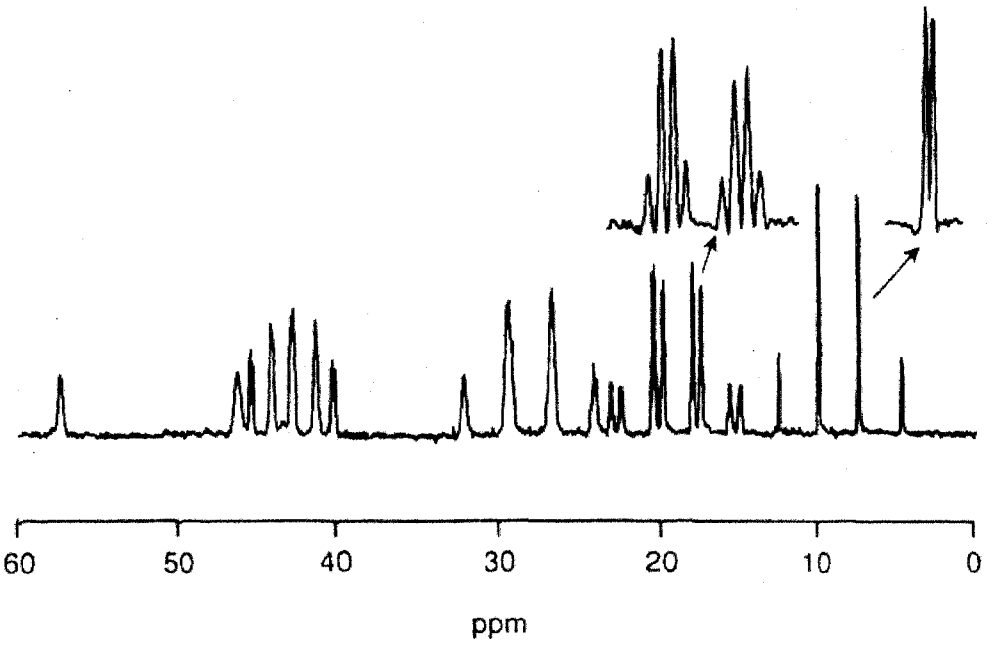
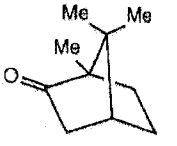
1. 1D Carbon NMR
   - 1D carbon spectrum
   - 1D carbon spectrum (proton decoupled)*
   - APT*
   - DEPT*
2. 2D proton NMR
   - COSY
   - DQF COSY*
   - long-range COSY
   - TOCSY
3. 2D carbon NMR
   - INADEQUATE
4. 2D proton-carbon NMR*
   - HMQC
   - HMQC (proton-decoupled)*
   - multiplicity-edited HSQC*
   - HMBC*
   - HSQC
   - HETCOR
5. The rest
   - 1D analogues
   - macromolecules, solids, multinuclear

1D Carbon NMR

1D spectrum

•high information content but low resolution and sensitivity



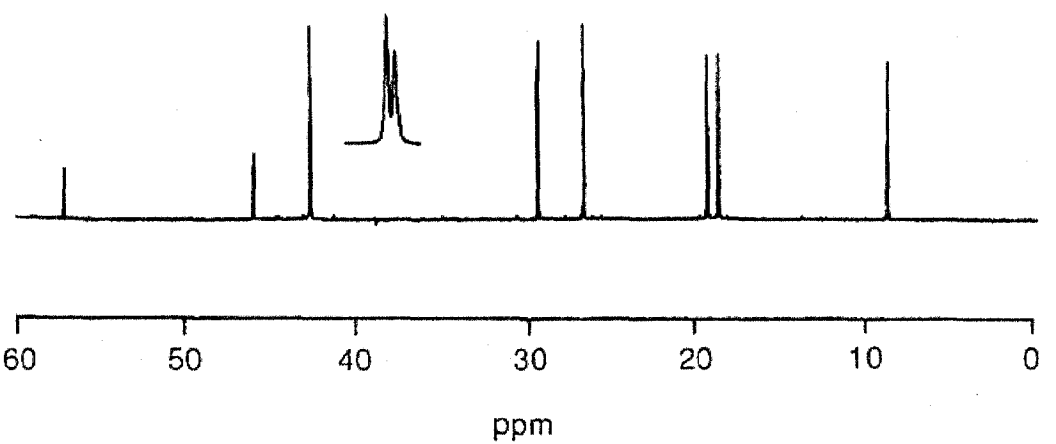


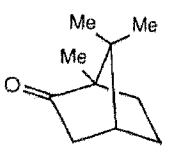
•spectrum reproduced from *Modern NMR Spectroscopy*, by Sanders and Hunter

1D Carbon NMR

proton-decoupled 1D spectrum

•high resolution and sensitivity but lower information content

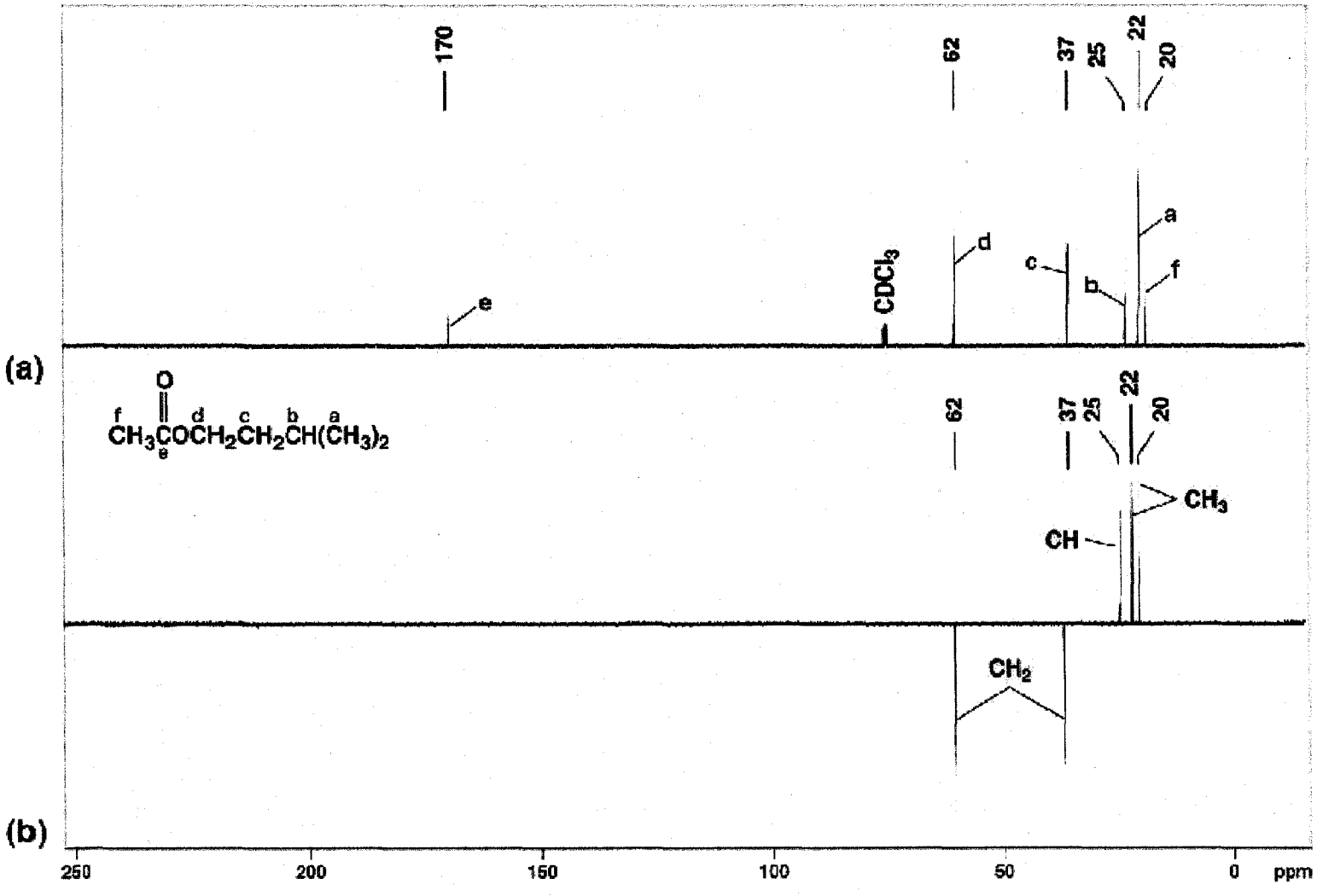




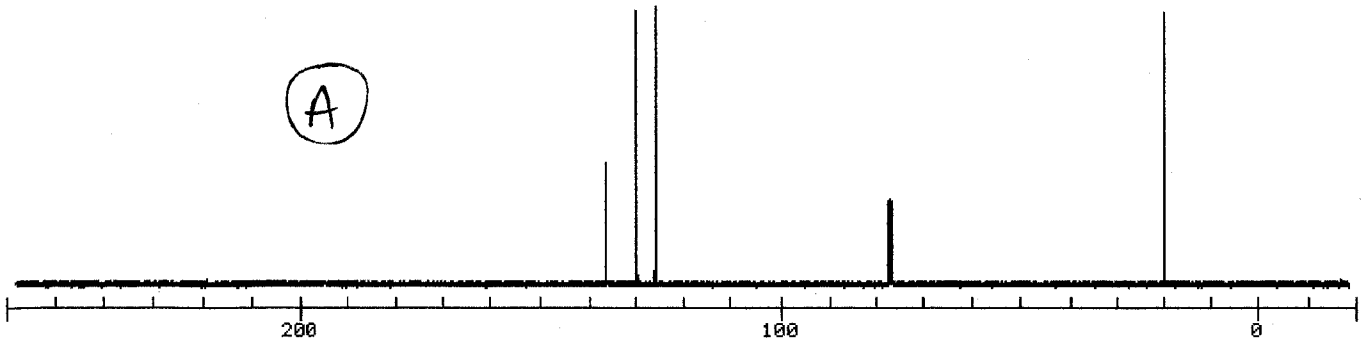
•spectrum reproduced from *Modern NMR Spectroscopy*, by Sanders and Hunter

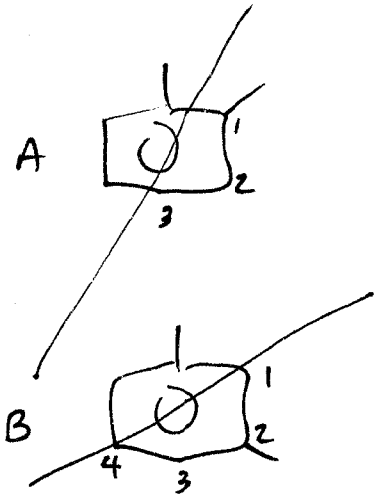
Isopentyl acetate

- 13C-NMR: (a) proton decoupled and (b) DEPT

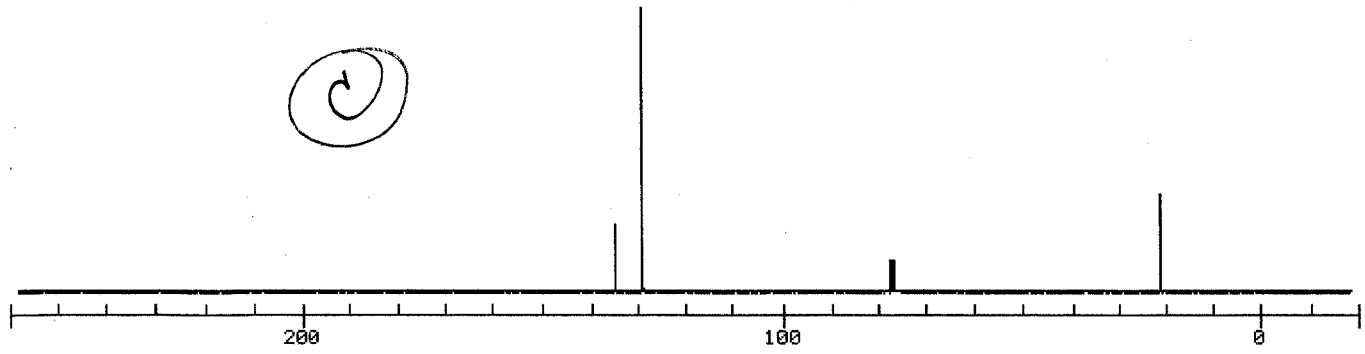


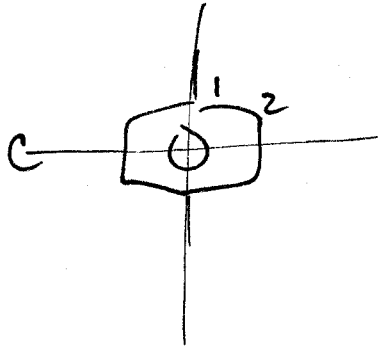
Same formula, different isomer. ^{13}C NMR.





Same formula, yet another isomer. ^{13}C NMR.

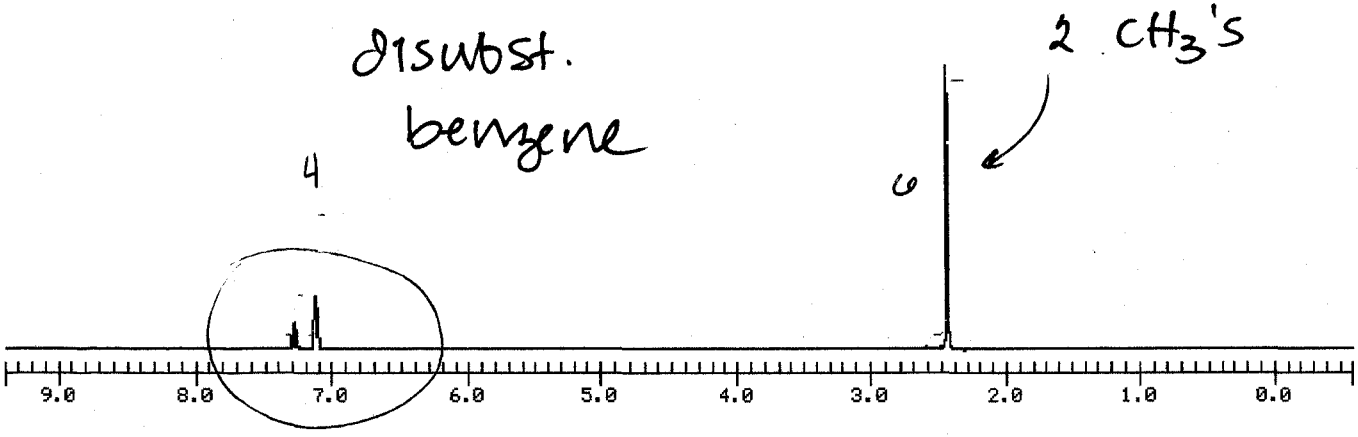




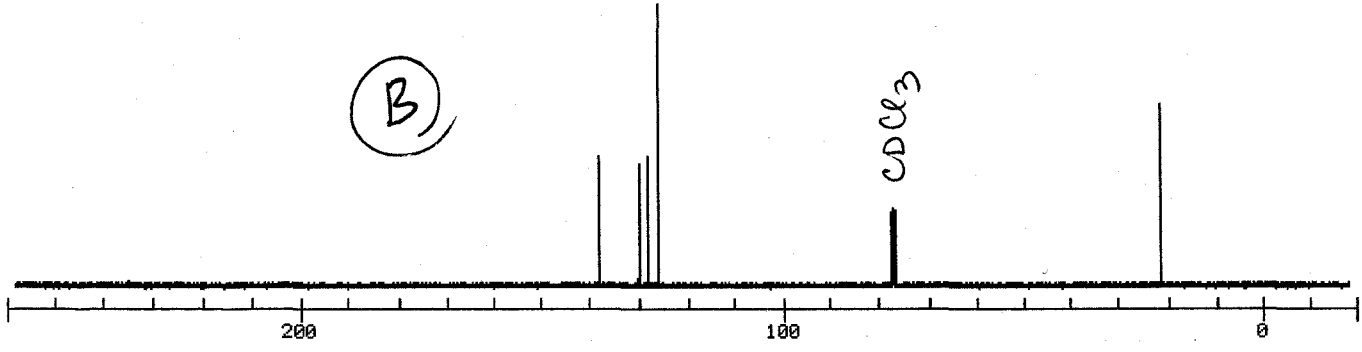
C_8H_{10} **SODAR = 4**

C_8H_{10}

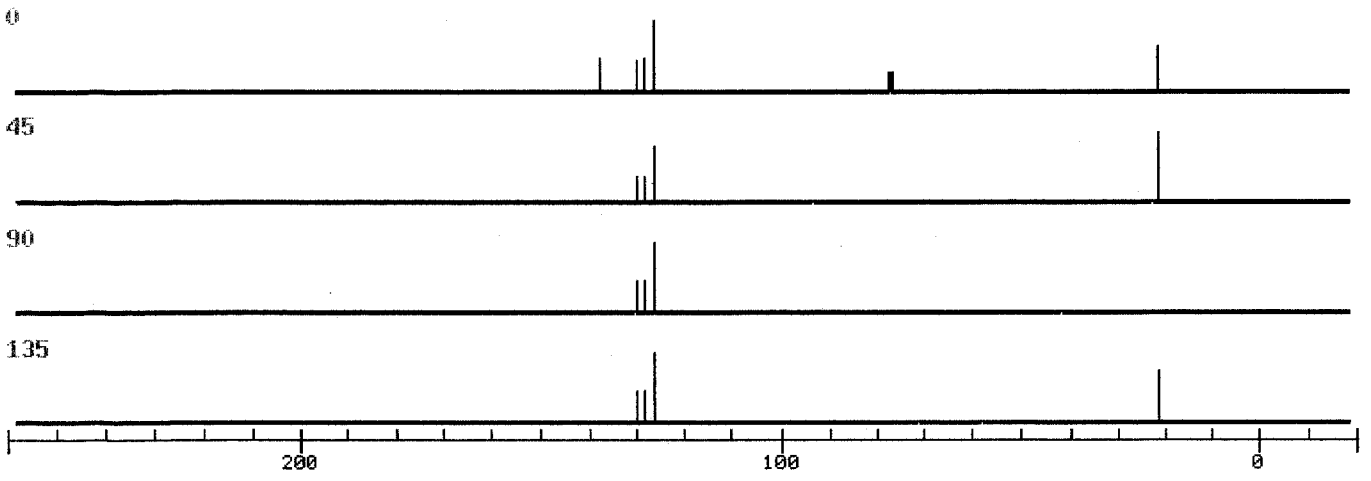
^{1}H NMR



^{13}C NMR



DEPT spectra



standard ^{13}C NMR

all C's w/ H's

CH

CH, CH_3 point up

CH_2 points down

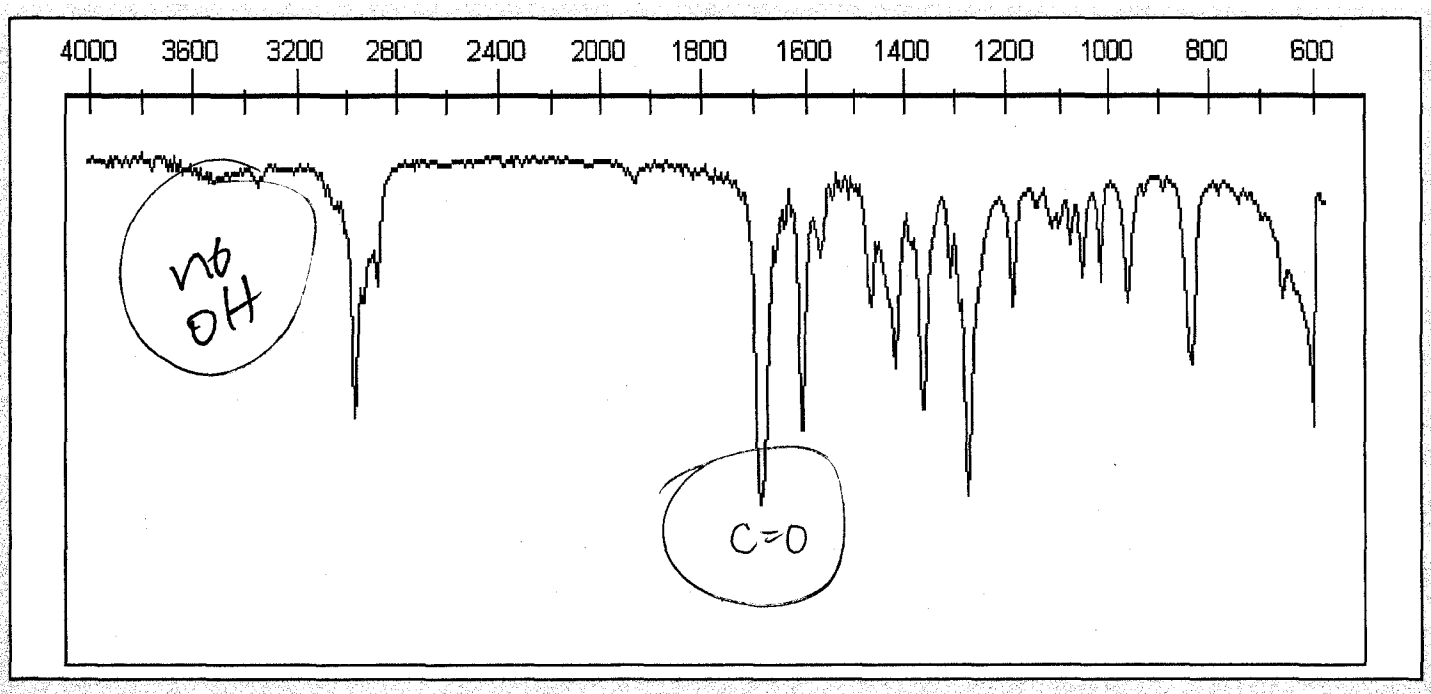
C_q do not appear in DEPT.

CH are positive in 90 + 135

CH_2 do not appear in 90; are negative in 135

CH_3 do not appear in 90; are positive in 135

All C's with H's appear in 45.



IR Spectrum

NMR Spectrum

Show Integration

Compound Name:
UNKNOWN #1

Analytical Data:
81.44 %C 8.70 %H

~~Molecular Formula:~~

9.86 9.86 0

Molecular Mass:
162.23

Notes

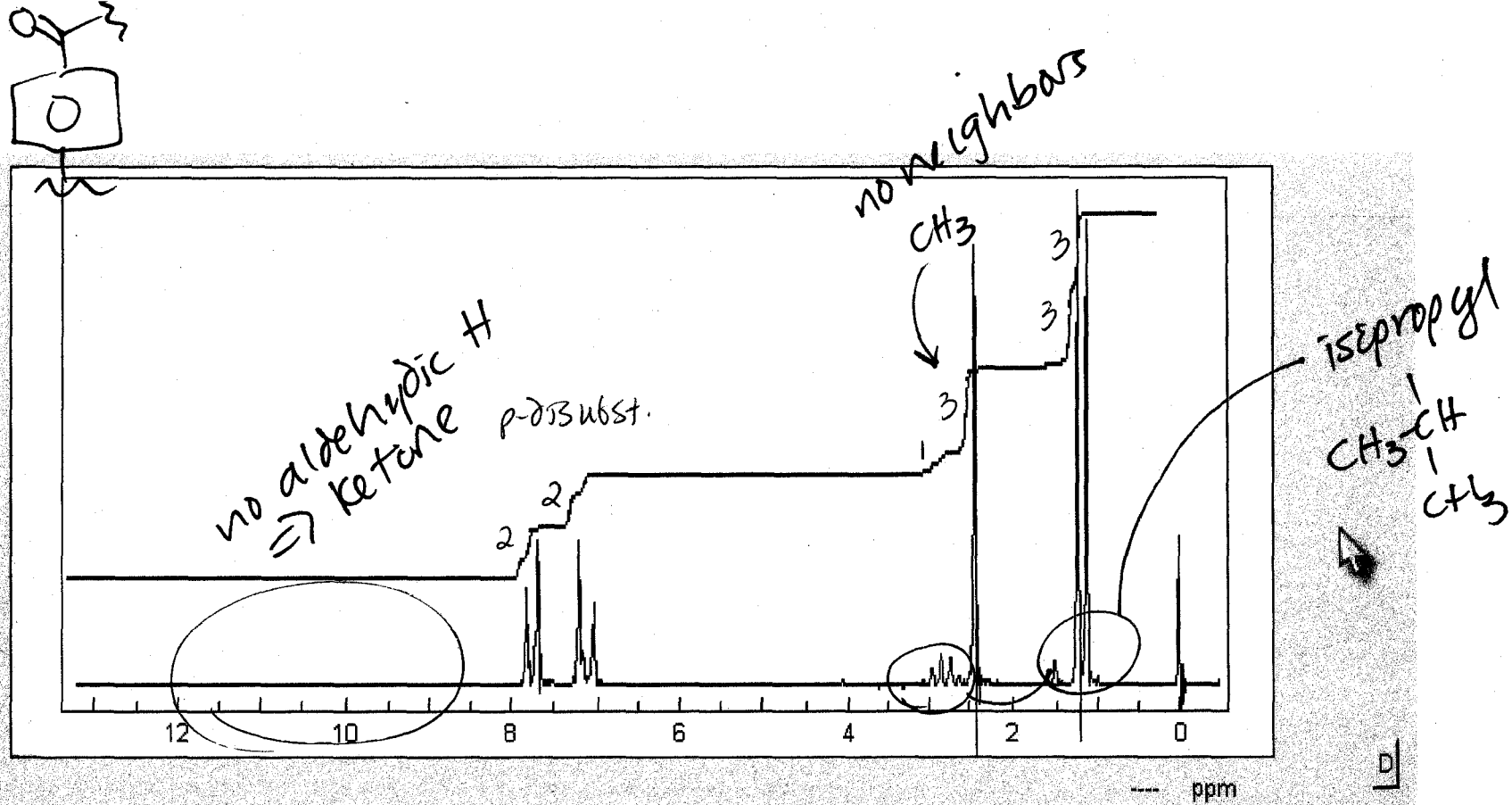
suspect benzene
C=O probably
a ketone

Show Structure | Add Label | Remove Labels

81.44 : 8.70 : 9.86
÷12 ÷1 ÷16
6.79 : 8.70 : 0.62
11 14 1

$C_{11}H_{14}O$

SODAR = 5



IR Spectrum

NMR Spectrum

Show Integration

Compound Name:
UNKNOWN #1

Analytical Data:
81.44 %C 8.70 %H

Molecular Formula:

9.84% O

Molecular Mass:
162.23

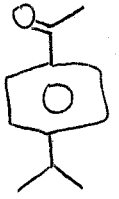
Notes

Show Structure | Add Label | Remove Labels

6.79 : 8.70 : 0.62

11 14 1

$C_{11}H_{14}O$ SODAR = 5



Chapter 14 - Aromatics

original aromatic: benzene C_6H_6 SOAR = 4.

"aromatic" means a compound whose structure + reactivity are similar to that of benzene.

All of these have at least one double bond.
Double bonds generally undergo addition rxns.

Reagent	Expect	Observe	Conclude
Br_2/CCl_4	decolorization (addition of Br_2)	NRX	benzene is very stable + unreactive
aq. $KMnO_4$	color change make vicinal diol	NRX	
H_2/cat.	fast rxn - add H_2 → alkane	slow rxn.	

If we force the rxn....

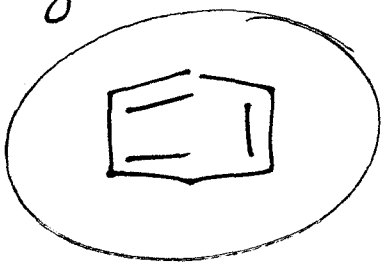
$C_6H_6 \xrightarrow[FeBr_3]{Br_2} C_6H_5Br$

substitution, not addition!

↑ only one product.

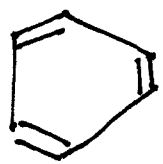
Go back to our possible structures- how many types of H do they each have?

Benzene must be extremely symmetrical.



structure proposed by Kekulé (1866)

we would expect two different bond lengths.



In fact, they are all the same

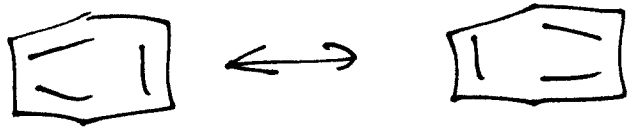
"Normal" C-C : 1.54 Å

Benzene bonds: 1.39 Å

"Normal" C=C : 1.34 Å

Benzene bonds are somewhere in between.

Why? Resonance



these are completely equivalent.

Resonance hybrid:  planar, hexagonal.

* If you're writing a mechanism - you must use a Kekulé structures. Why? mechanism show the movement of e's - you have to "localize" them.