Chemistry 30B Discussion - Week 3: Structure Determination - DCF

There are 10 problems in this problem set. You will be provided with a chemical formula, mass spectrum, IR spectrum, ^{1}H NMR spectrum, & a ^{13}C NMR spectrum. Use this information to determine the structure of the unknown compounds.

In addition to determining the structure you will need to explain the following experimental data by doing the following.

First, you need to indicate the number of degrees of unsaturation of the system. As a reminder, the equation is given:

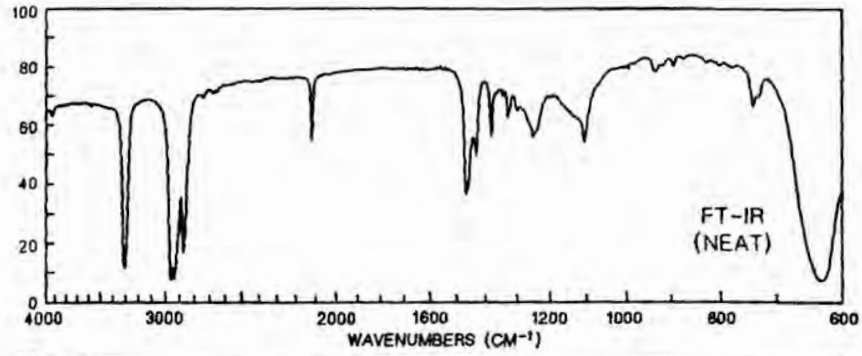
Degree of Unsaturation = [2 + (2 x #Carbons) + #Nitrogens - #Hydrogens - #Halogens]/2
(note: I did not forget oxygen, it isn't part of the equation)

In the mass spectra you need to identify the key molecular fragments and their corresponding molecular structure, not that signals in mass spectrometry come only from charged species.

Indicate the species involved and type of vibration for the imporatnt signals in the IR spectra.

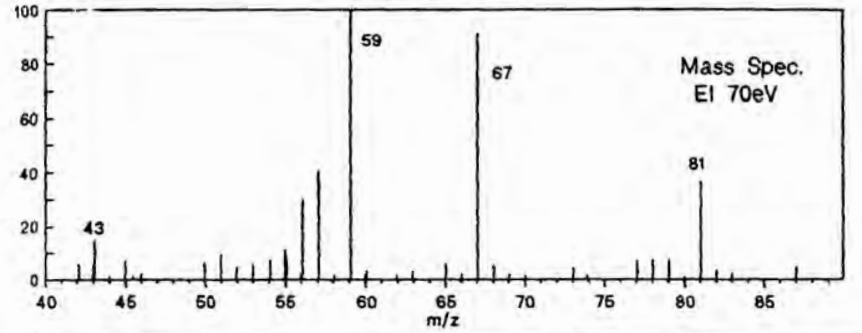
Finally, assign the ^{1}H & ^{13}C NMR signals for each compound. Indicate, if not already done, if the signal is a singlet (s), doublet (d), triplet (t), or multiplet (m).

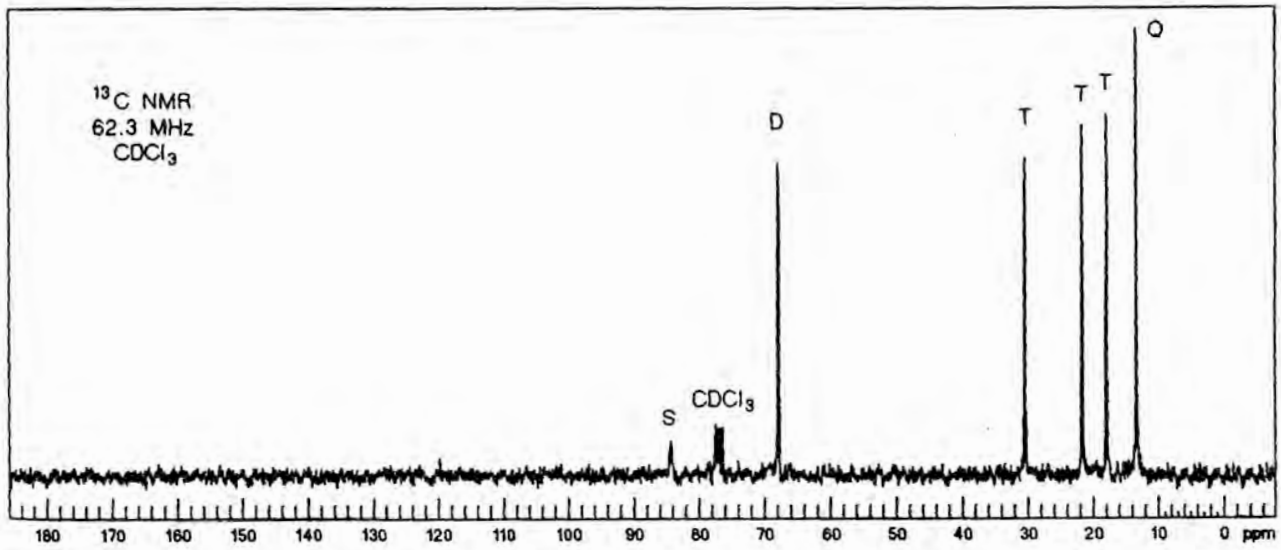
#1 - C_6H_{10}

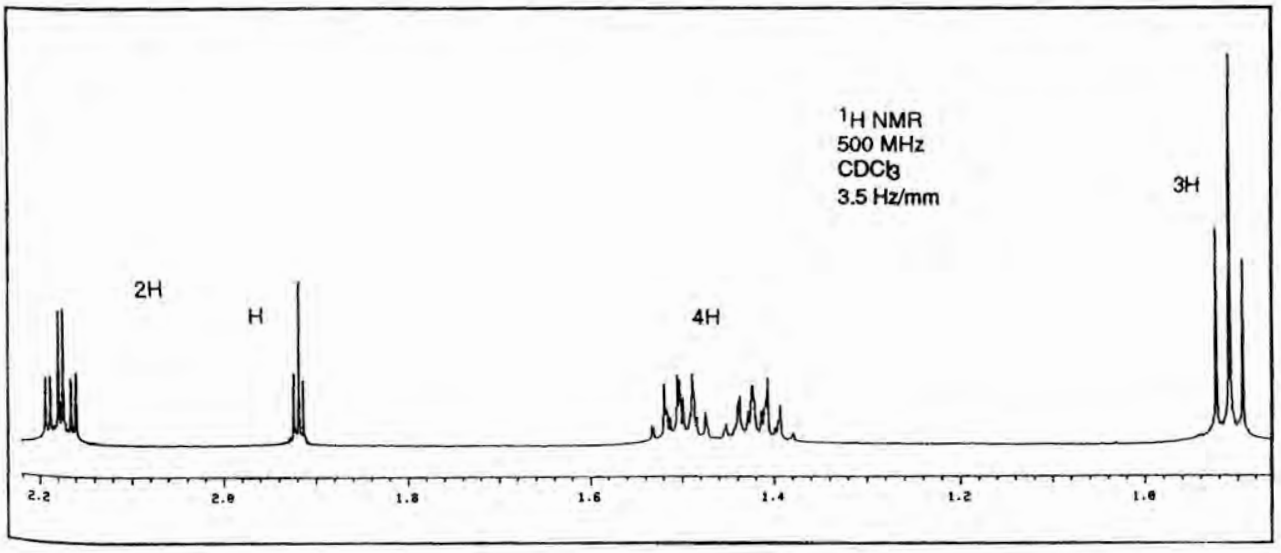


Exact M.S. (EI) = 81.0704

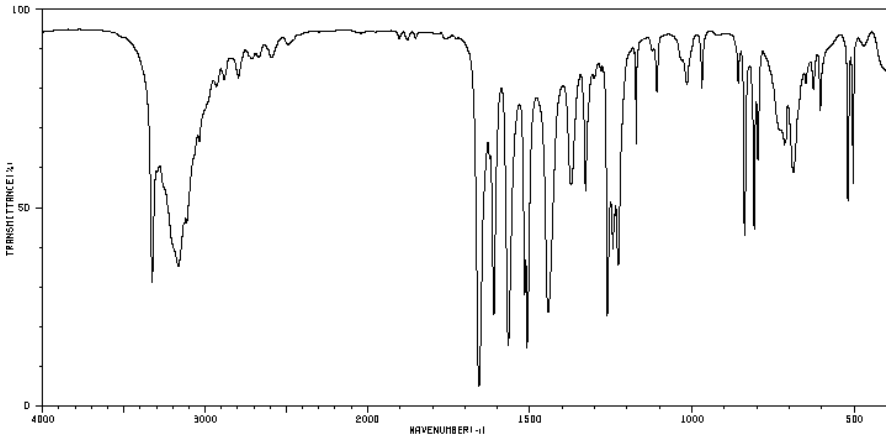
$UV\lambda_{max} = 220 (\varepsilon = 1{,}200)$



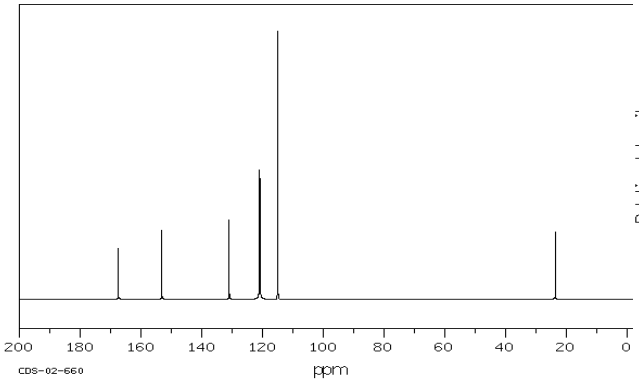


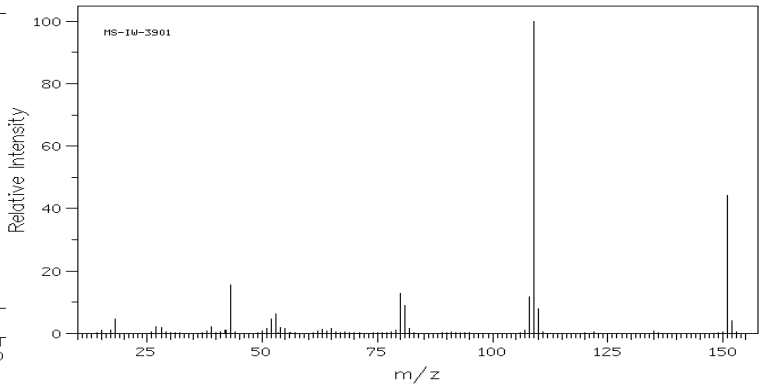


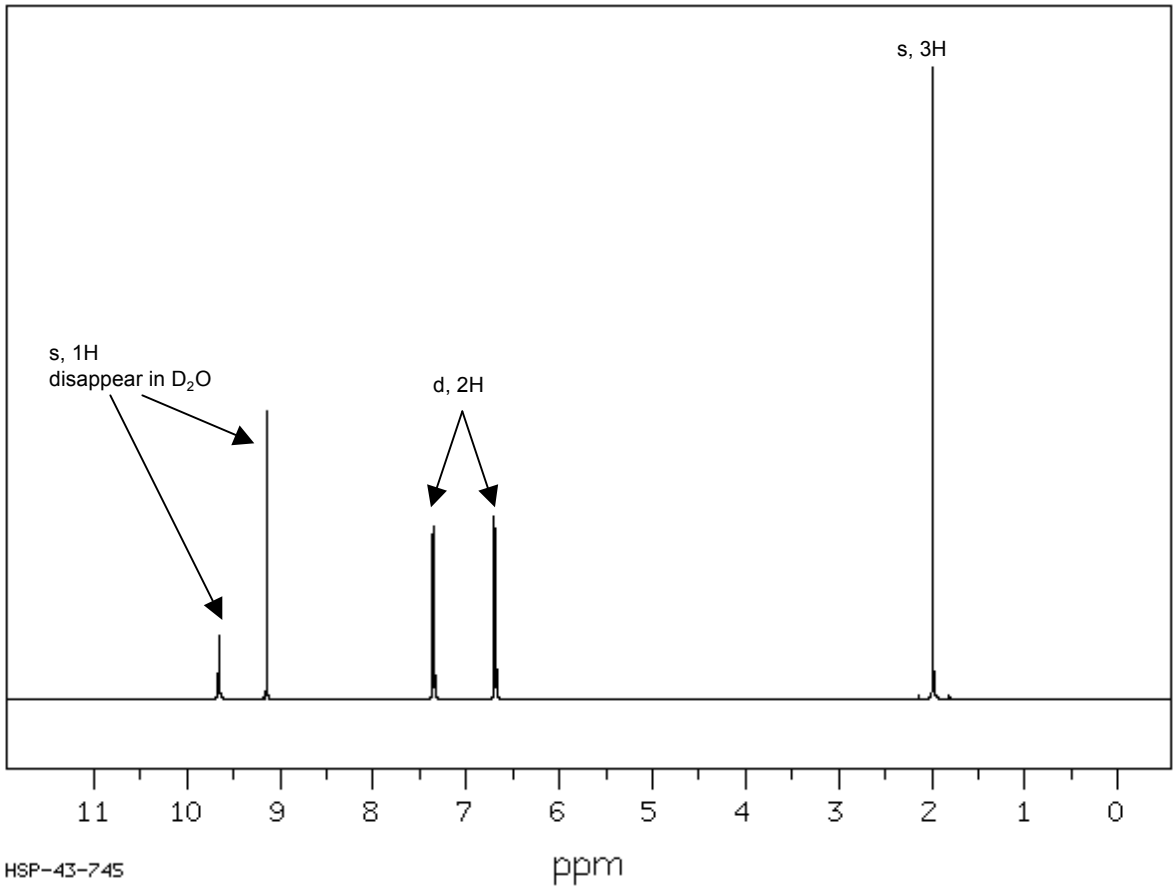
#2 - $C_8H_9NO_2$



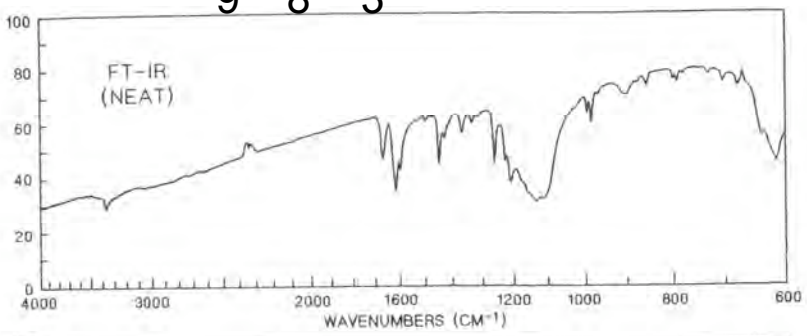
What is the common name of this compound?



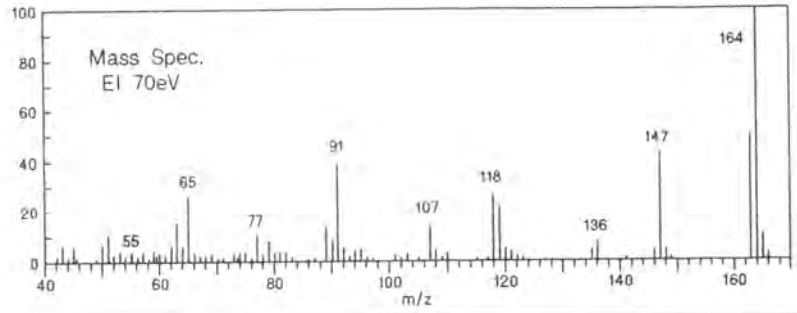


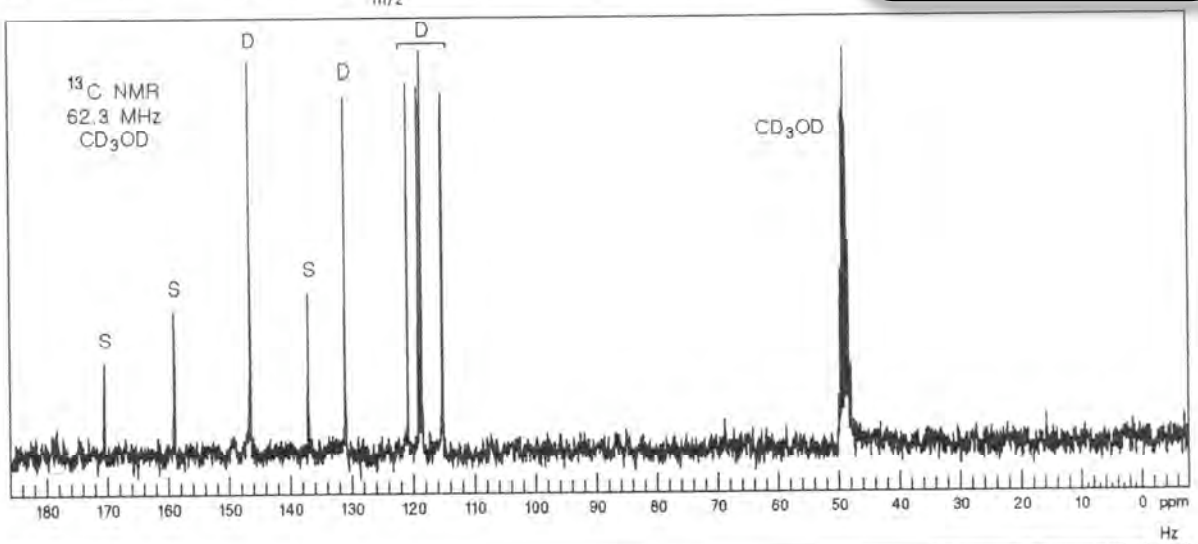


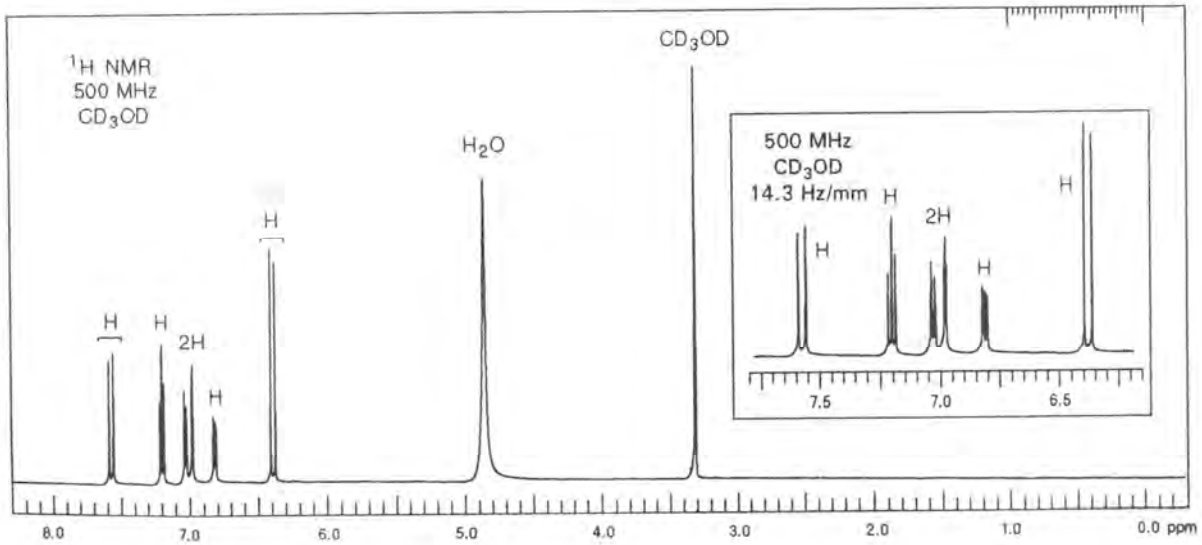
#3 - $C_9H_8O_3$



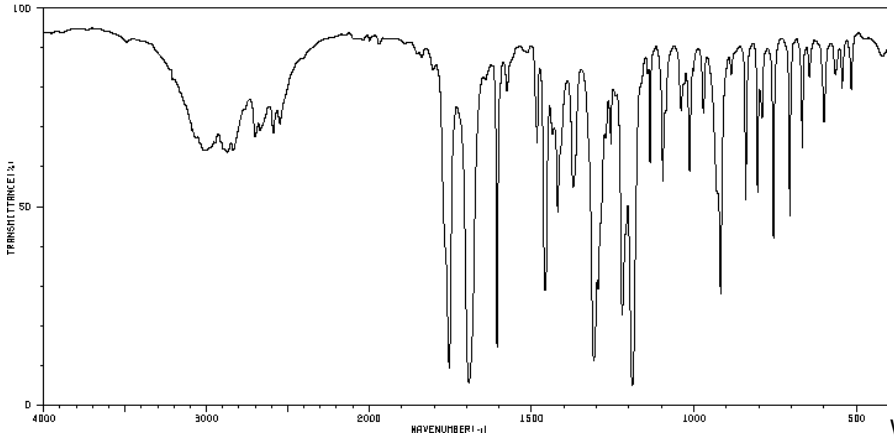
UV λ_{max} = 214 (ε = 16,000)
233 (ε = 13,000)
276 (ε = 19,000)



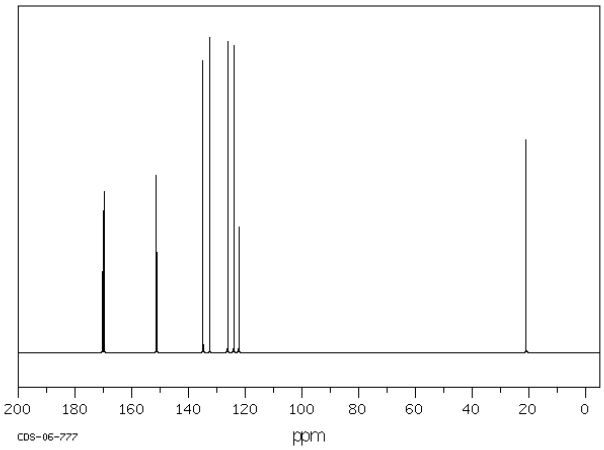


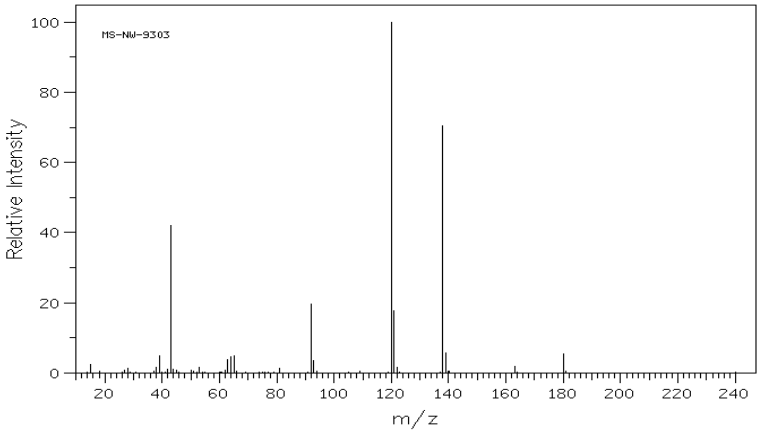


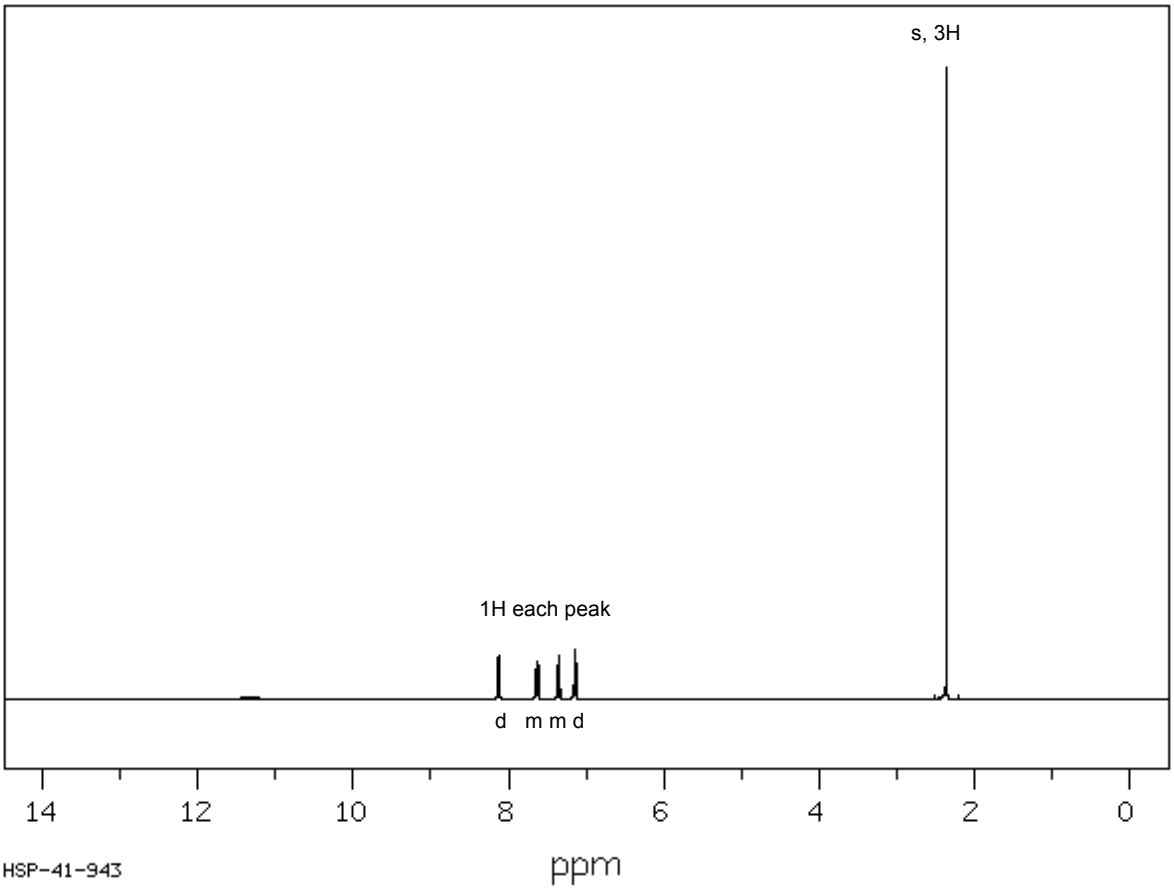
#4 - $C_9H_8O_4$



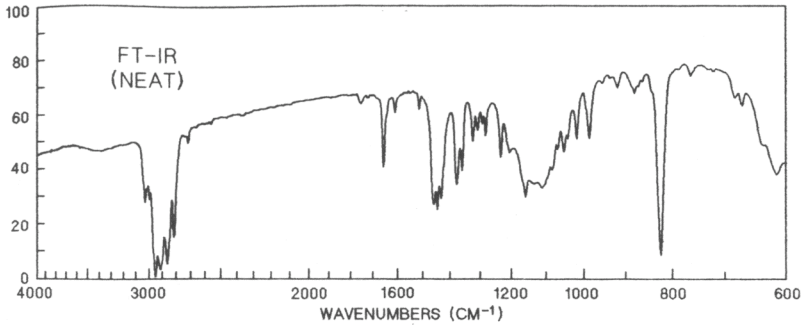
What is the common name of this compound?



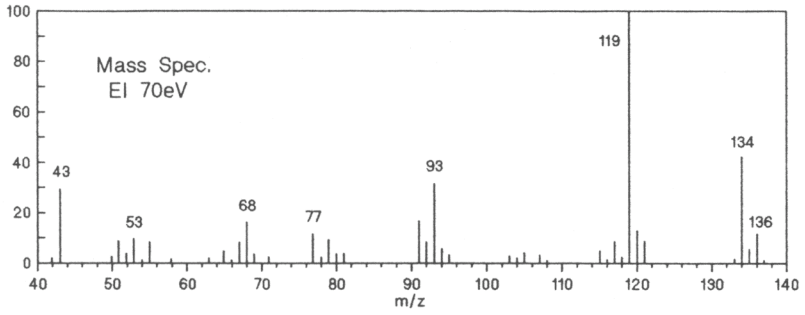


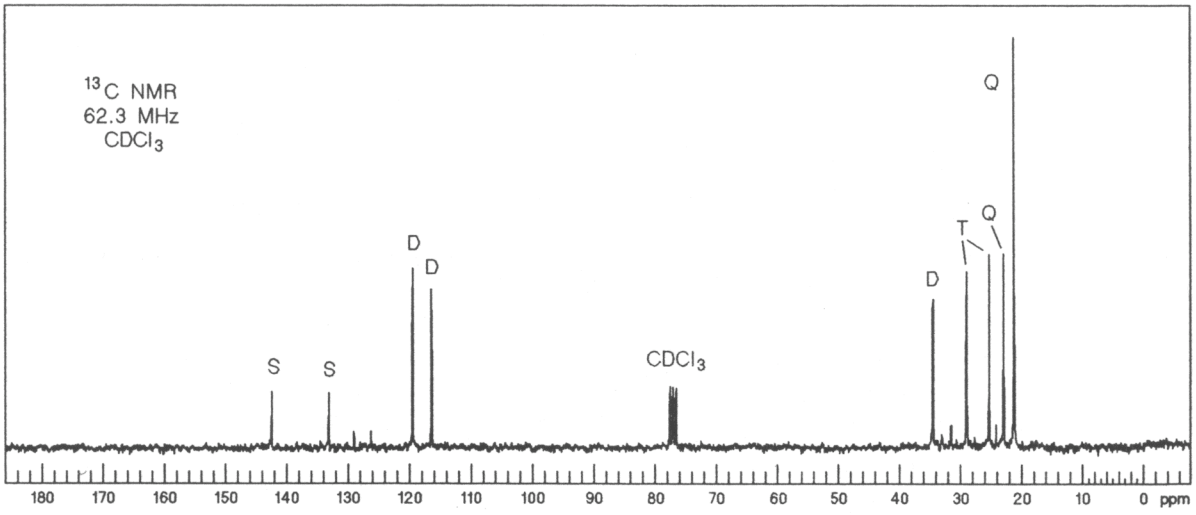


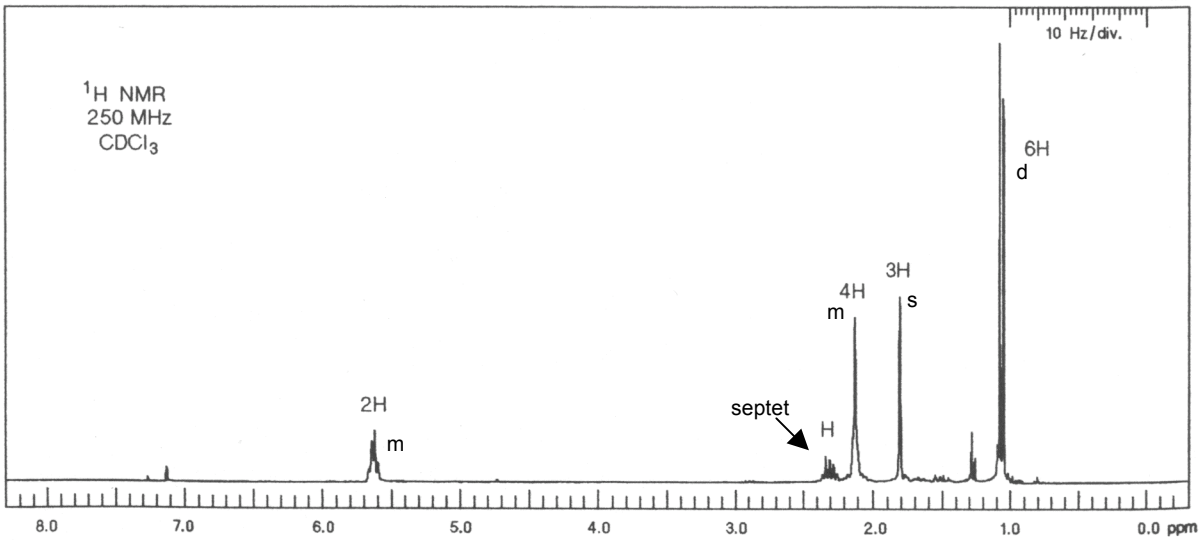
#5 - $C_{16}H_{10}$



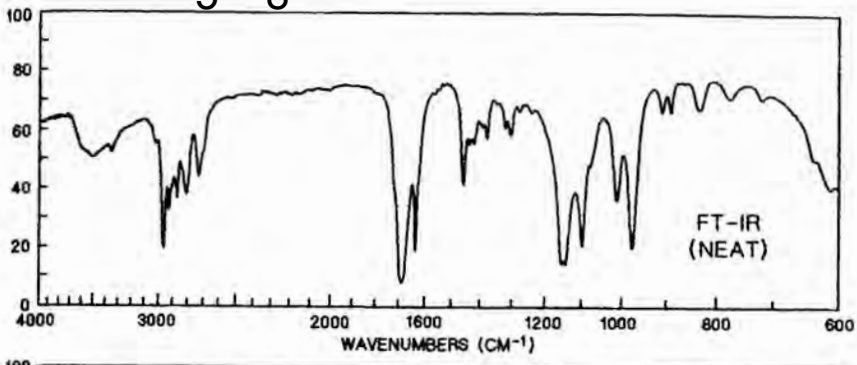
$UV\lambda_{max} = 268\ (\varepsilon = 8000)$





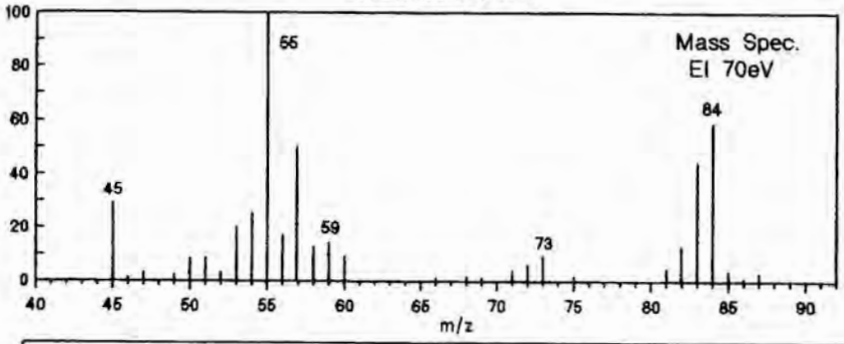


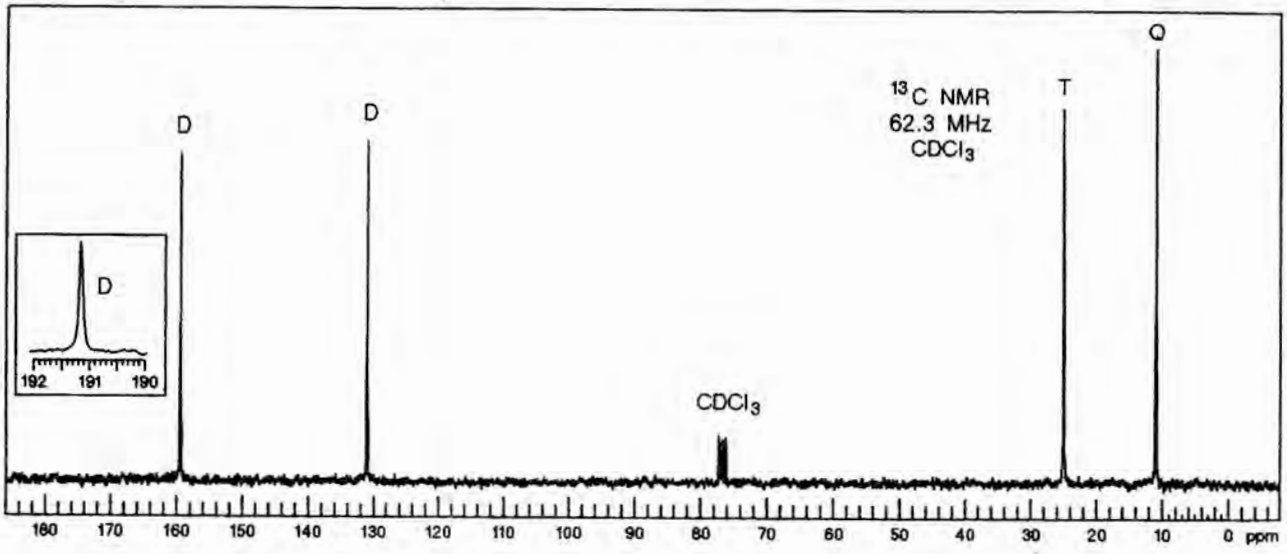
#6 - C_5H_8O

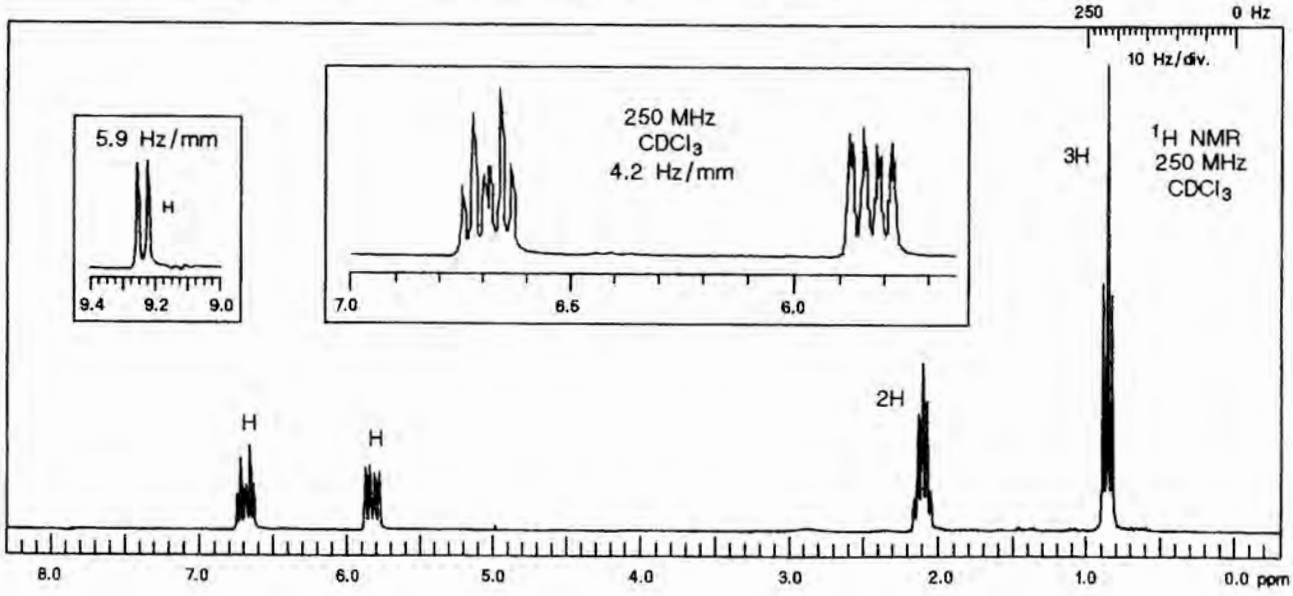


Exact M.S. (EI) = 84.0575

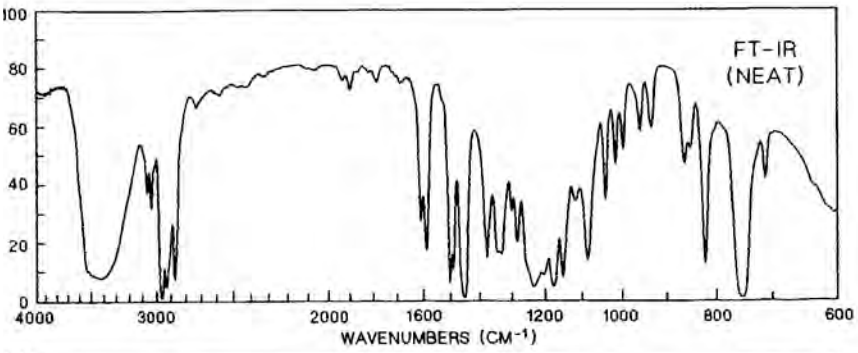
$UV\lambda_{max}$ = 209 (ε = 16,000)
328 (ε = 50)





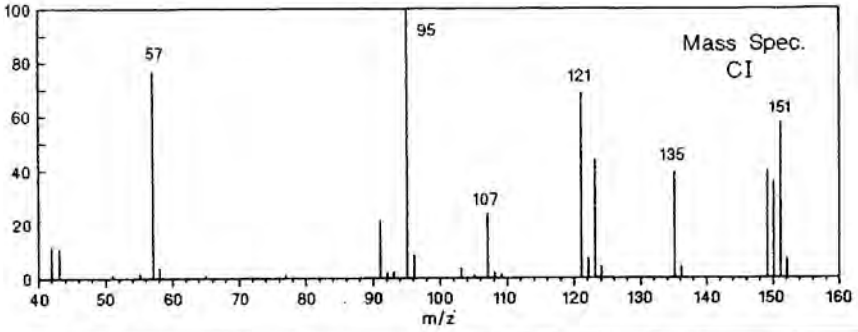


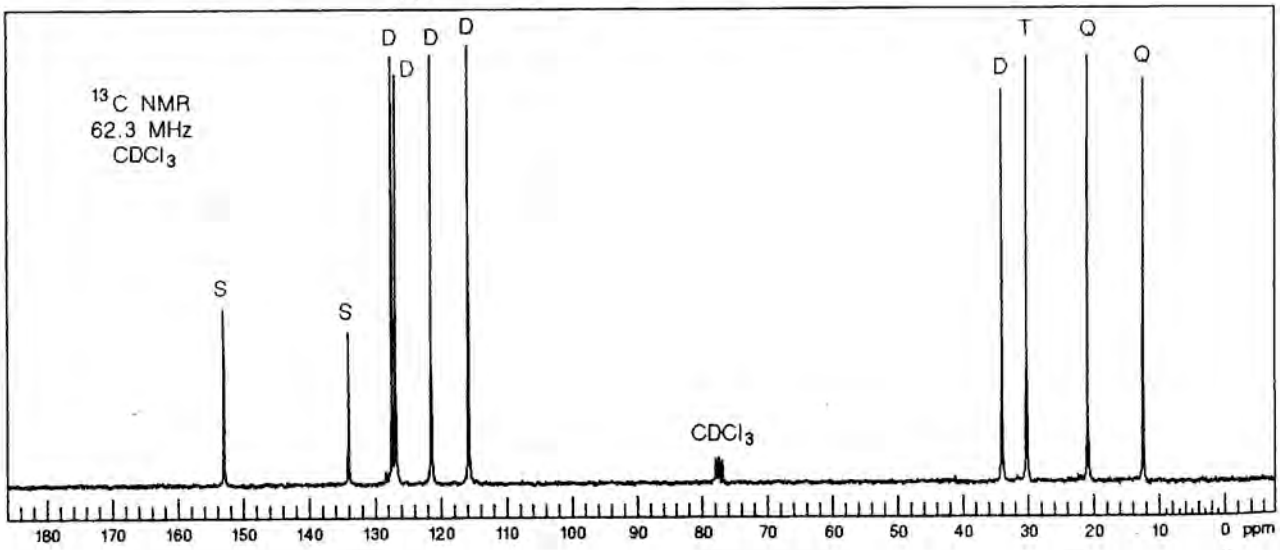
#7 - $C_{10}H_{14}O$

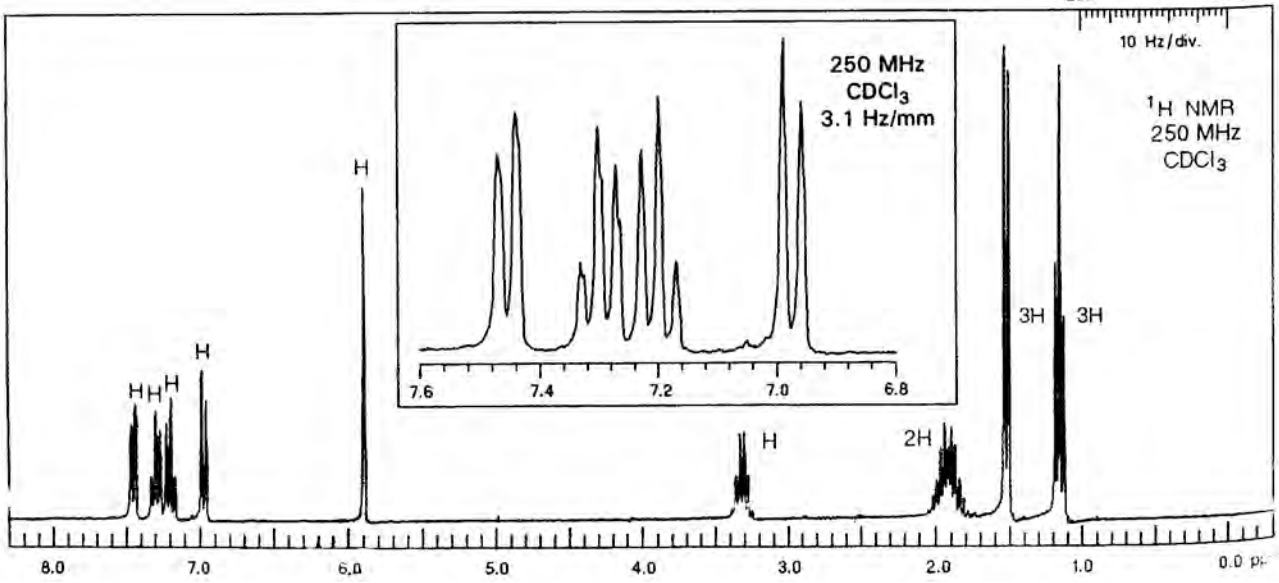


Exact M.S. (CI) = 151.1123

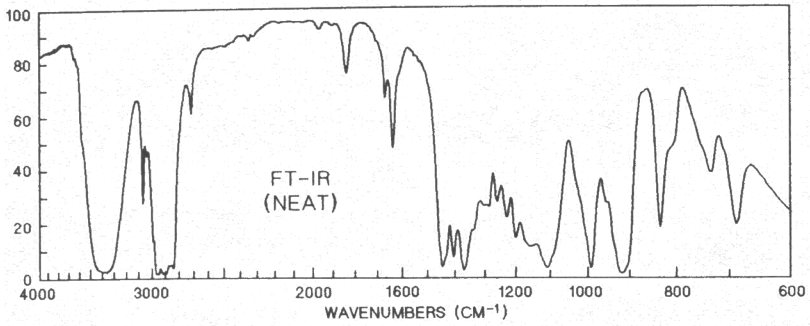
UV λ_{max} = 215 (ε = 6000)
274 (ε = 1500)

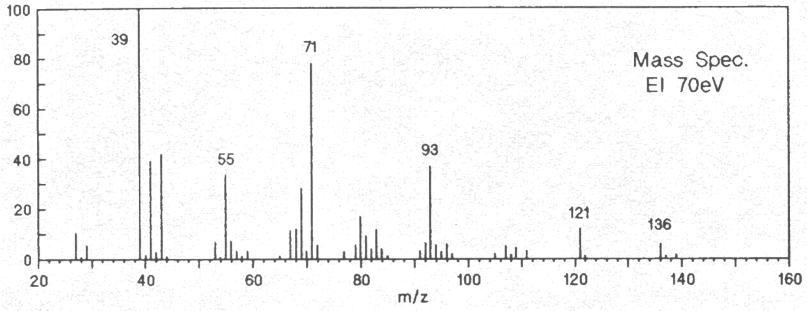


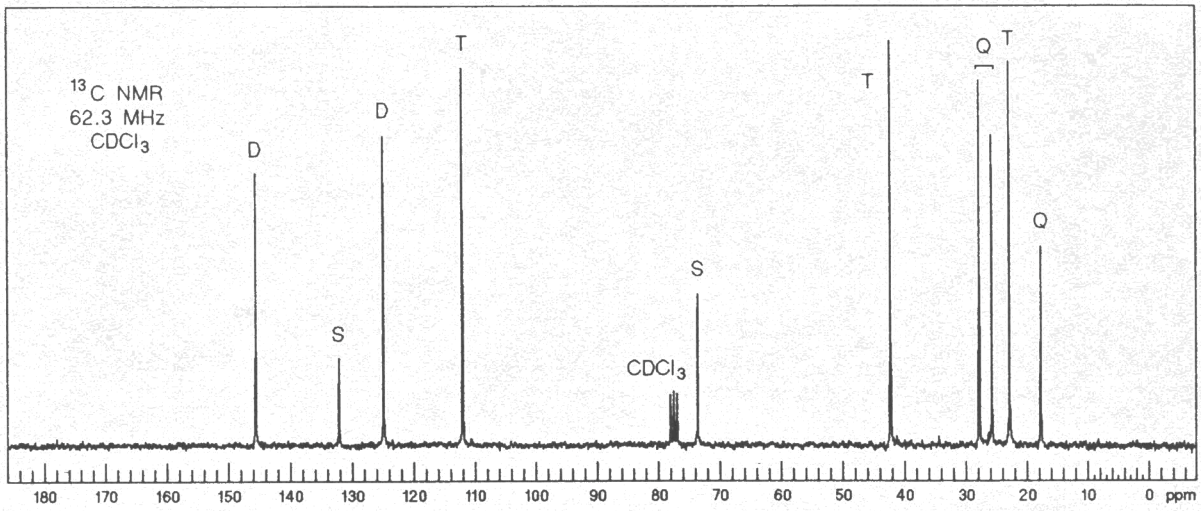


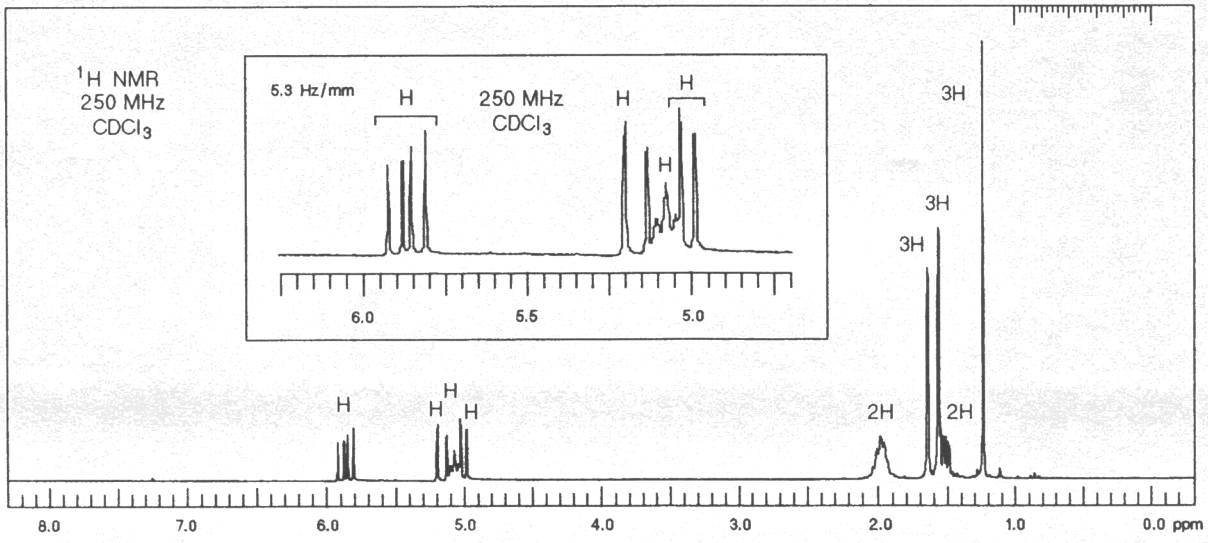


#8 - $C_{10}H_{18}O$

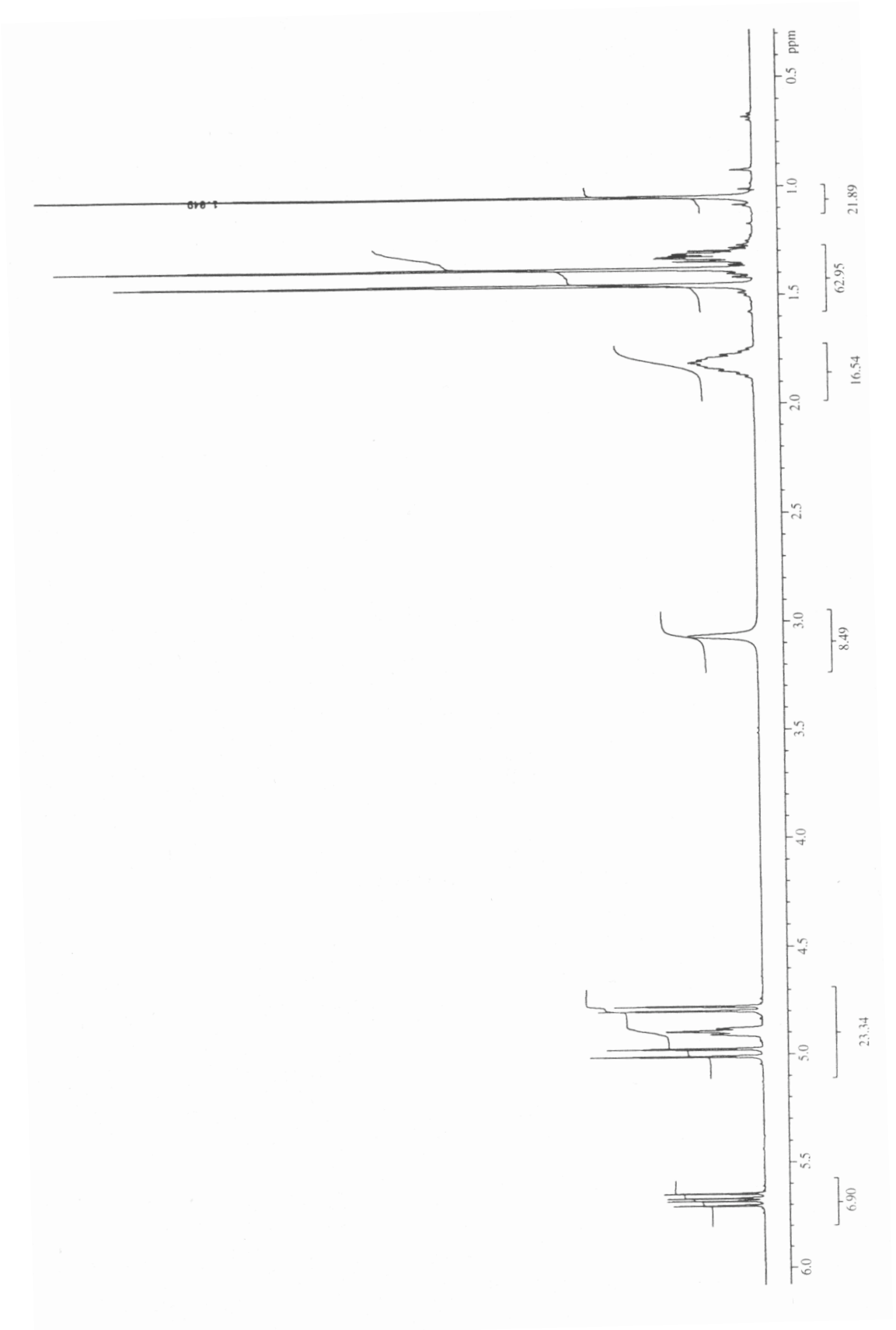

FT-IR
(NEAT)
WAVENUMBERS (CM⁻¹)


Mass Spec.
EI 70eV
m/z

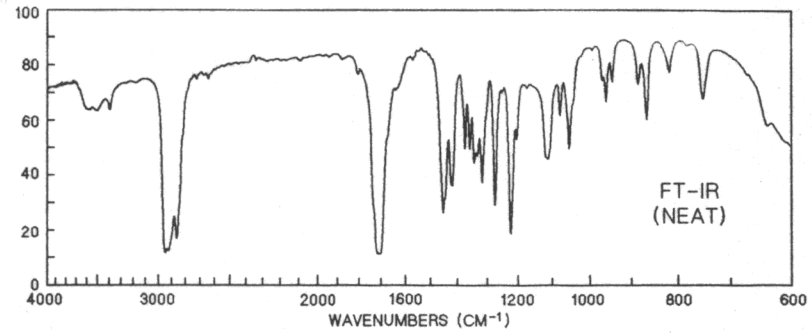

13C NMR
62.3 MHz
CDCl3
ppm


1H NMR
250 MHz
CDCl3
5.3 Hz/mm
ppm

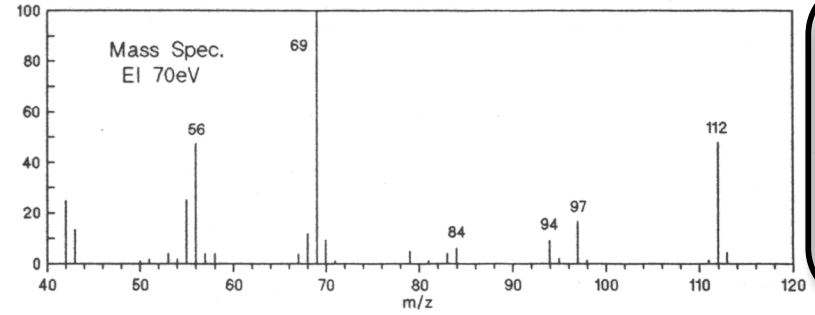
#8 - $C_{10}H_{18}O$ Full Page ^{1}H NMR

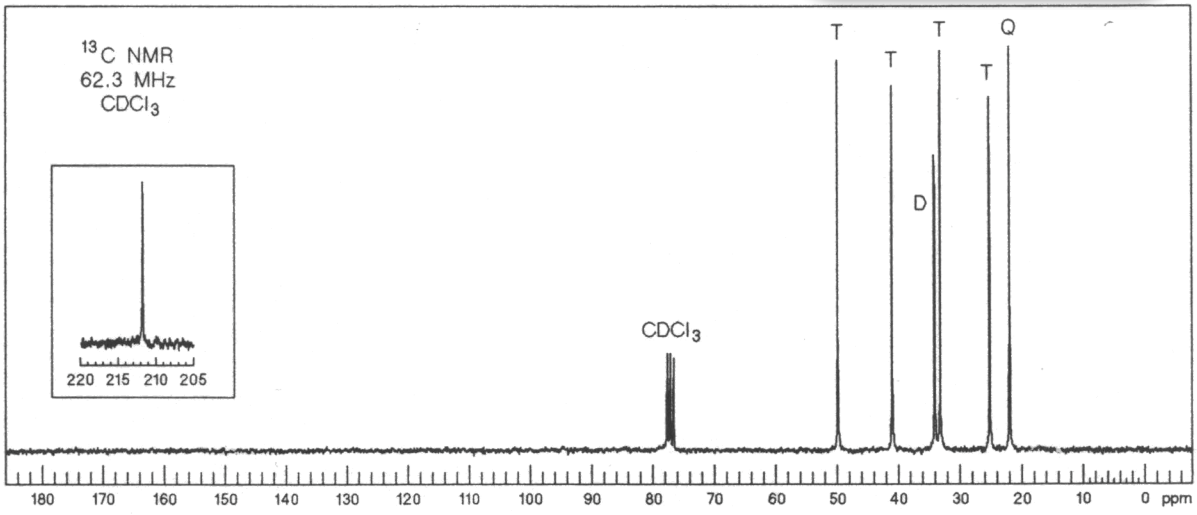


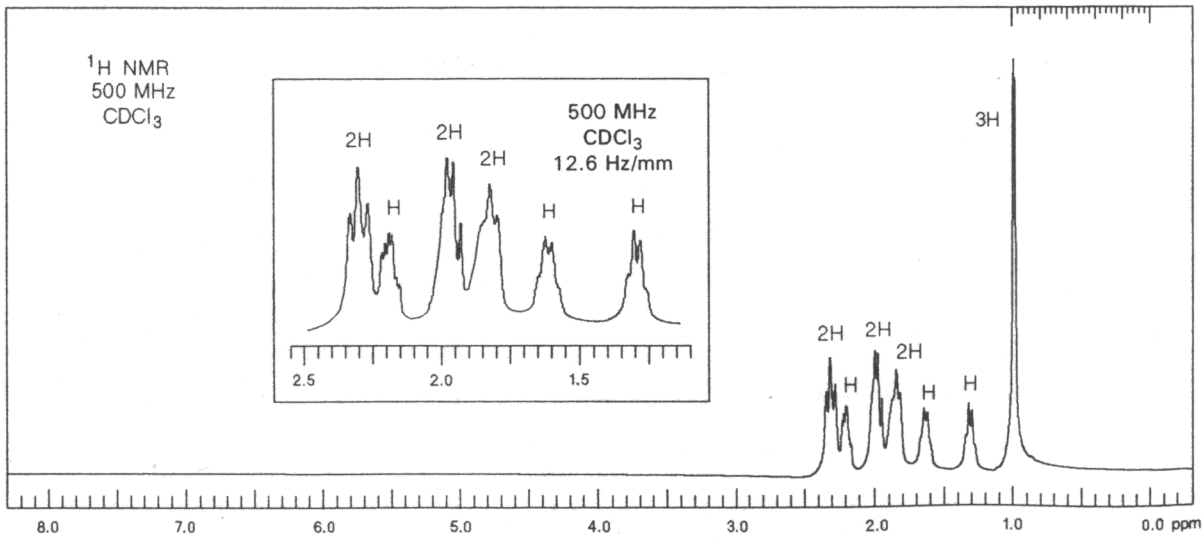
#9 - $C_7H_{12}O$



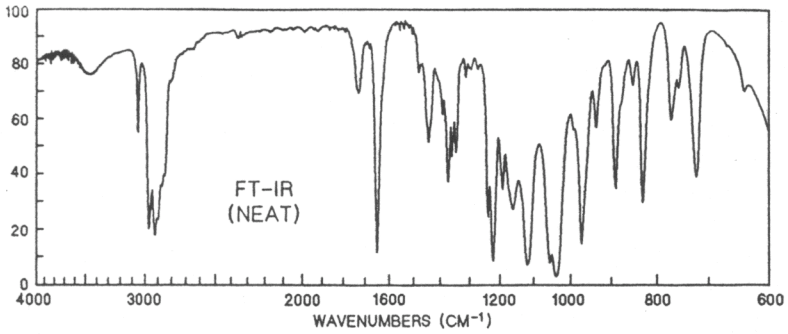
$UV\lambda_{max} = 291\ (\varepsilon = 15)$

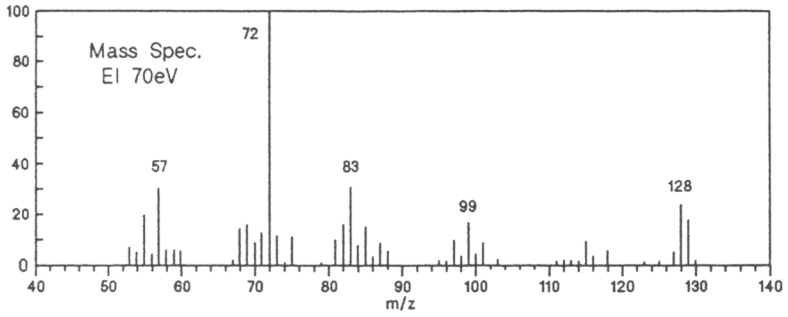


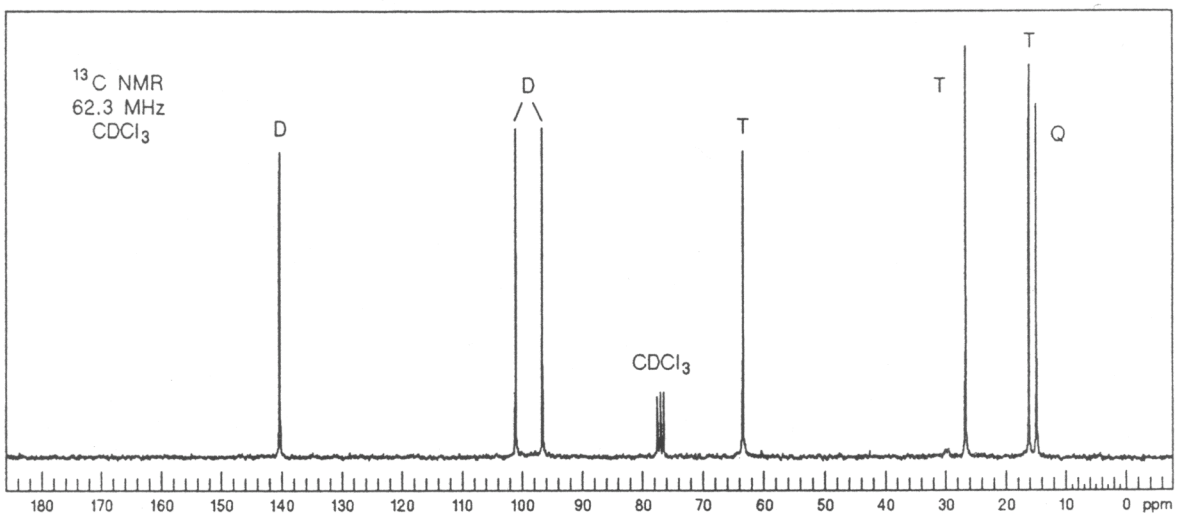


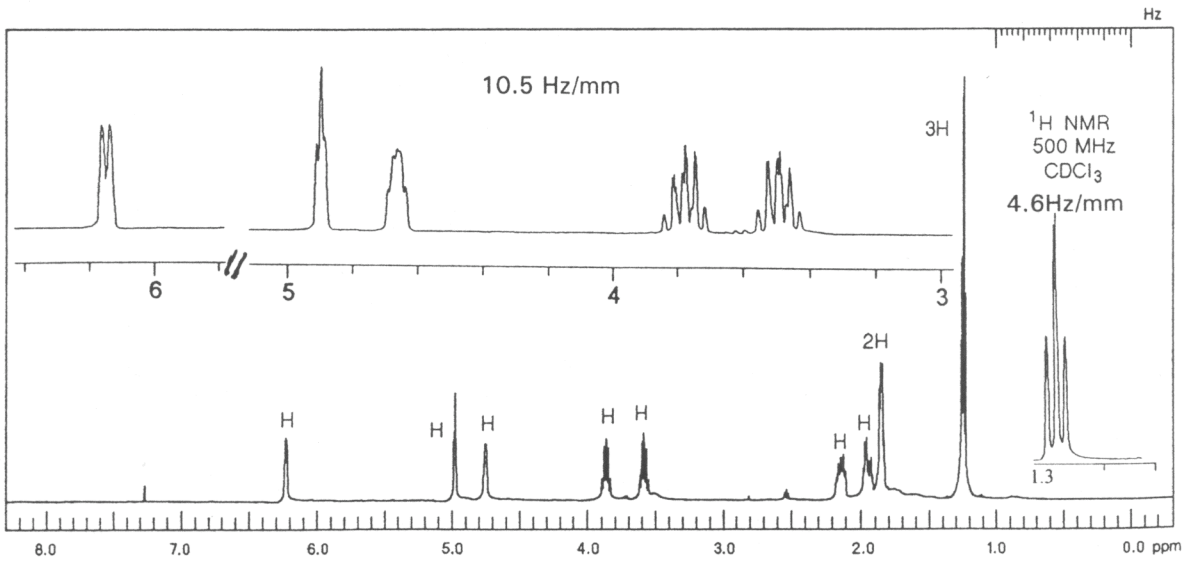


#10 - $C_7H_{12}O_2$


FT-IR
(NEAT)
WAVENUMBERS (CM-1)


Mass Spec.
EI 70eV
72
57
83
99
128
m/z


13C NMR
62.3 MHz
CDCl3
D
D
T
CDCl3
T
T
Q
ppm


Hz
10.5 Hz/mm
3H
1H NMR
500 MHz
CDCl3
4.6Hz/mm
2H
H
H
H
H
H
H
H
1.3
ppm