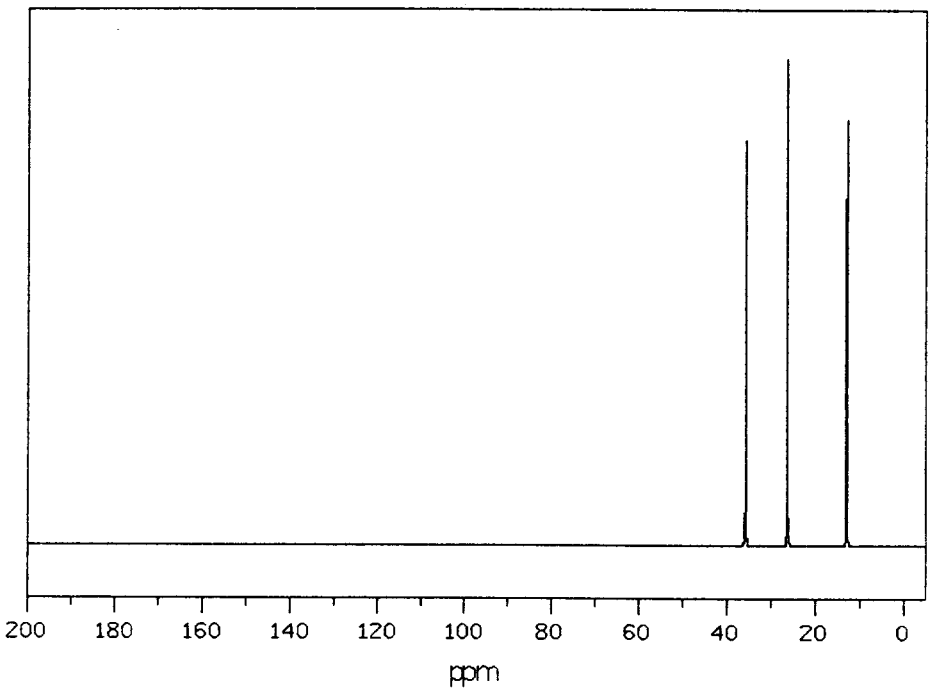
Mass Spectrum



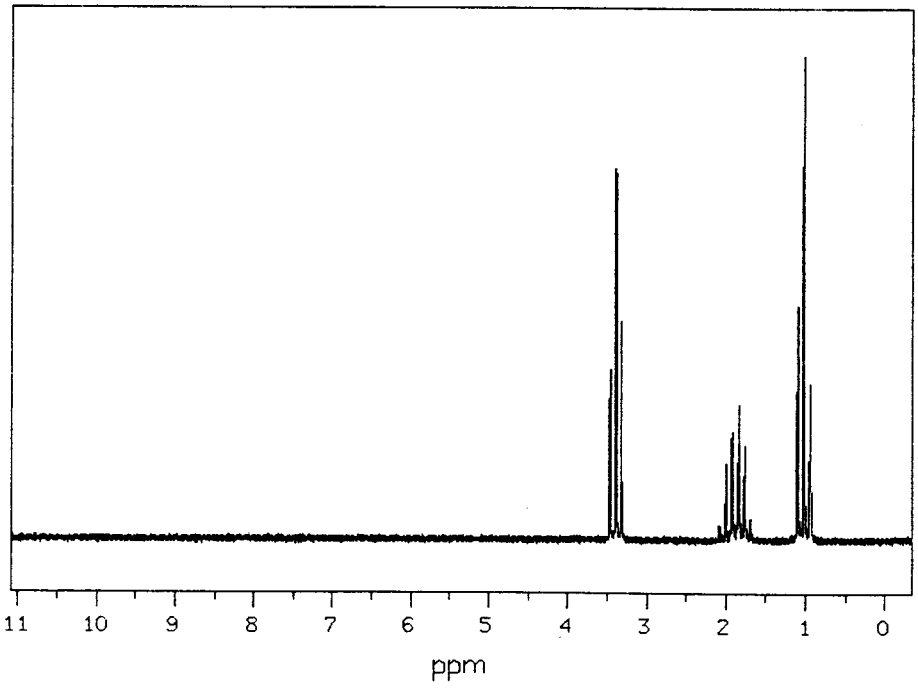
IR Spectrum



13C-NMR Spectrum (3 peaks)



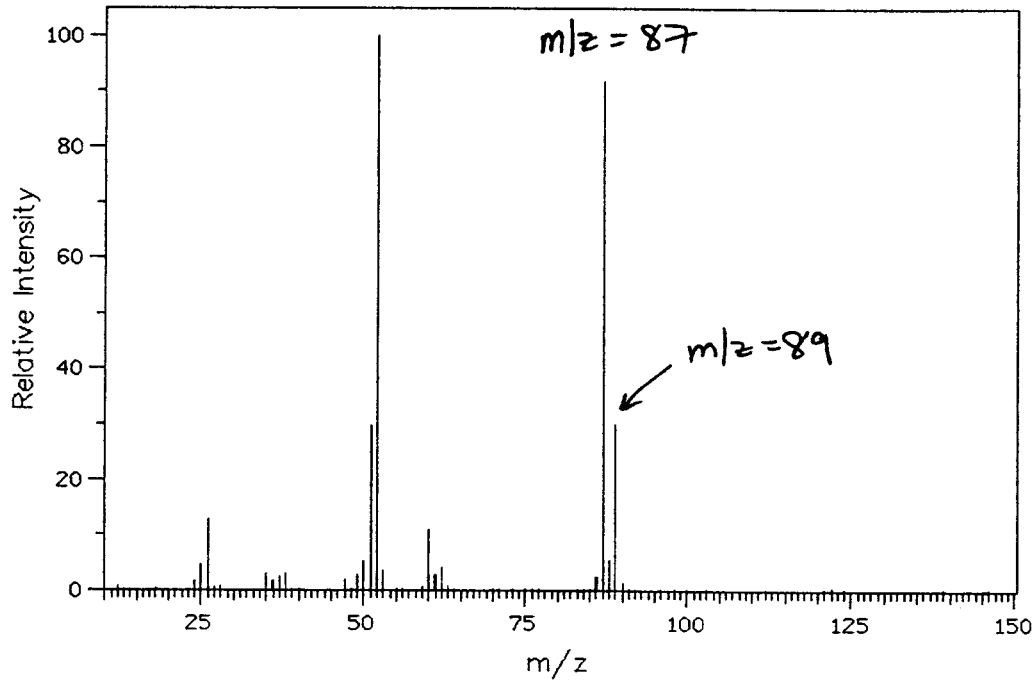
1H-NMR Spectrum



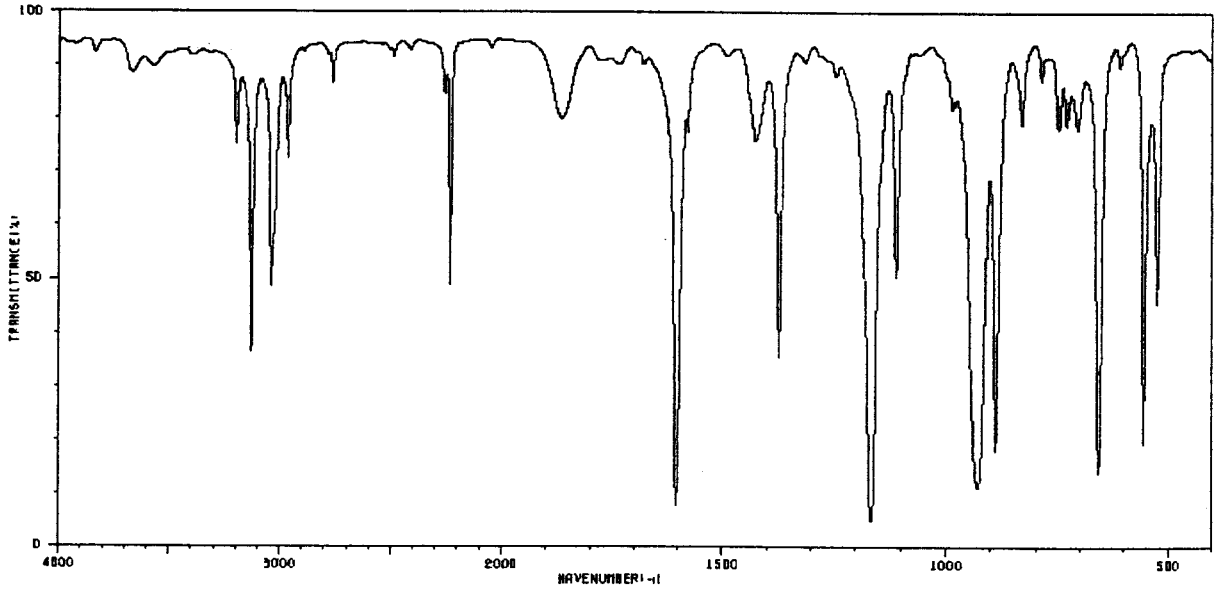
From left to right: triplet (2H), sextet (2H), triplet (3H)

Compound C

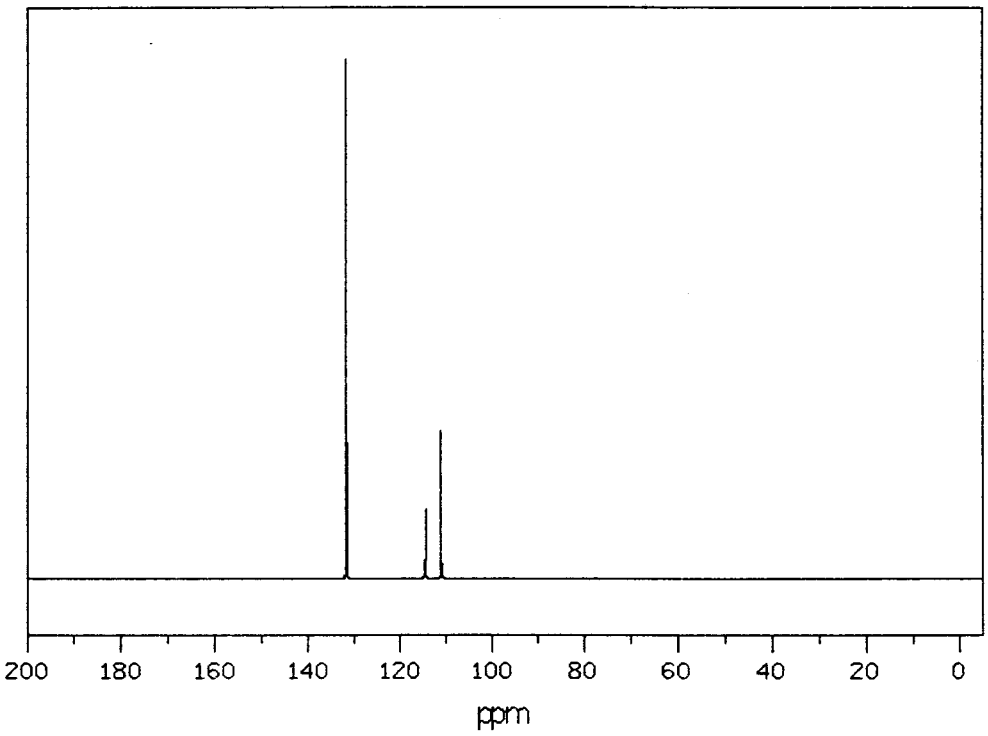
Mass Spectrum



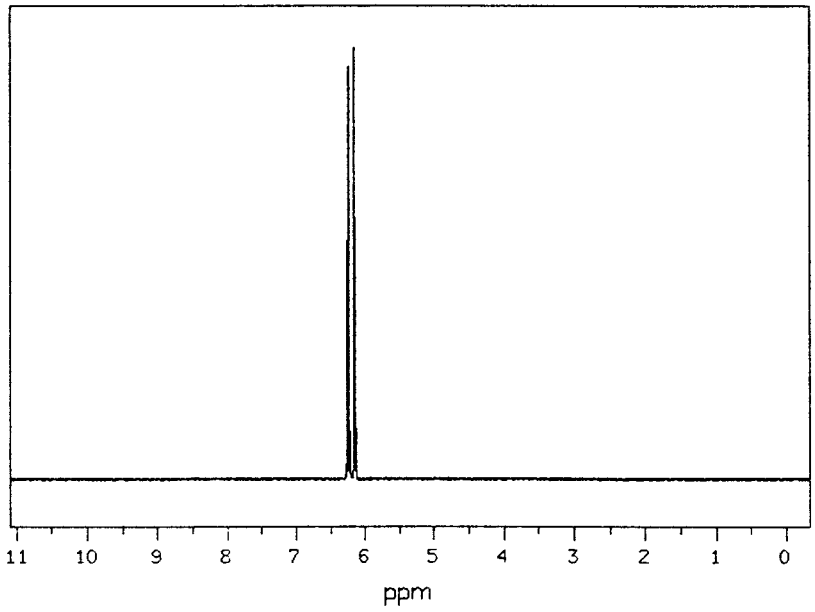
IR Spectrum



13C-NMR Spectrum (3 peaks)



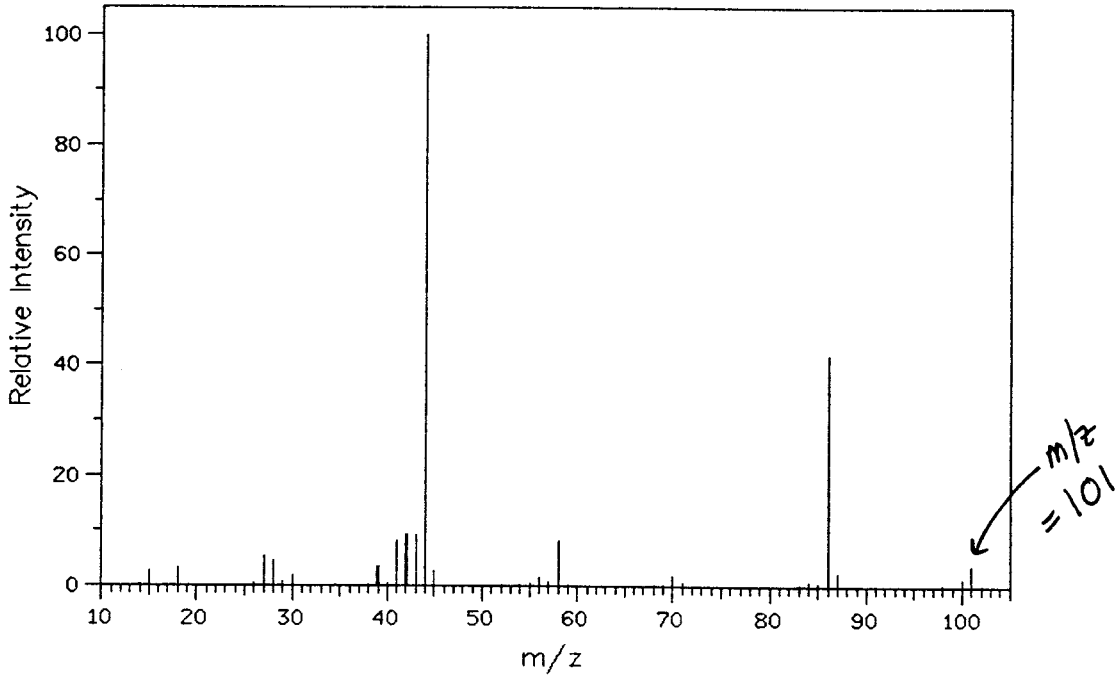
1H-NMR Spectrum



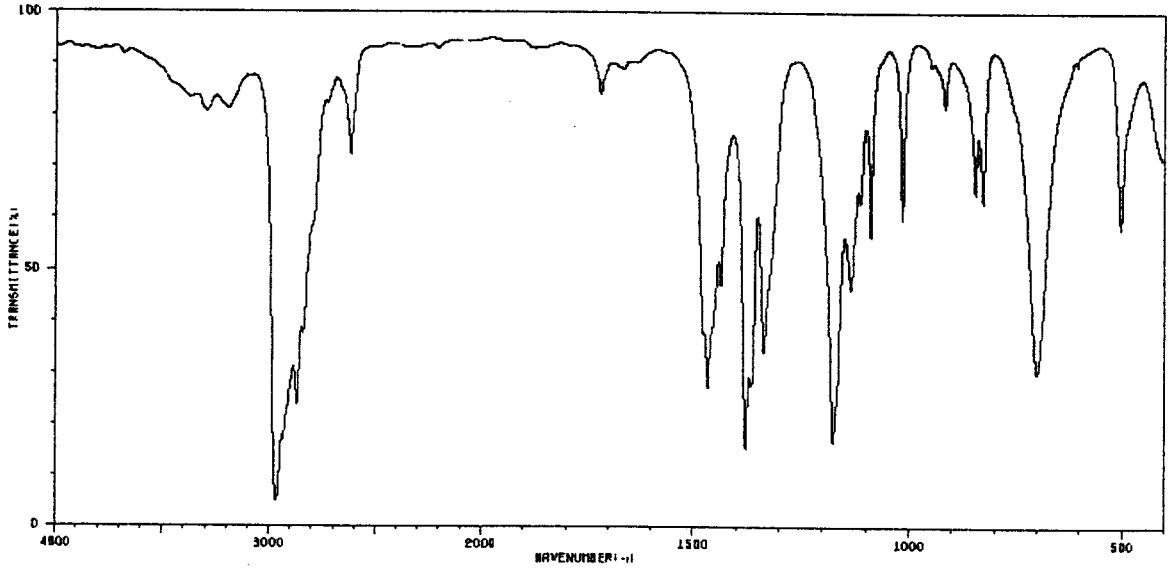
Each of the peaks above is actually a doublet with a very small coupling constant (~2 Hz); i.e., the spectrum contains 2 doublets

Compound D

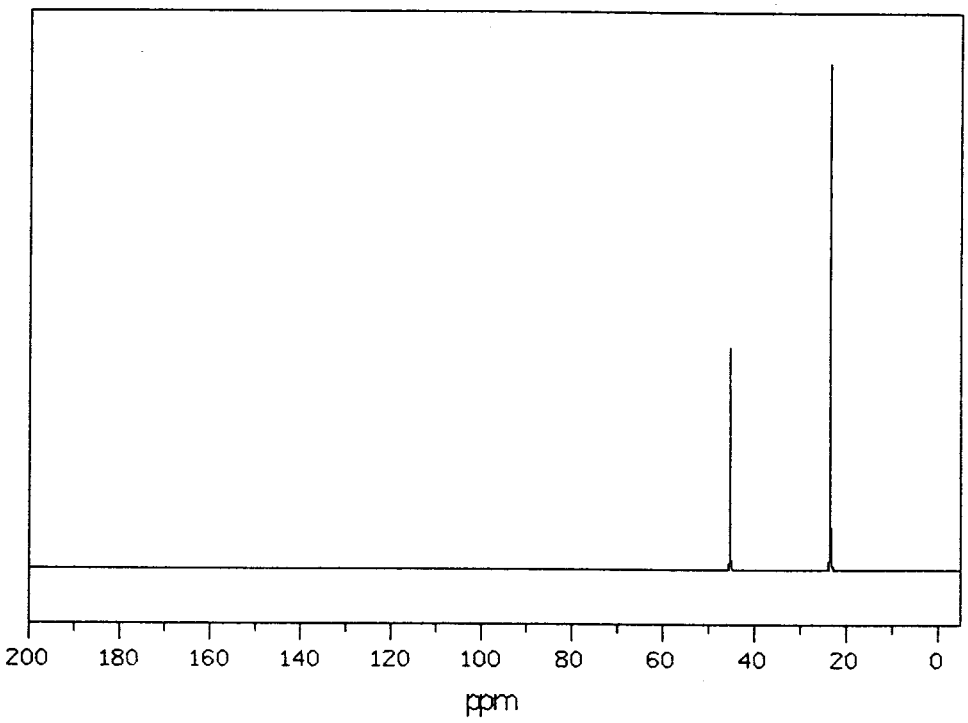
Mass Spectrum



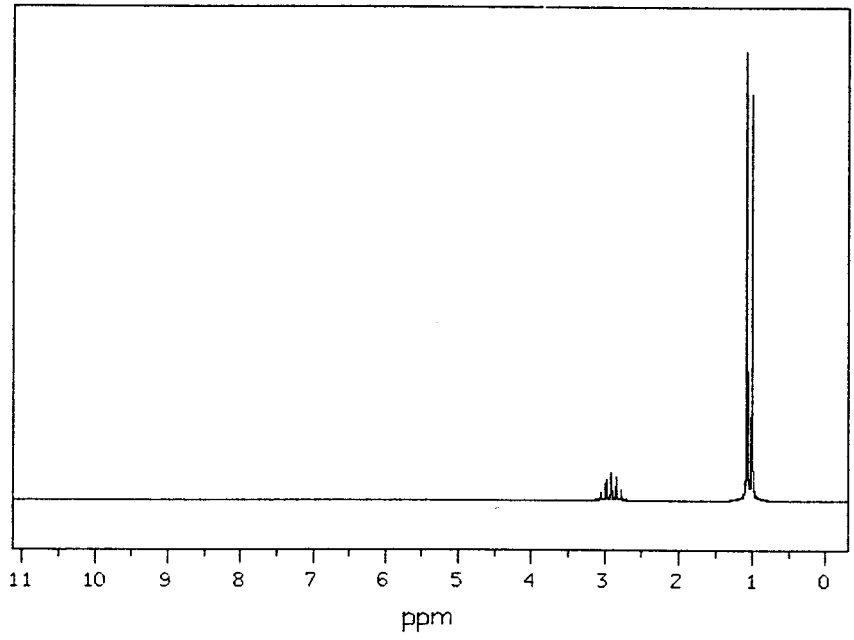
IR Spectrum



13C-NMR Spectrum (2 peaks)



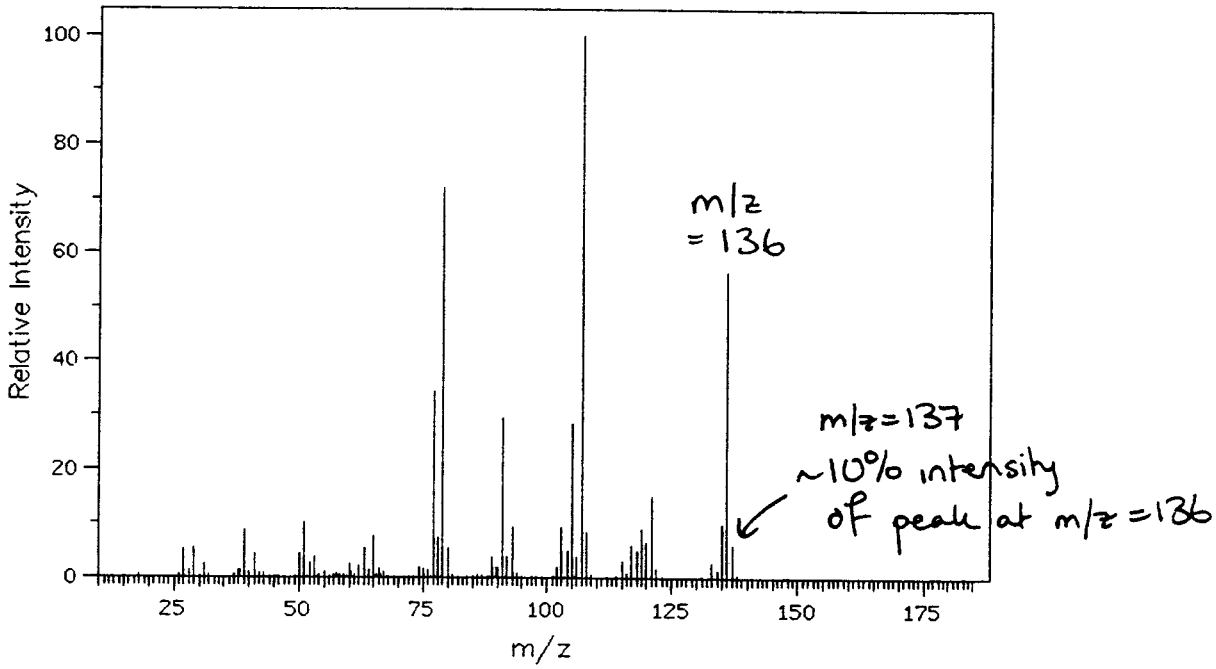
1H-NMR Spectrum



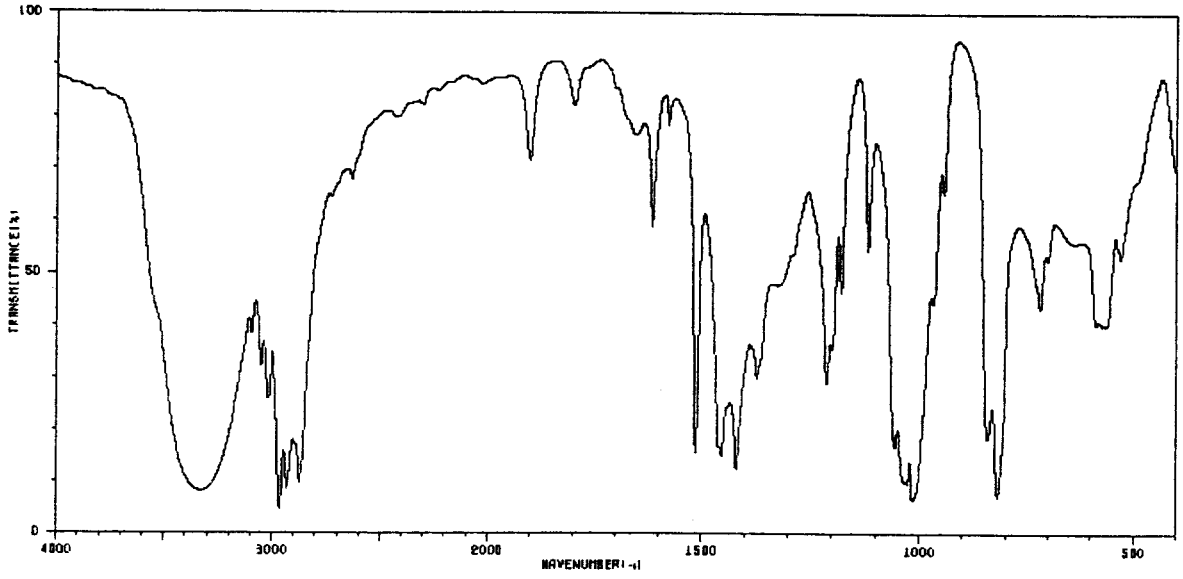
From left to right: septet (1H), doublet (6H)

Compound E

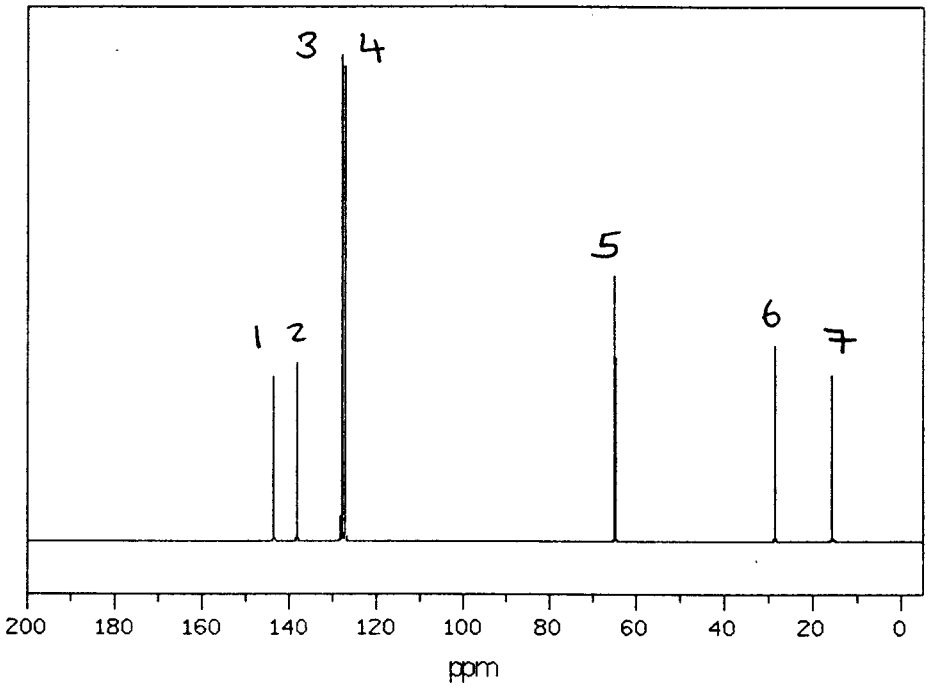
Mass Spectrum



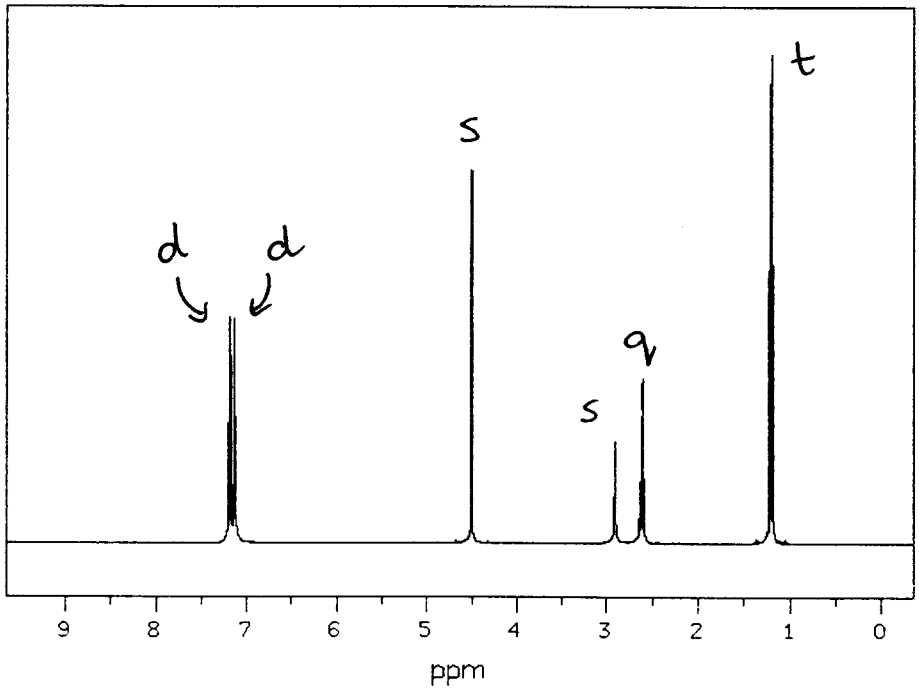
IR Spectrum



13C-NMR Spectrum (4 peaks above 100 ppm, 3 peaks below 100 ppm)



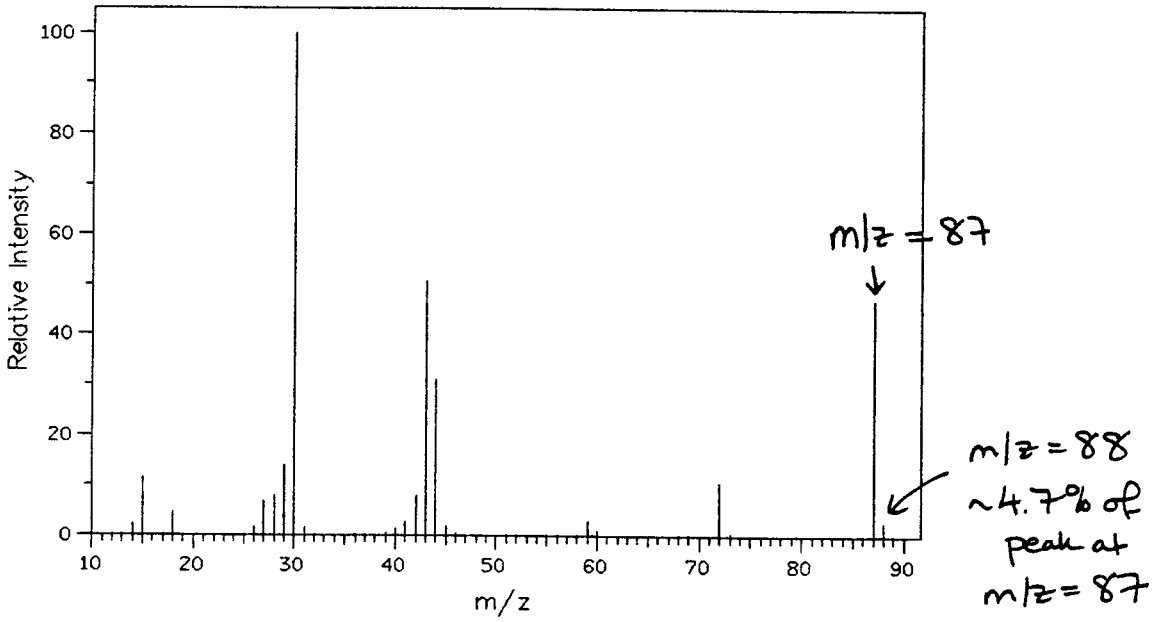
1H-NMR Spectrum



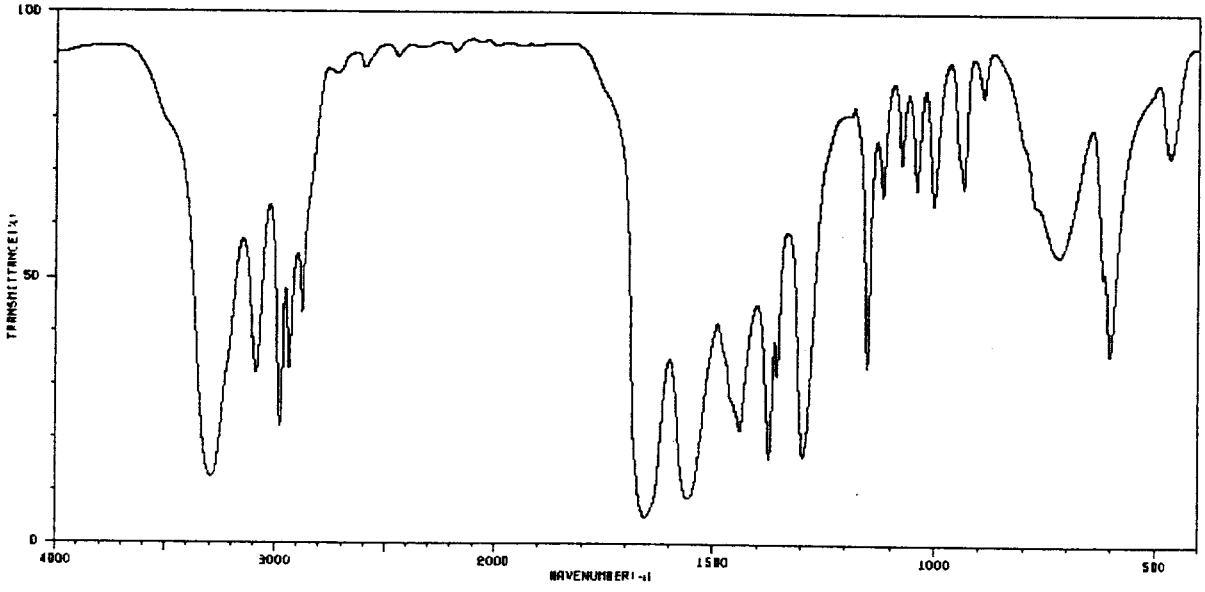
From left to right: two doublets (2H each), singlet (2H), singlet (1H), quartet (2H), triplet (3H)

Compound F

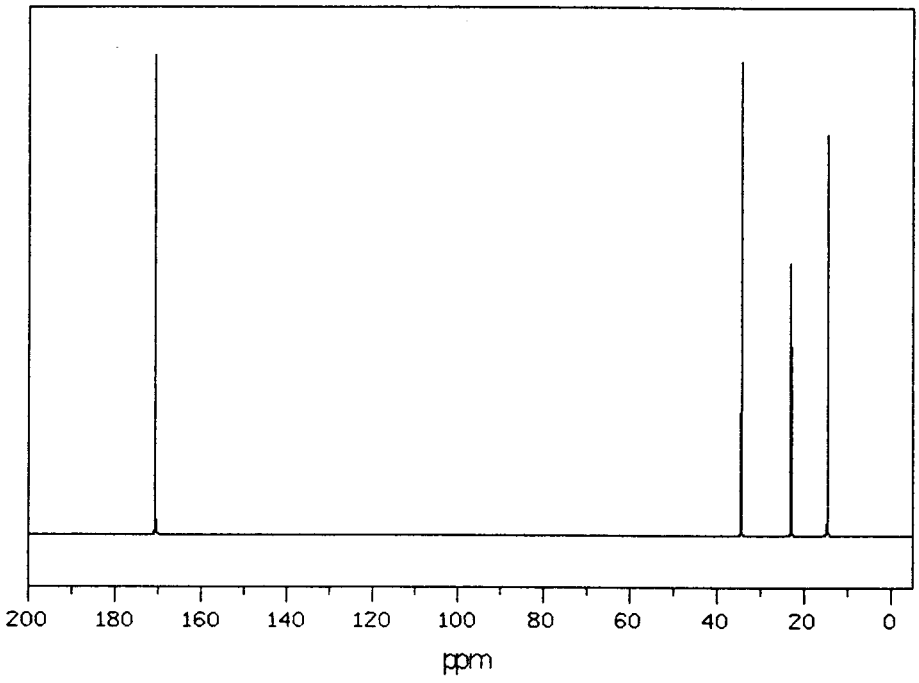
Mass Spectrum



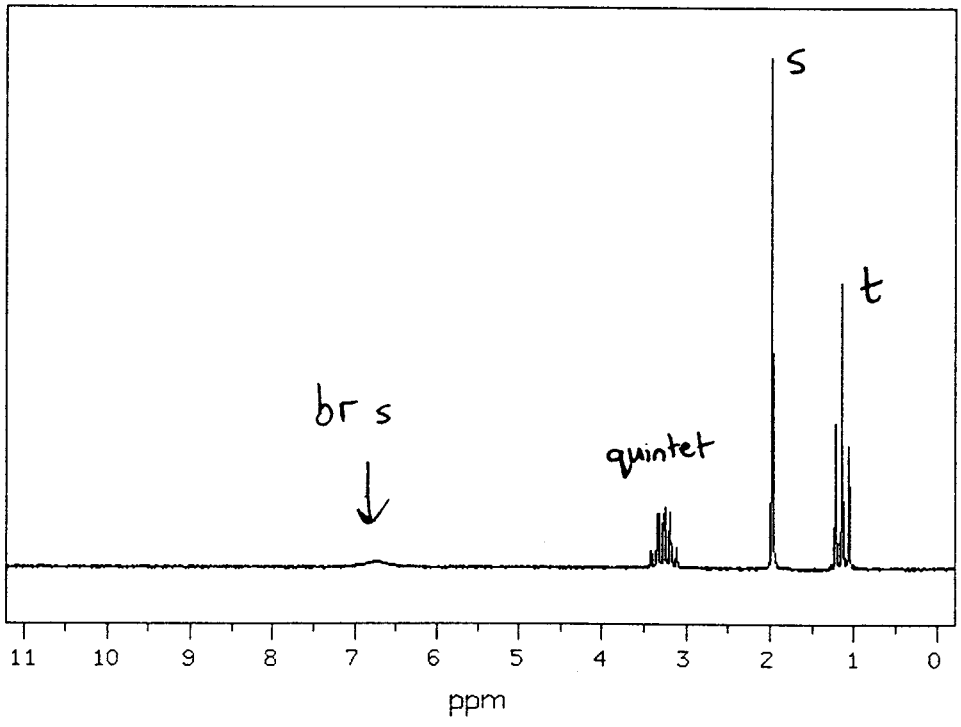
IR Spectrum



13C-NMR Spectrum (4 peaks)



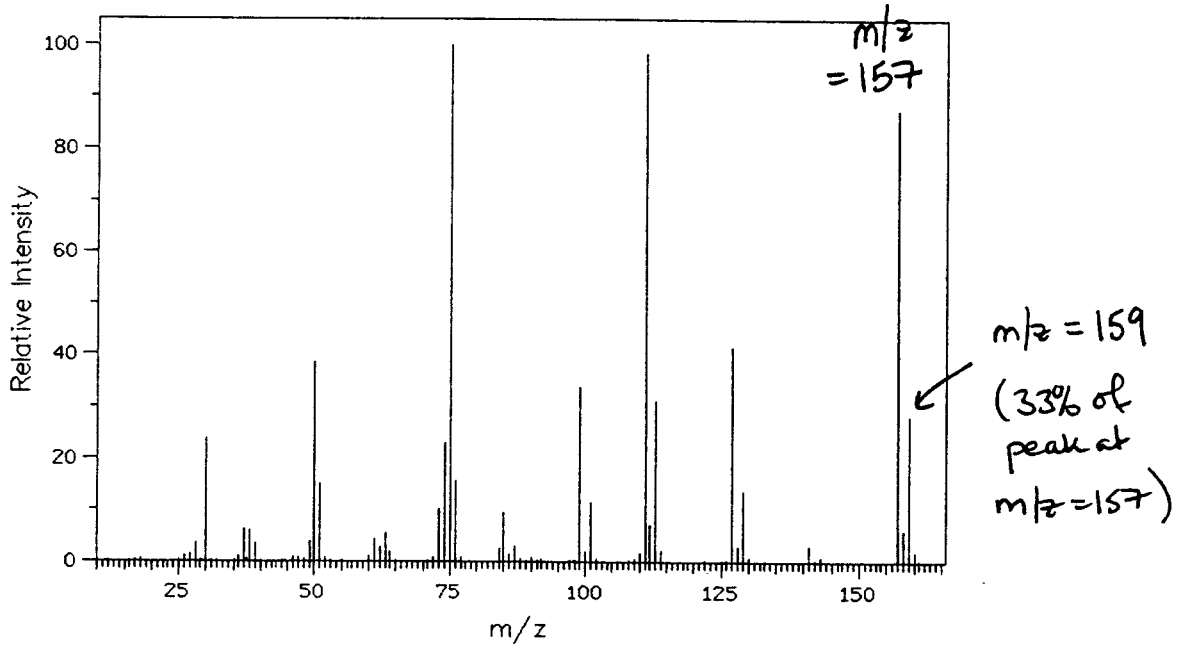
1H-NMR Spectrum



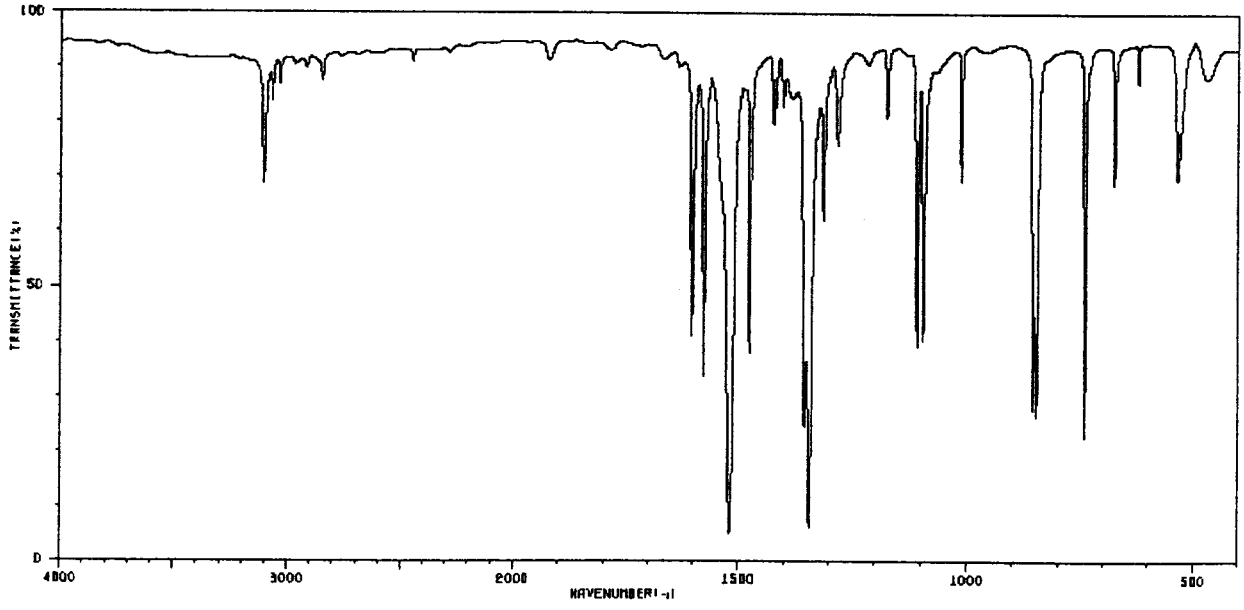
From left to right: very broad singlet (1H), quintet (2H), singlet (3H), triplet (3H)

Compound G

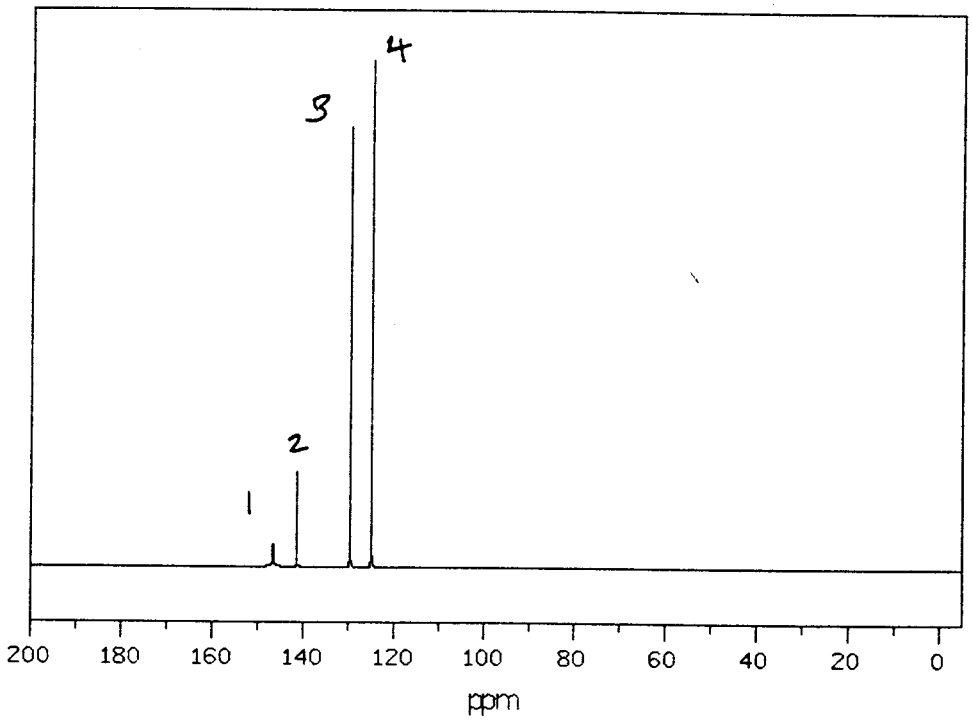
Mass Spectrum



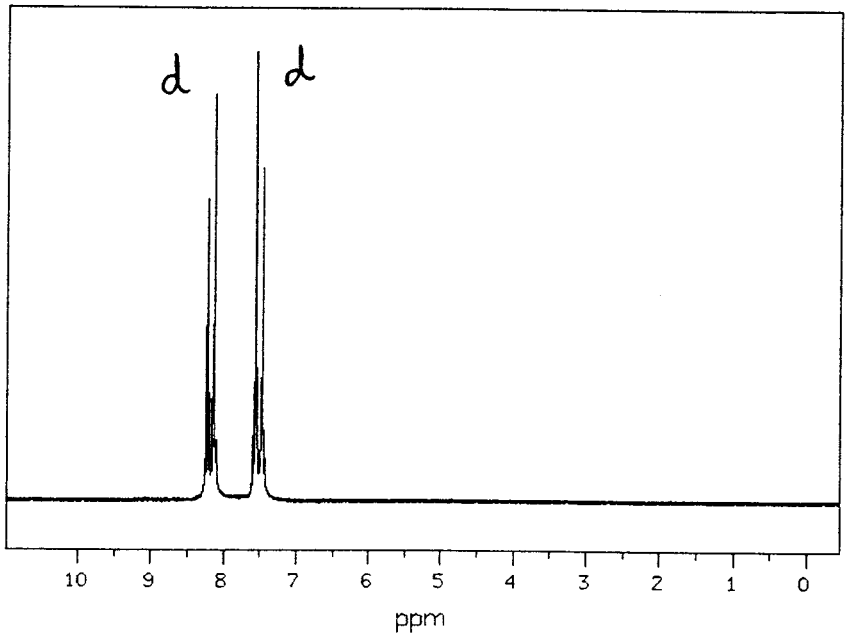
IR Spectrum



13C-NMR Spectrum (4 peaks)



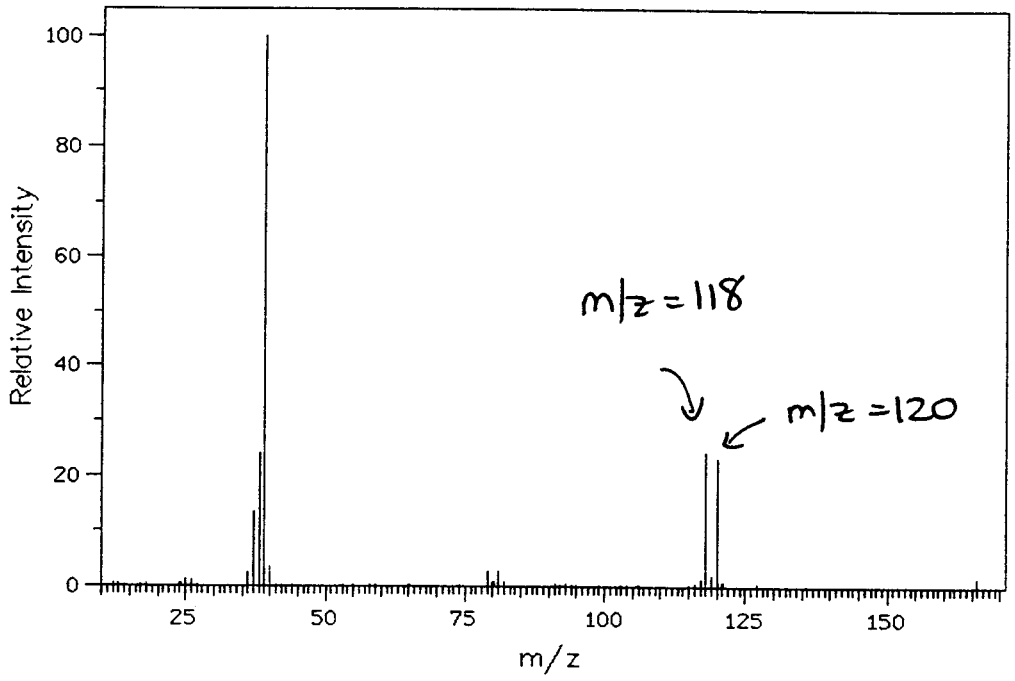
1H-NMR Spectrum



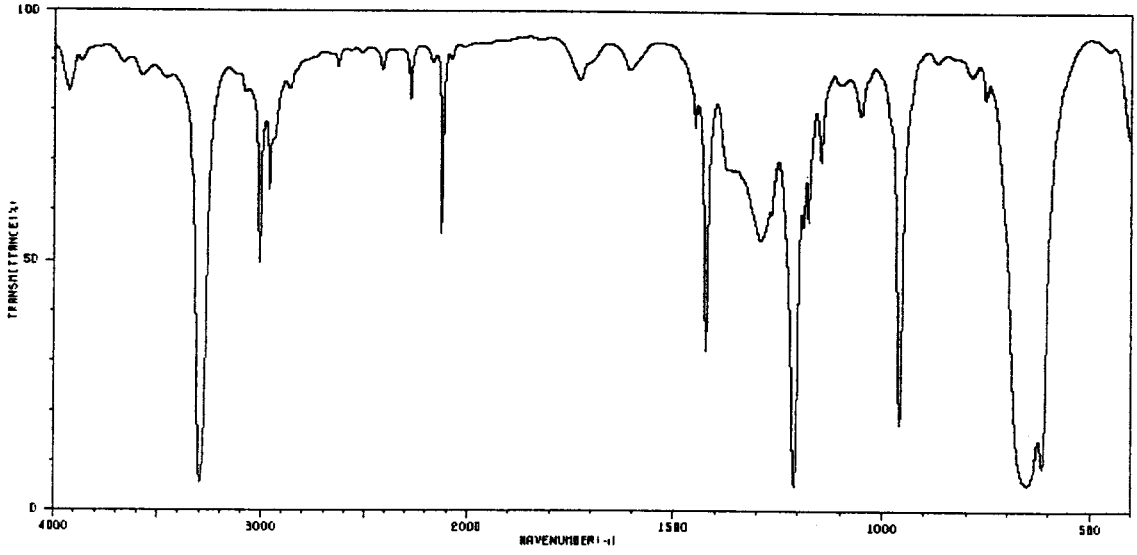
From left to right: doublet (1H), doublet (1H)

Compound H

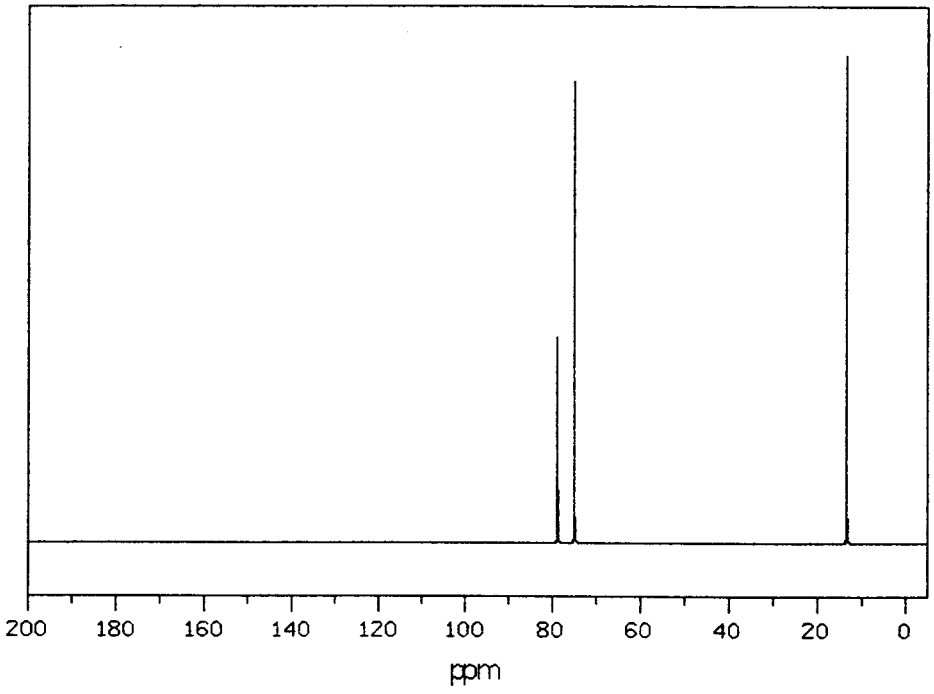
Mass Spectrum



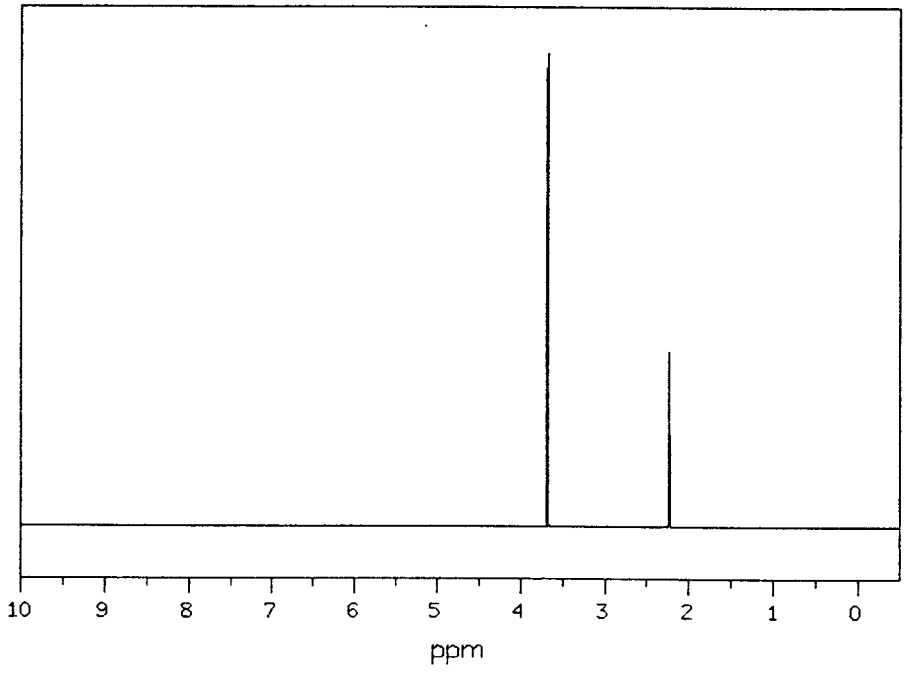
IR Spectrum



13C-NMR Spectrum (3 peaks)



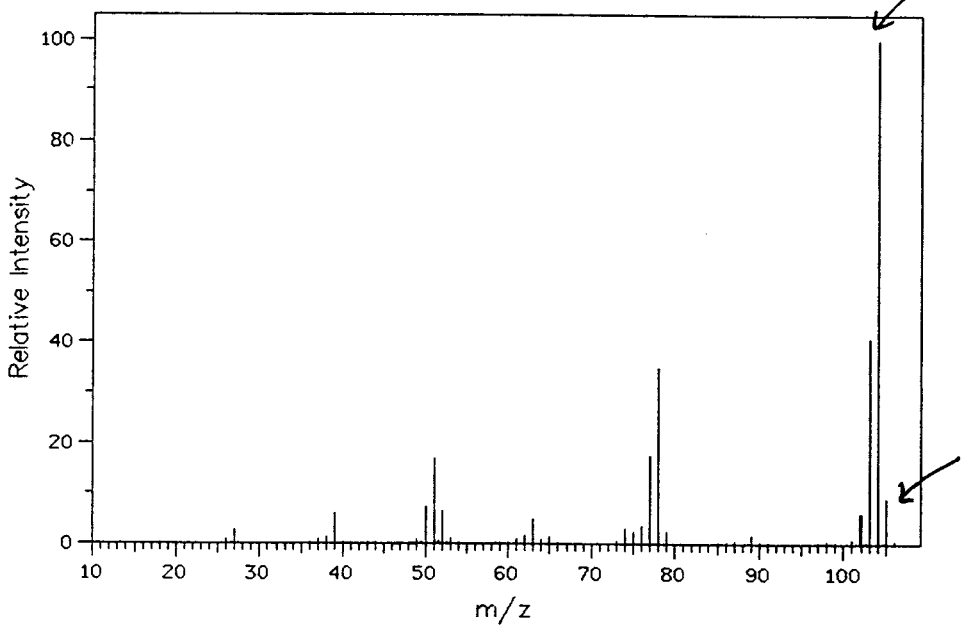
1H-NMR Spectrum



From left to right: singlet (2H), singlet (1H)

Compound J

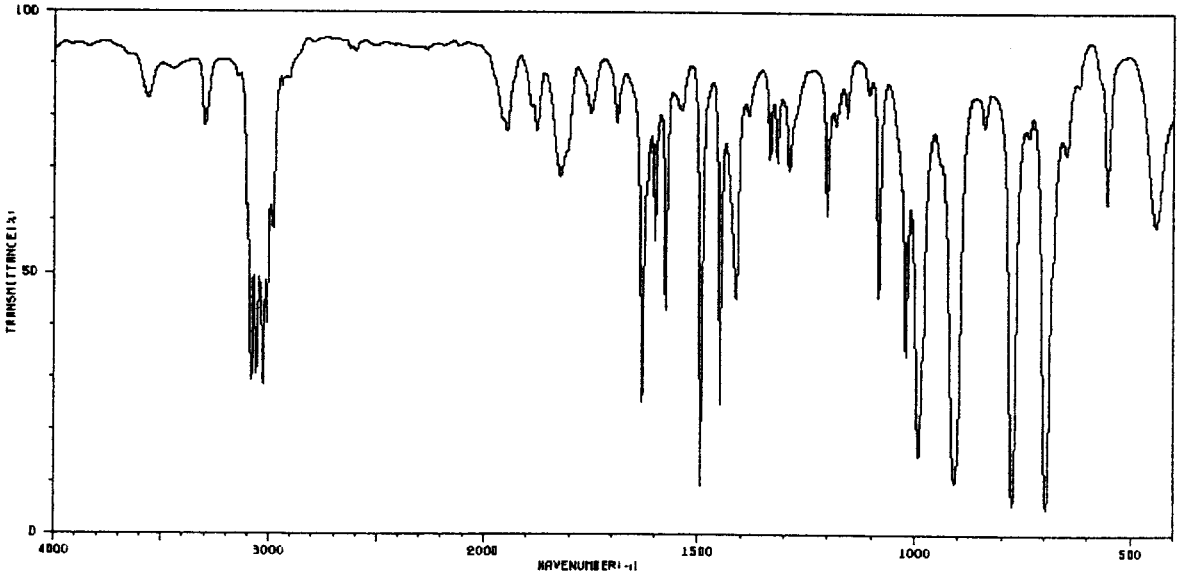
Mass Spectrum



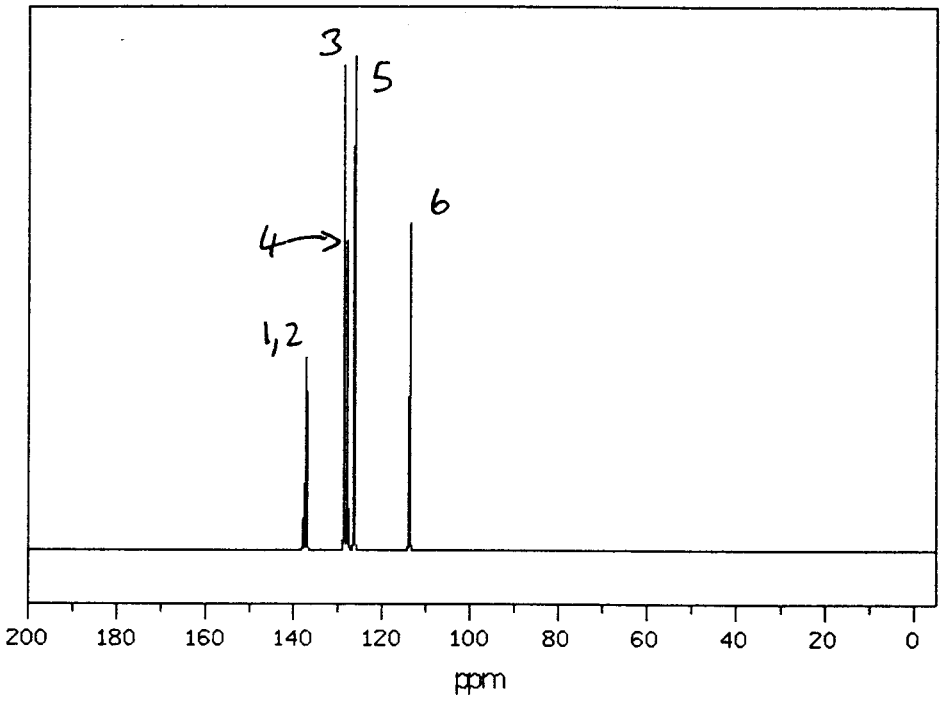
m/z = 104

m/z = 105 (9.3% of peak at m/z = 104)

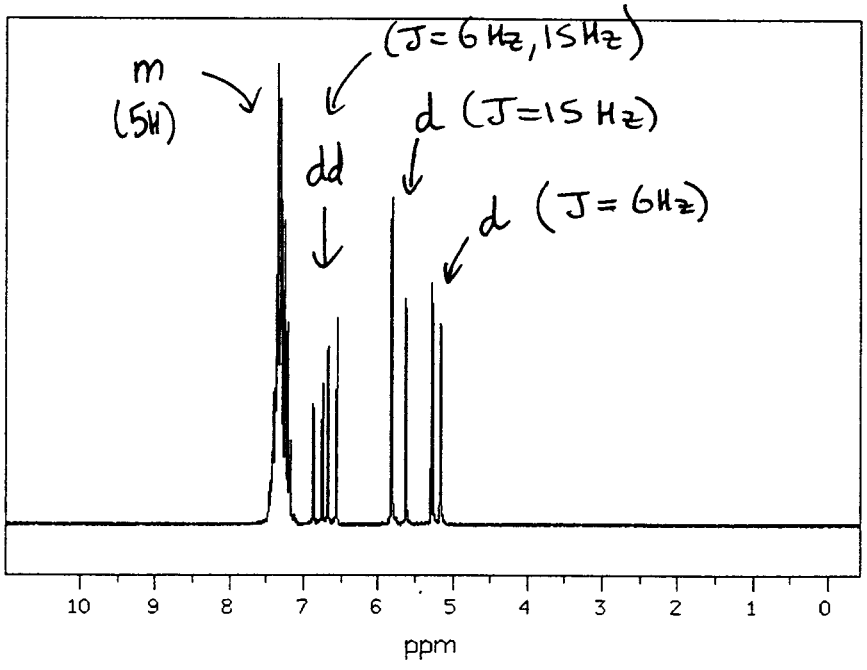
IR Spectrum



13C-NMR Spectrum (trust me, there are 6 peaks between 100 and 150 ppm)



1H-NMR Spectrum



From left to right: multiplet (5H), doublet of doublets (1H), doublet (1H), doublet (1H)