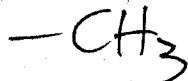


Useful numbers to know for ^1H -NMR

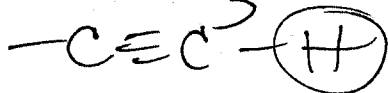
ppm

group

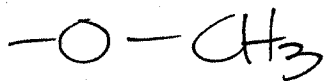
1



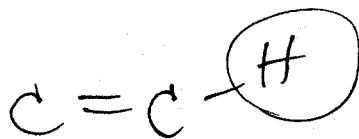
3



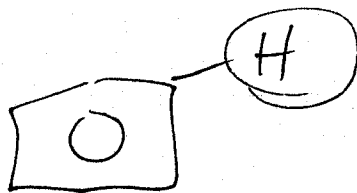
4



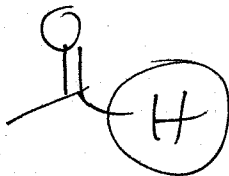
5



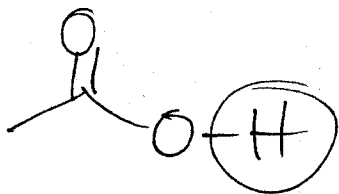
7



9



12



Types of NMR Instruments

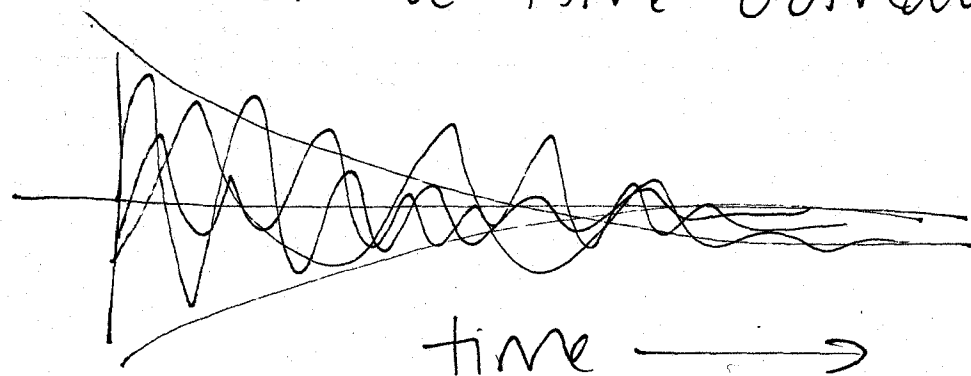
CW - Continuous wave - scans through RF one at a time - chart output goes along w/ frequency scan.

- not very sensitive (requires concentrated samples)

- usual mode for 60 MHz machines.

FT - Fourier transform - need a computer!

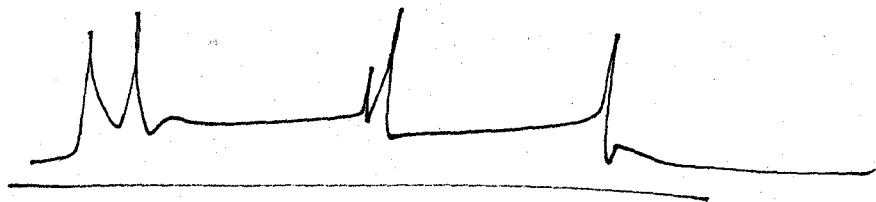
hit sample w/ pulse containing all freq's.
collect a time-domain spectrum - FID



lots of superimposed sine waves - one for each type of H.

computer does the FT

time domain \rightarrow frequency domain



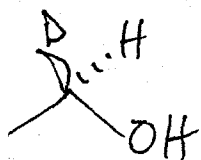
- very sensitive / high resolution
- can use dilute sample

"Equivalencies" of protons

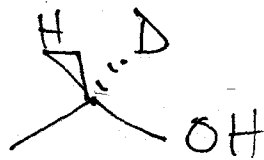
1. homotopic $\left\{ \begin{array}{l} \text{chemically equiv.} \\ \text{chemical-shift equiv.} \end{array} \right.$

ex. CH_3 in $\text{CH}_3\text{CH}_2\text{OH}$

2. enantiotopic - ex. CH_2 in $\text{CH}_3\text{CH}_2\text{OH}$

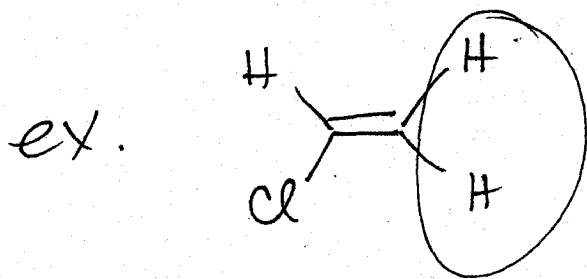


vs.



still chemical-shift equiv.
under normal (achiral) NMR
conditions.

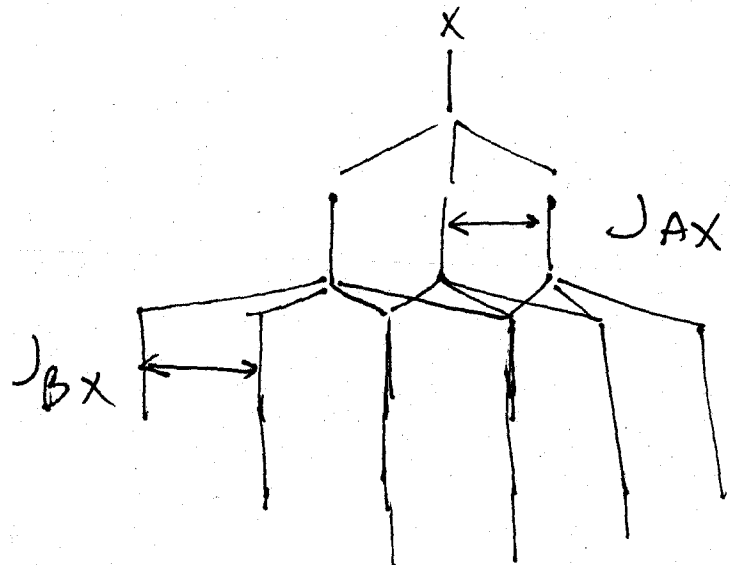
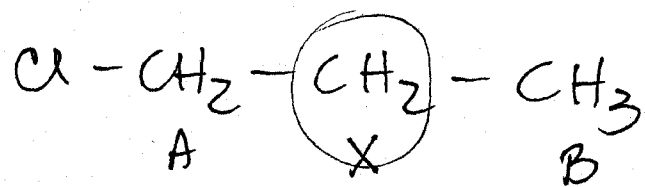
3. diastereotopic - replacing each of the
protons in tom generates diastereomers.



these are not
chemical-shift equiv.
show up in different
places in NMR.

-also can conceivably split each other.

Recall $n+1$ rule - only works when all the
coupling constants (J values) are about
the same.



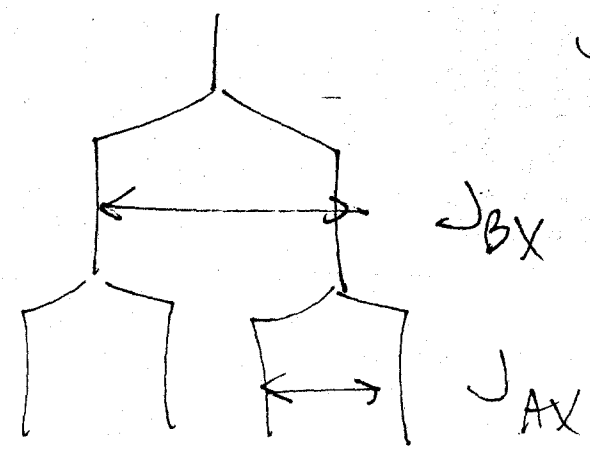
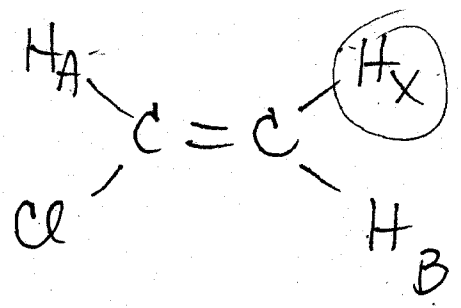
$n+1$ says:

5 neighbors \Rightarrow 6 lines

Because $J_{AX} \approx J_{BX}$

the lines overlap
wind up w/ 6 lines

What if $J_{AX} \neq J_{BX}$?



$J_{AX} \ll J_{BX}$

SKIP

9.12 2D NMR

9.13 → 9.18 mass spec

9.10 Rate Processes

9.11 - ^{13}C NMR $\sim 0.1\%$ of C's

⇒ no spin-spin splitting
(chances of having adjacent ^{13}C 's
is slim to none)

⇒ no integrals

(see handout
on blackboard)

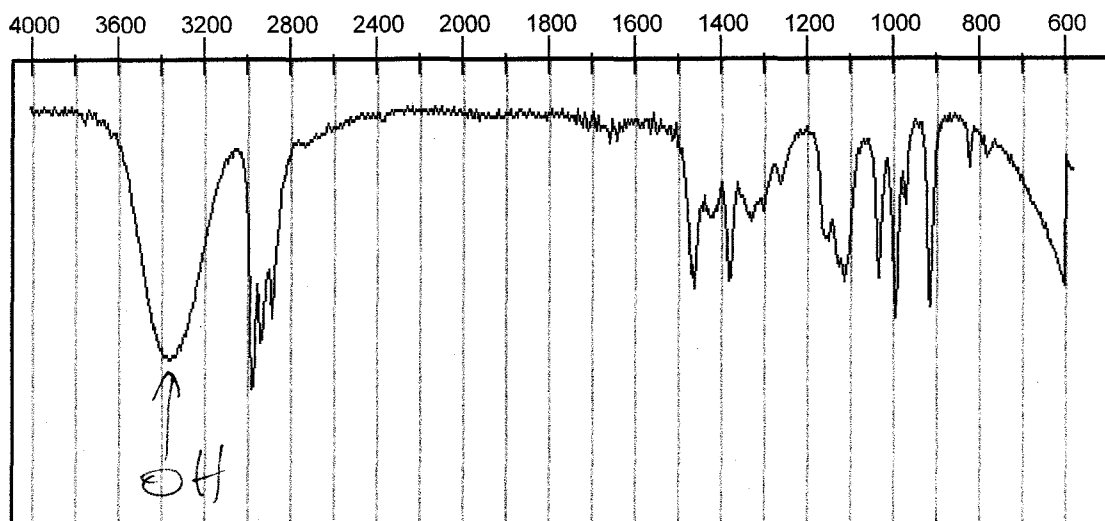
scale 0 → 200 ppm

Spectral Interpretation

MHS

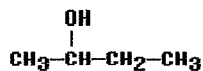
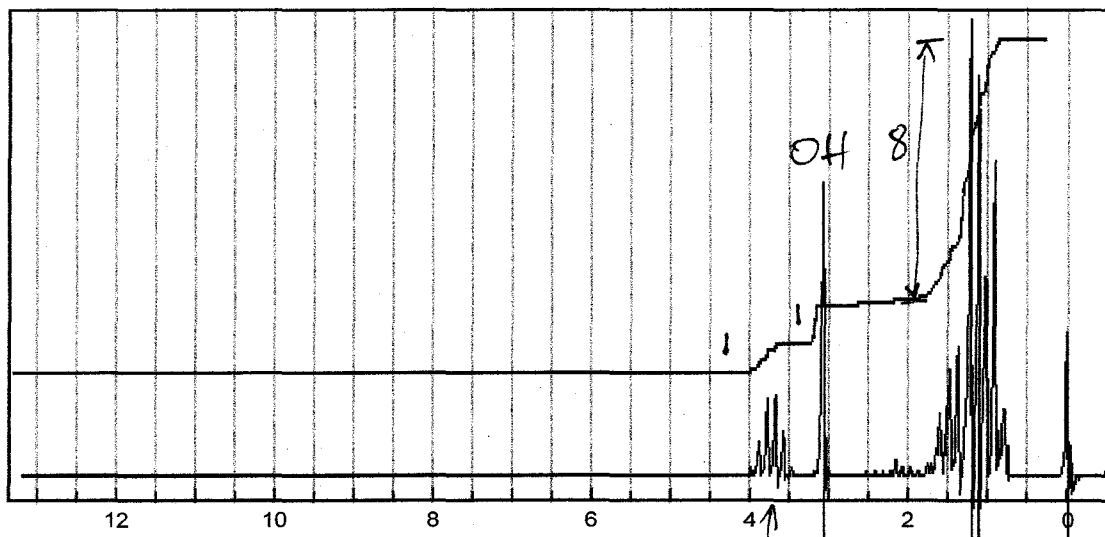
Dec 01 2008

Known Compound: 2-butanol

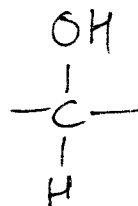


Formula: $C_4H_{10}O$

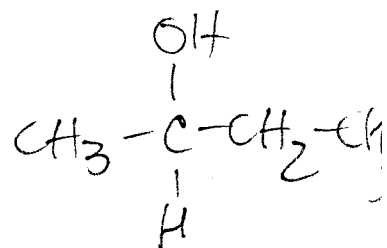
SODAR = \emptyset { no rings
no π bonds



has the
OH



6 lines
5 neighbors
 $CH_3 + CH_2$

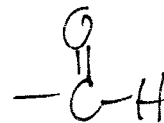
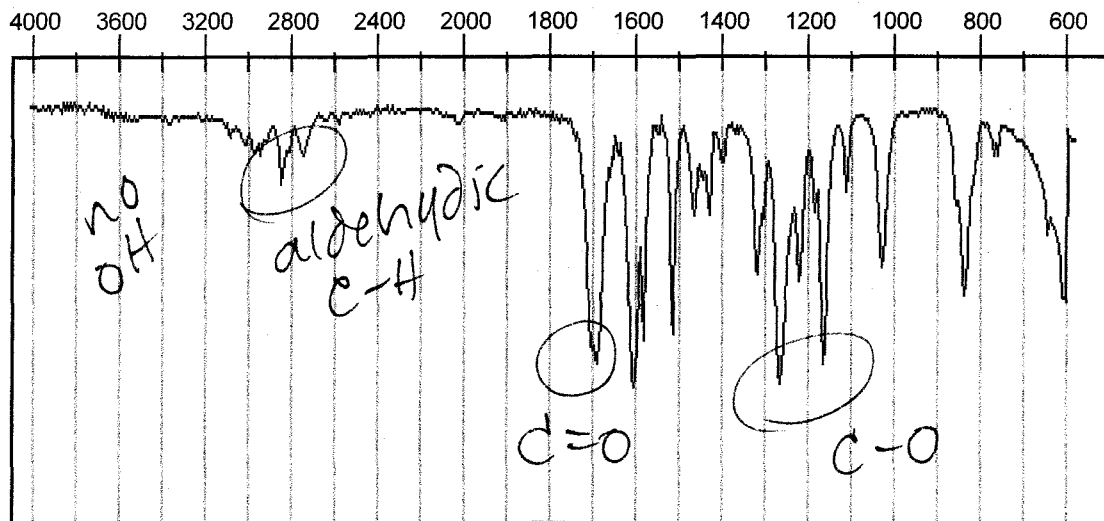


Spectral Interpretation

MHS

Dec 01 2008

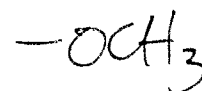
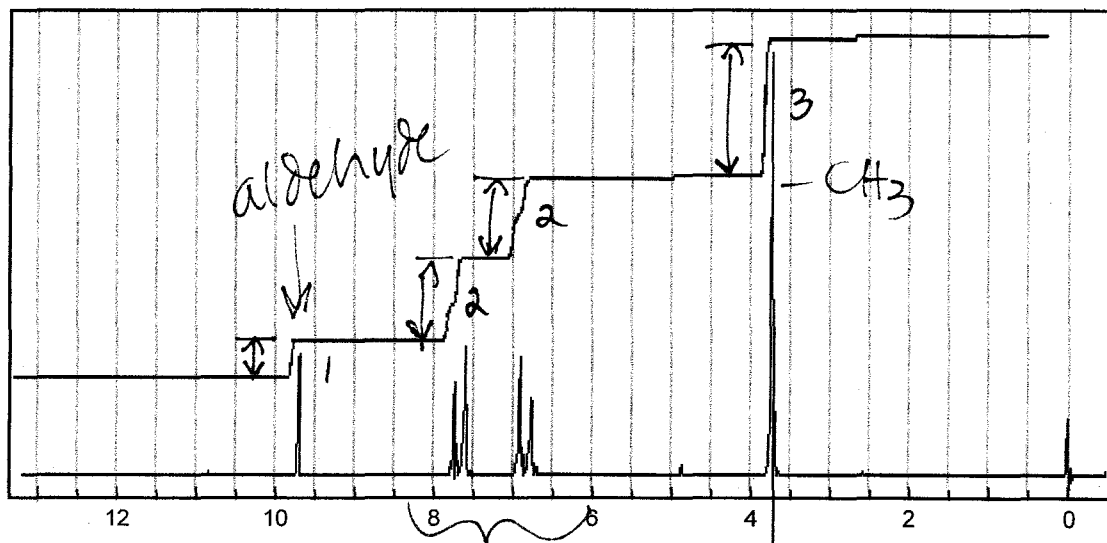
Known Compound: 4-methoxybenzaldehyde



Formula: $\text{C}_8\text{H}_8\text{O}_2$

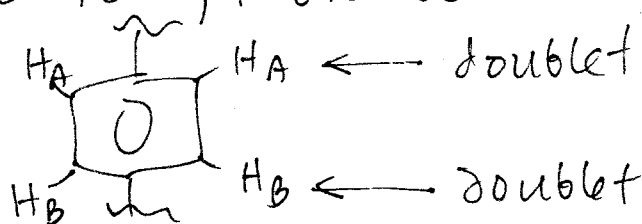
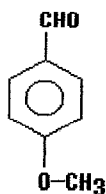
SODAR = 5

think aromatics



disubst benzene

this is 1,4 disubst.

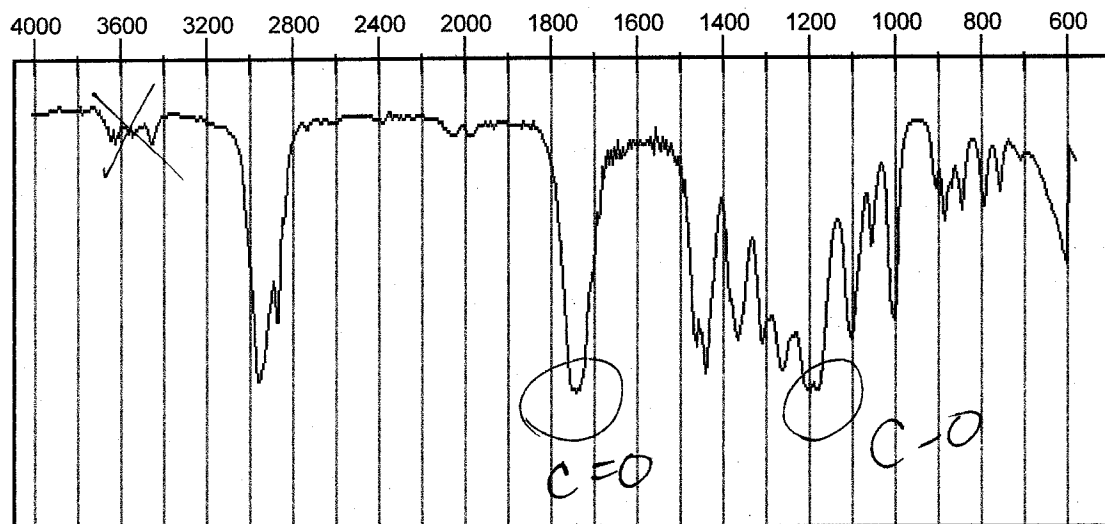


Spectral Interpretation

MHS

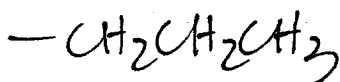
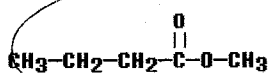
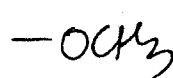
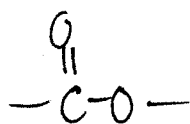
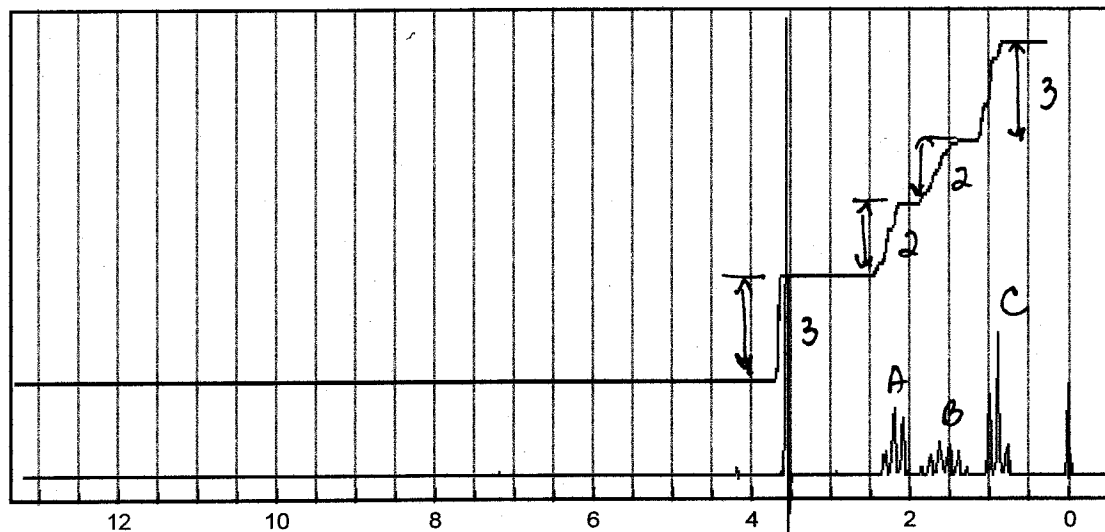
Dec 01 2008

Known Compound: methyl butanoate



probably
an
ester

Formula = $C_5H_{10}O_2$ SODAR = 1



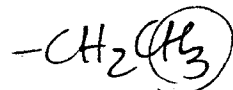
$-OCH_3$ no neighbors
+ downfield so near
the O

A: CH_2 w/ 2 neighbors
 $-(CH_2)CH_2-$

B: CH_2 w/ 5 neighbors



C: CH_3 w/ 2 neighbors

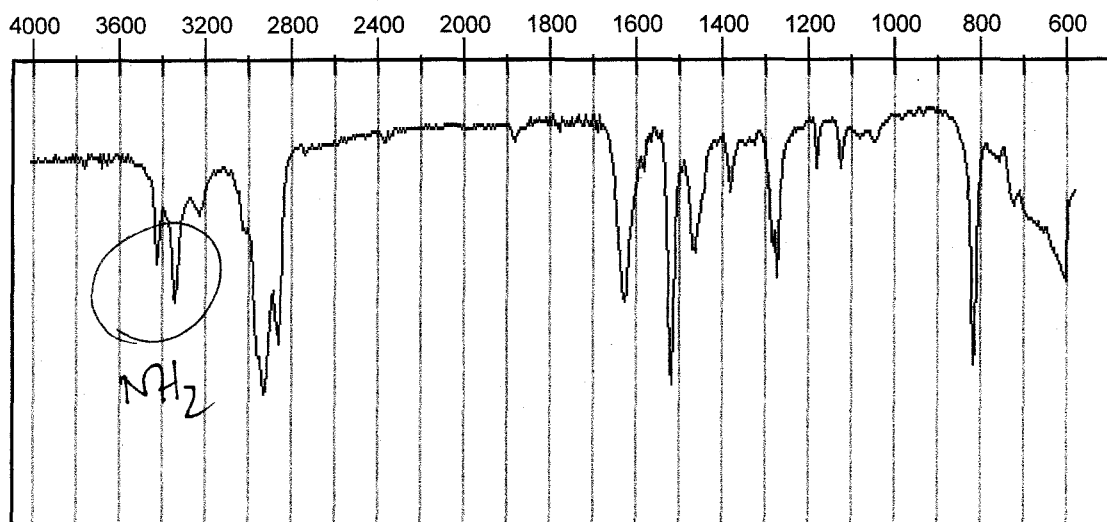


Spectral Interpretation

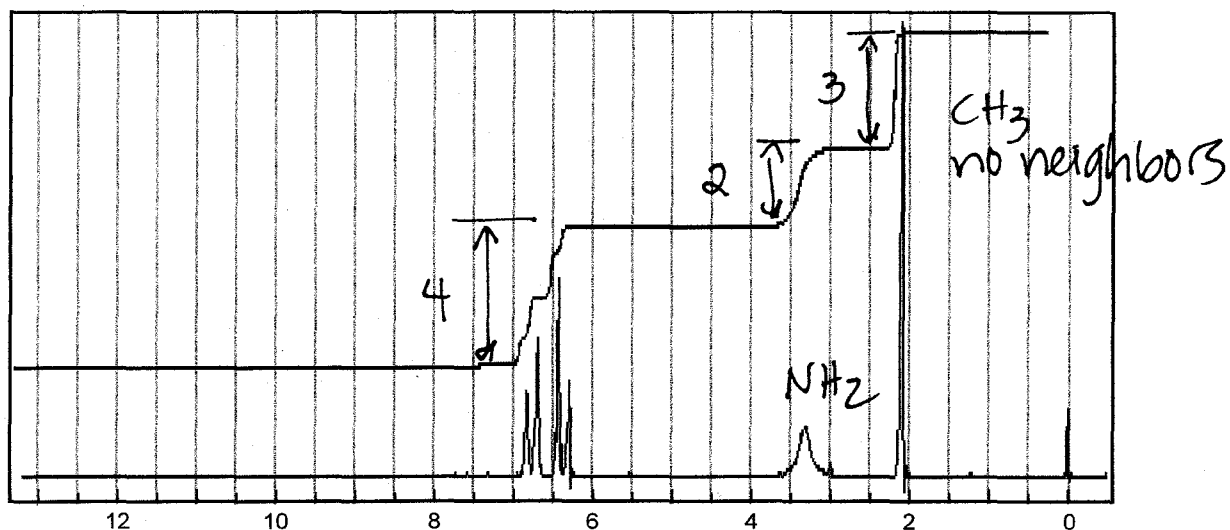
MHS

Dec 01 2008

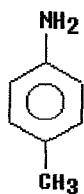
Known Compound: p-toluidine



Formula: C_7H_9N SODAR = 4



1,4 disubst aromatic



Fragments: $-CH_3$
 $-NH_2$

