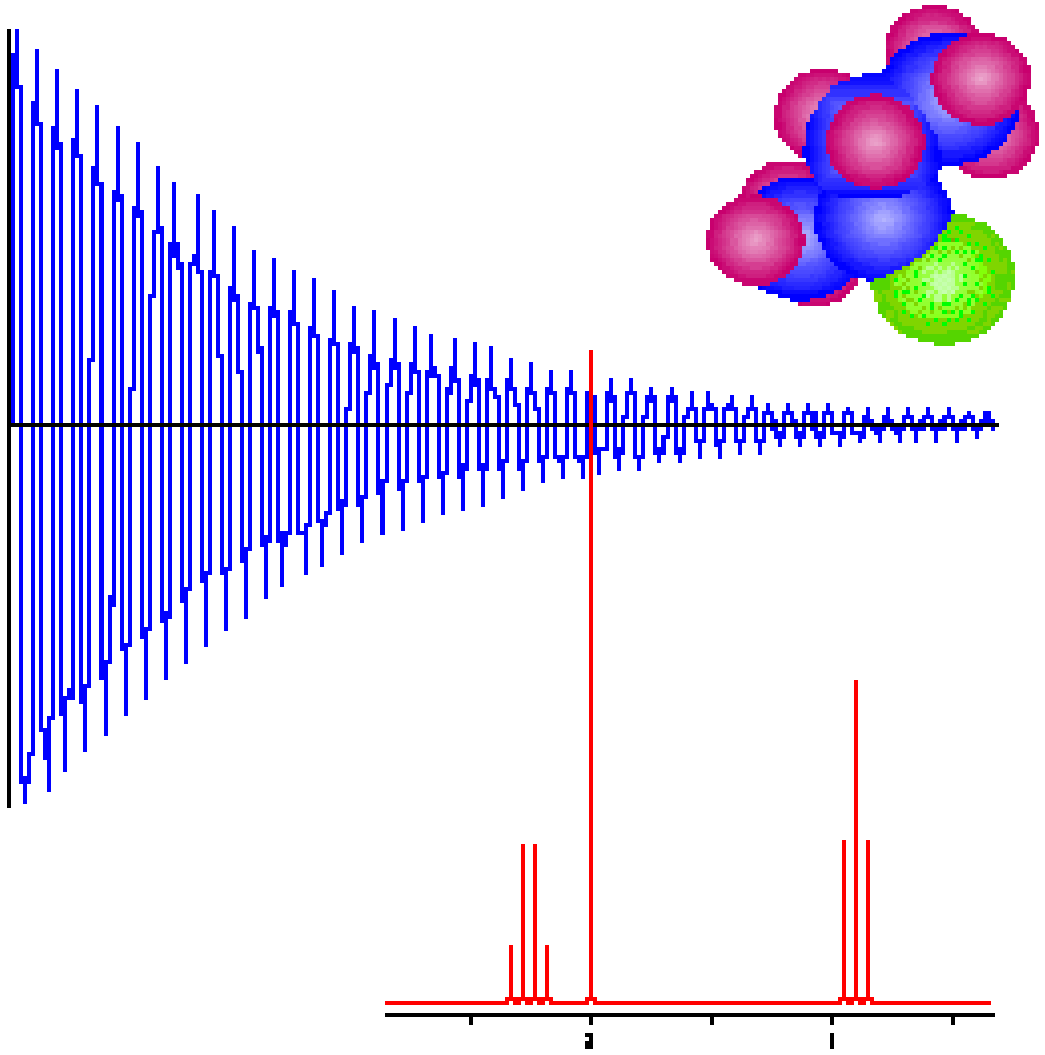
Proton NMR Spectroscopy



Introduction to ^{1}H NMR

nuclear magnetic resonance (NMR) is a spectroscopy technique which is on the absorption of EMR from the radiofrequency region 4 to 900 MHz by nuclei of the atom.

Two types:

^{1}H-NMR (proton nuclear magnetic resonance)

Gives information about the number and type of (H-atoms) in the molecule

e.g. CH_3CH_2OH contain 3 types of (H-atoms) and they are adjacent to each other and their ratio 3:2:1

^{13}C-NMR

Introduction to ^{1}H NMR

proton nuclear magnetic resonance spectroscopy is one of the most powerful tools for elucidating the number of hydrogen or proton in the compound.

N.B.

mass number (M) is the total number of protons and neutrons)

Atomic number is the number of electrons and gives information about the reactivity of atom

Spin Quantum number (I):

It is the spin which created in atoms or molecules due to continuous movement of electrons and neutrons.

Which nuclei have a “spin”?

- If mass # and atomic # are both even, I = 0 and the nucleus has **no spin**.

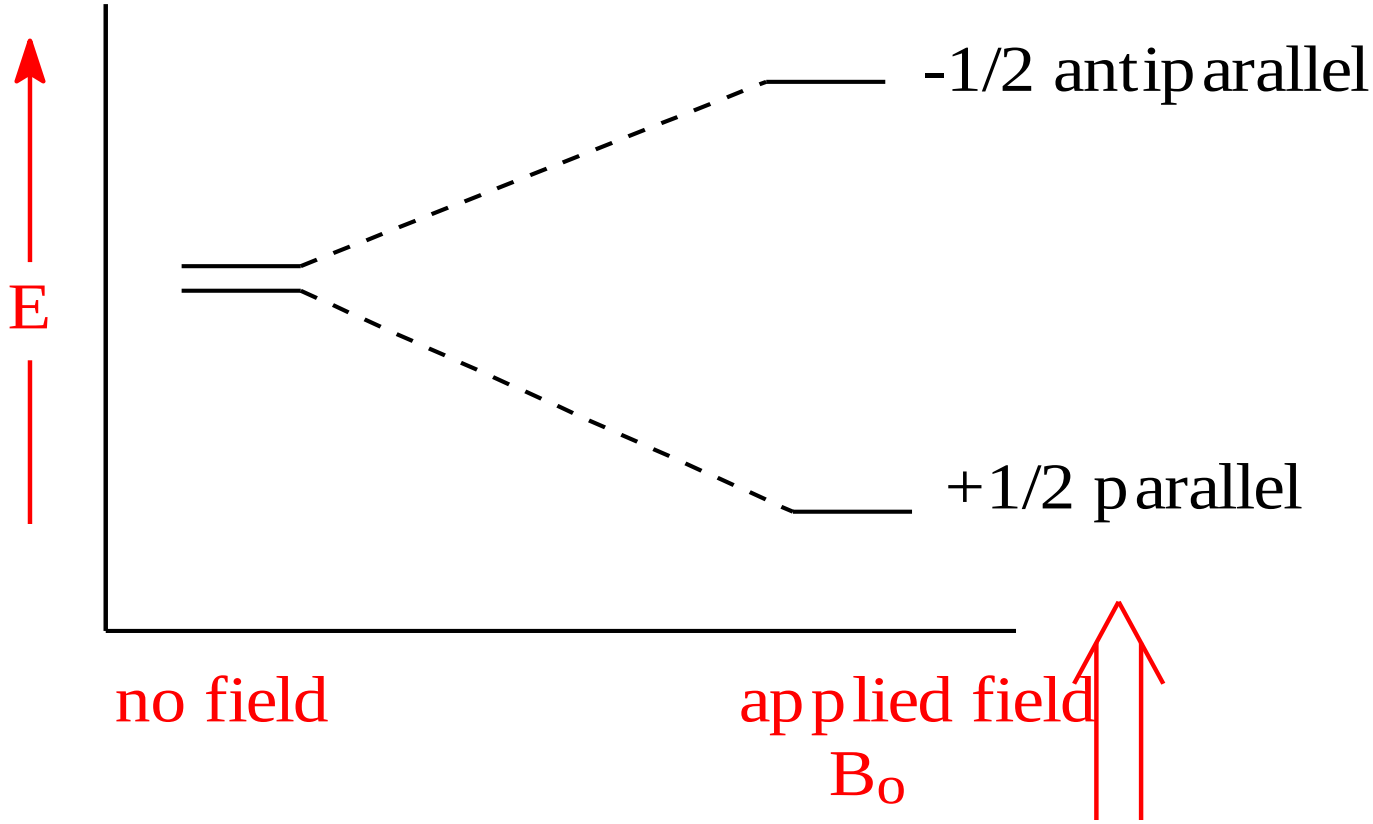
e.g. Carbon-12, Oxygen-16

- For each nucleus with a spin, the # of allowed spin states can be quantized:
- For a nucleus with I, there are 2I + 1 allowed spin states.

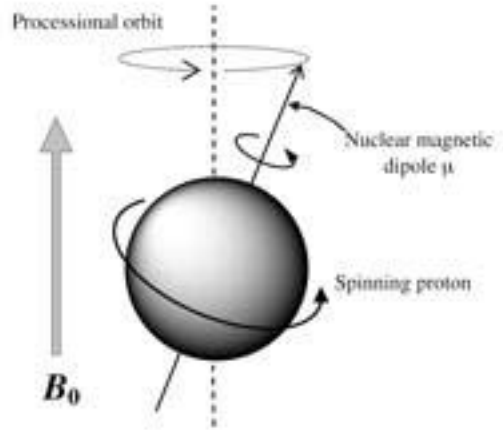
^{1}H, ^{13}C, ^{19}F, ^{31}P all have I = 1/2

$$\Delta E = \gamma(h/2\pi)Bo$$

Spin states split in the presence of B_0

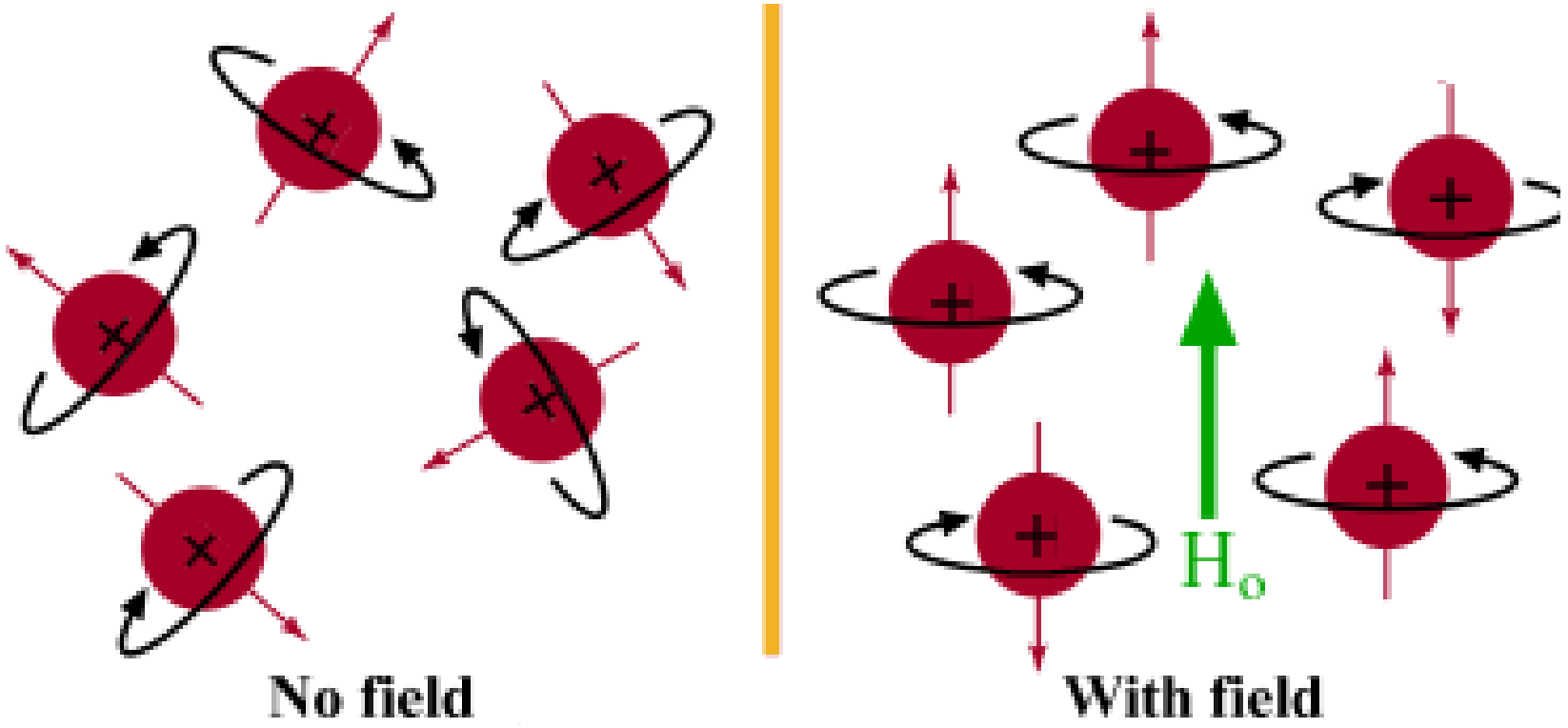


When a **nucleus** aligned with a **magnetic** field, B_0, absorbs radiation frequency (Rf), it can change spin orientation to a higher energy spin state. By relaxing back to the parallel (+1/2) spin state, the nucleus is said to be in **resonance**. Hence,

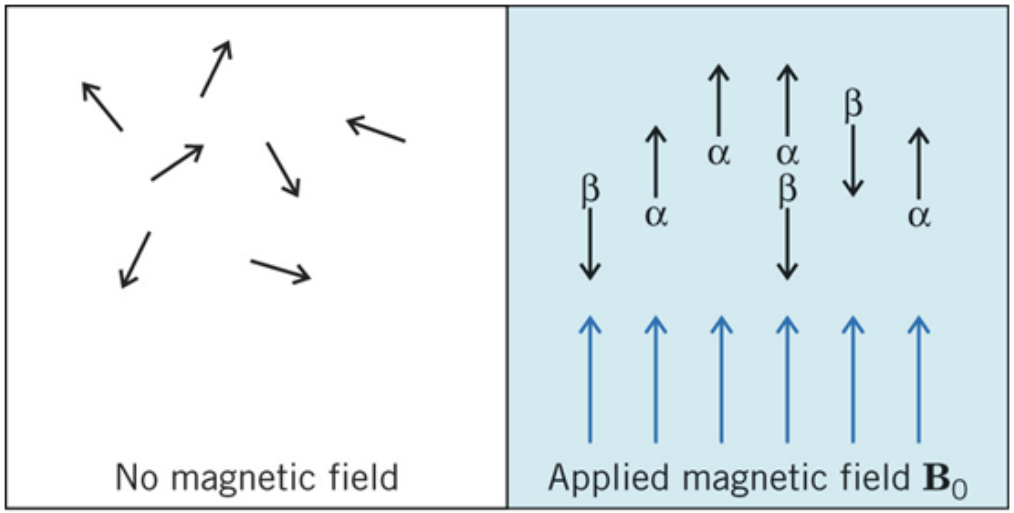


NMR

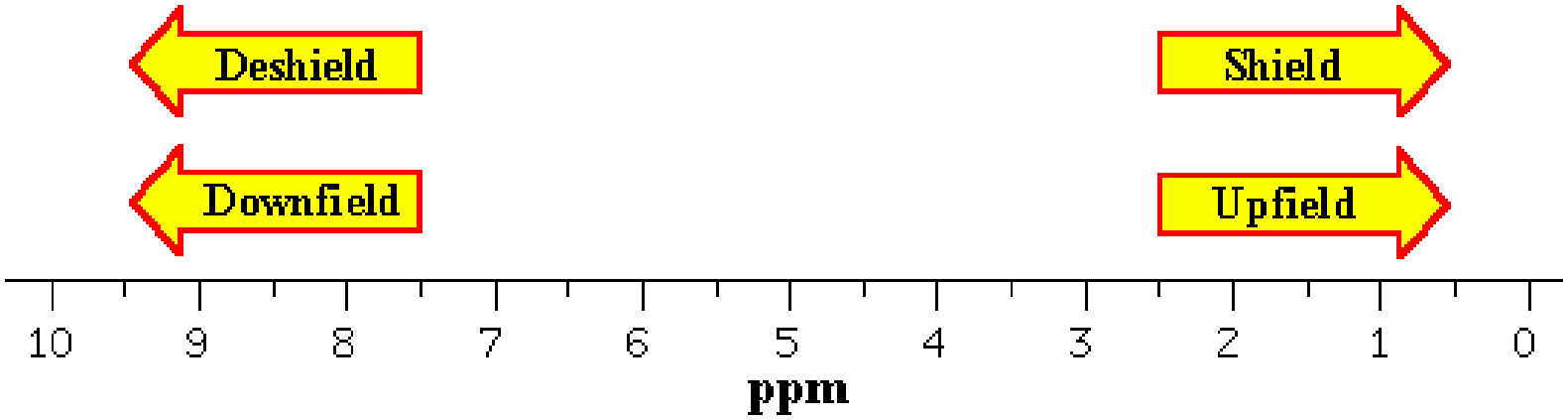
Presence of Magnetic Field



- **Nuclei aligned with the magnetic field are lower in energy than those aligned against the field**
- **The nuclei aligned with the magnetic field can be flipped to align against it if the right amount of energy is added (DE)**
- **The amount of energy required depends on the strength of the external magnetic field**



Typical 1H NMR Scale is 0-10 ppm



Ppm and taw?

What is the shielding and deshielding?

Shielded proton is

Deshielded proton is

What Does an NMR Spectrum Tell You?

- # of chemically unique H's in the molecule
  # of signals
- The types of H's that are present e.g. aromatic, vinyl, aldehyde …
  chemical shift
- The number of each chemically unique H
  integration
- The H's proximity to eachother
  spin-spin splitting

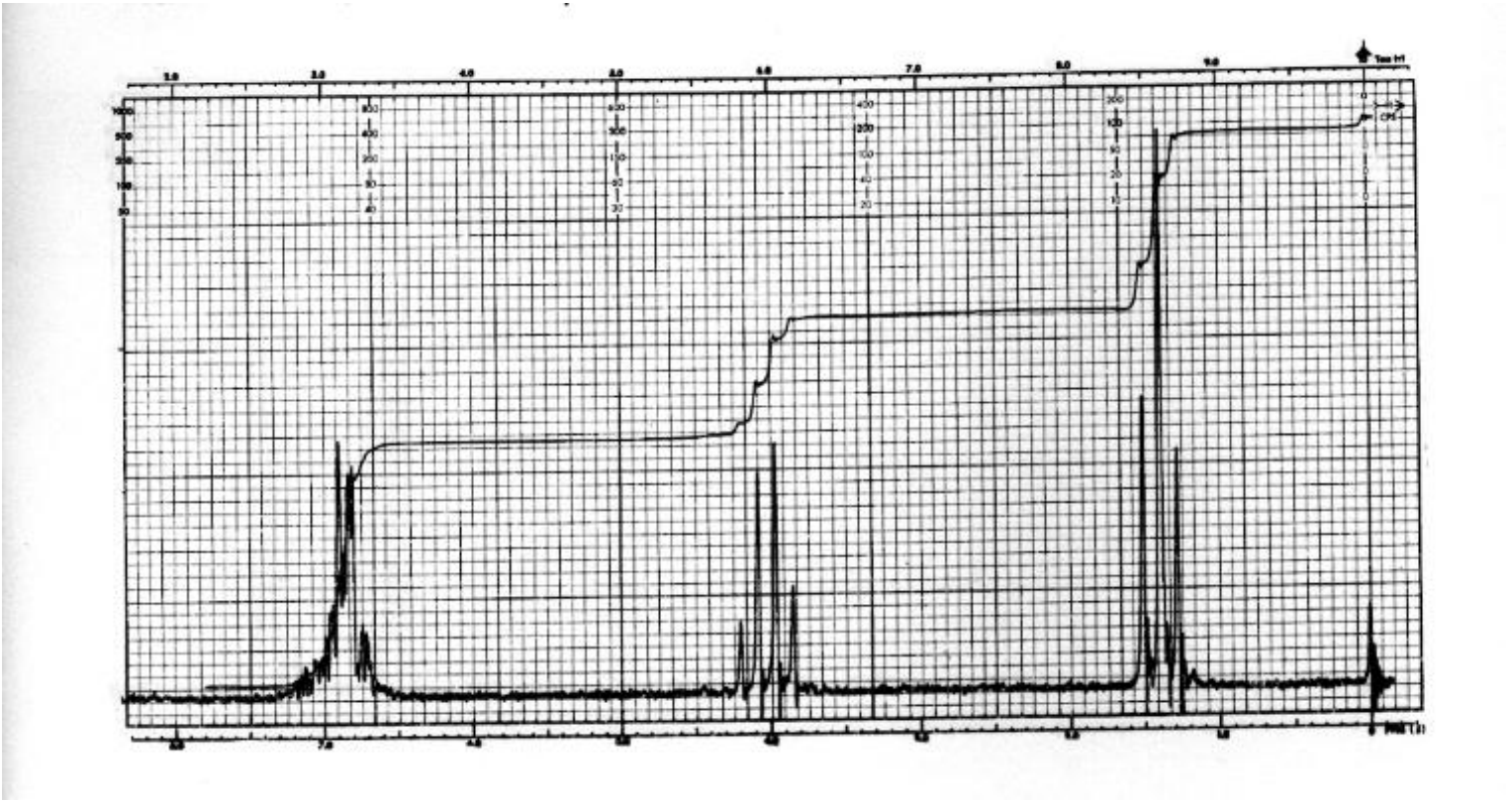
Information from ^{1}H-NMR spectra:

1. **Number of signals: How many different types of hydrogens in the molecule.**
2. **Position of signals (chemical shift): What types of hydrogens.**
3. **Relative areas under signals (integration): How many hydrogens of each type.**
4. **Splitting pattern: How many neighboring hydrogens.**

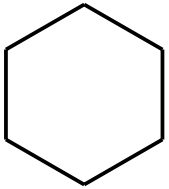
1. Number of signals: How many different types of hydrogens in the molecule.

Magnetically equivalent hydrogens resonate at the same applied field.

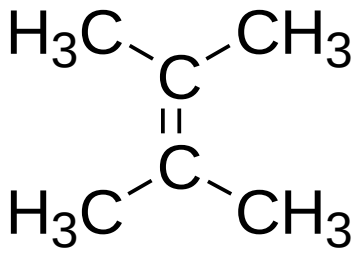
Magnetically equivalent hydrogens are also chemically equivalent.



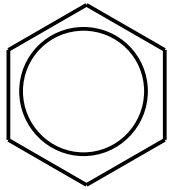
number of signals?



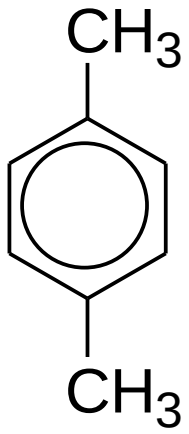
one



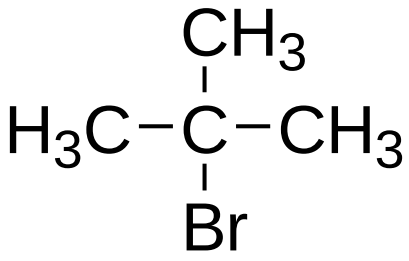
one



one



two



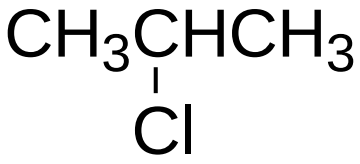
one

CH_3CH_2-Br

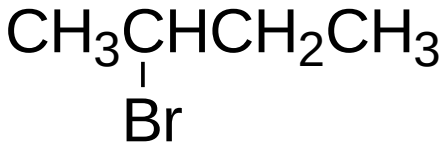
two

$CH_3CH_2CH_2$-Br

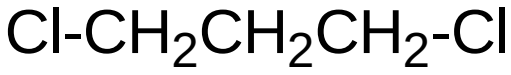
three



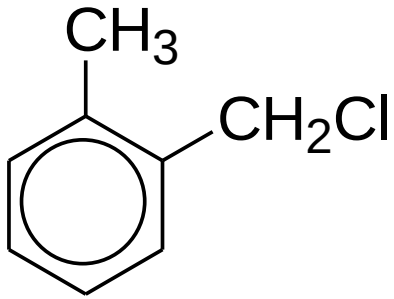
two



four



two



three

2. Position of signals (chemical shift): what types of hydrogens.

primary	0.9 ppm	
secondary	1.3	
tertiary	1.5	
aromatic	6-8.5	
allyl	1.7	
benzyl	2.2-3	
chlorides	3-4	H-C-Cl
bromides	2.5-4	H-C-Br
iodides	2-4	H-C-I
alcohols	3.4-4	H-C-O
alcohols	1-5.5	H-O- (variable)

Note: combinations may greatly influence chemical shifts. For example, the benzyl hydrogens in benzyl chloride are shifted to lower field by the chlorine and resonate at 4.5 ppm.

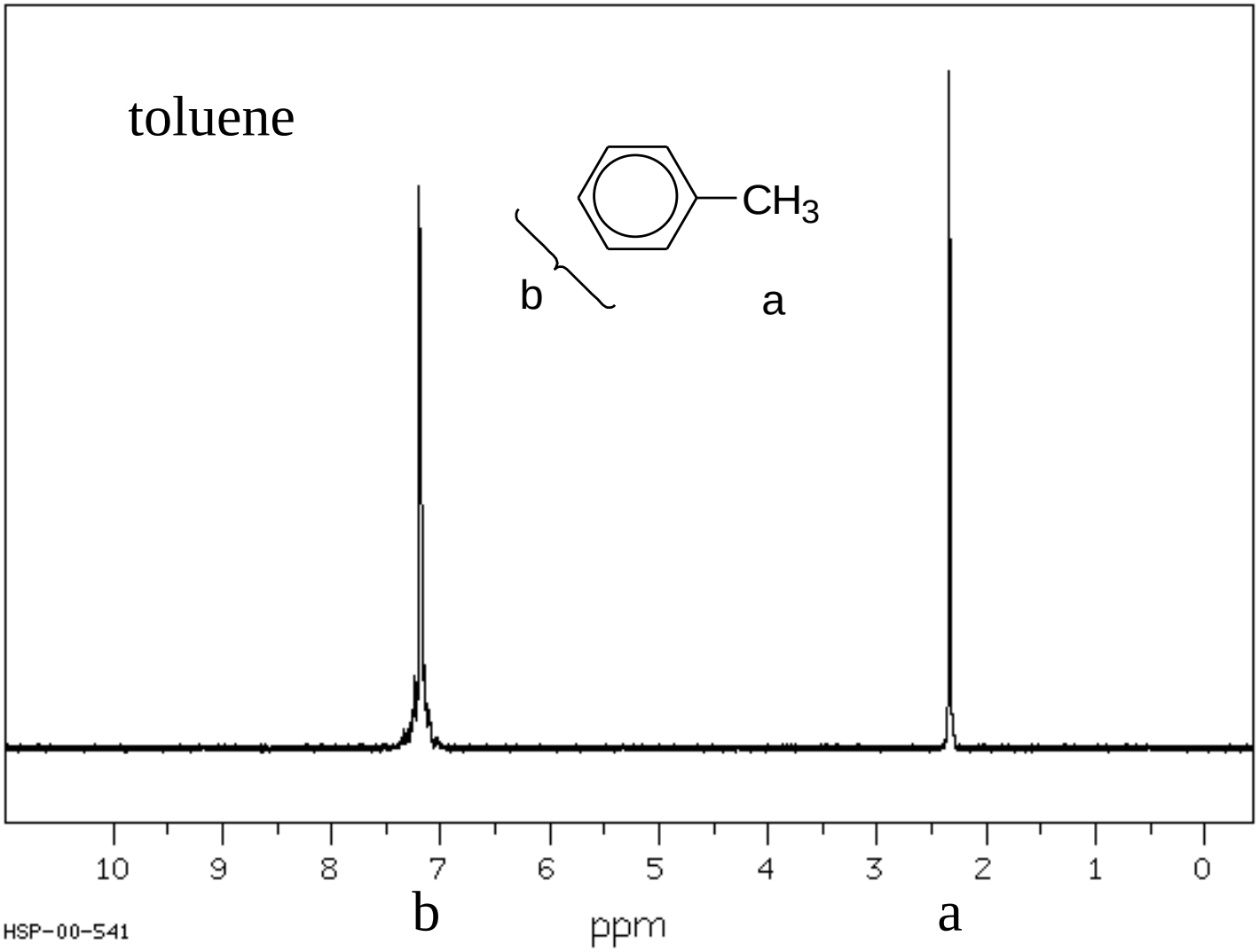
reference compound = tetramethylsilane $(CH_3)_4Si$ @ 0.0 ppm

remember: **magnetic field →**

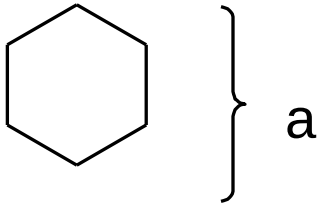
← chemical shift

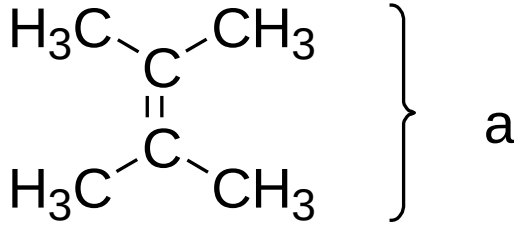
convention: let most upfield signal = a, next most upfield = b, etc.

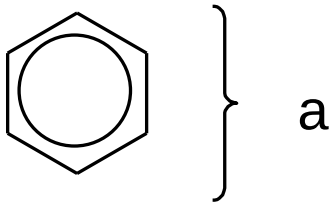
… c b a tms

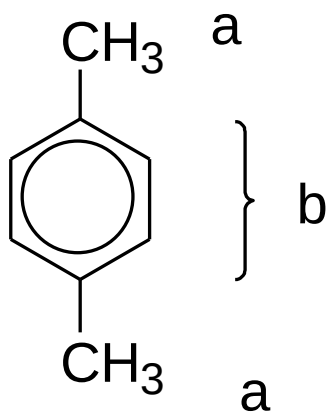

toluene
CH3
b
a
10
9
8
7
6
5
4
3
2
1
0
b
ppm
a
HSP-00-541

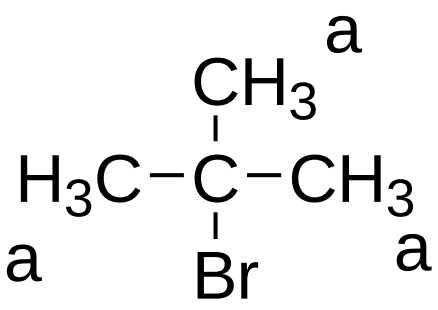
3- chemical shifts

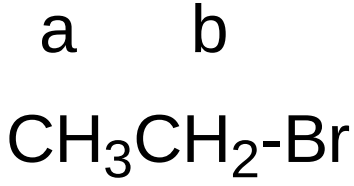


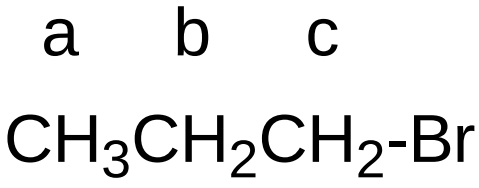


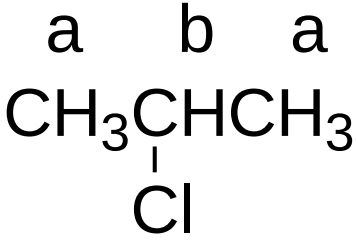


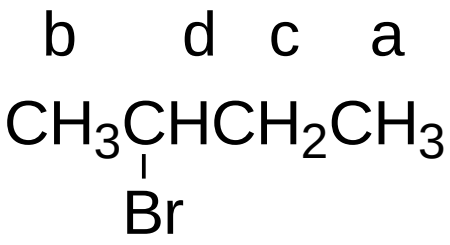


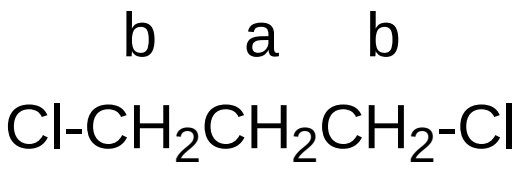

a
CH3
H3C
C
CH3
a
Br
a

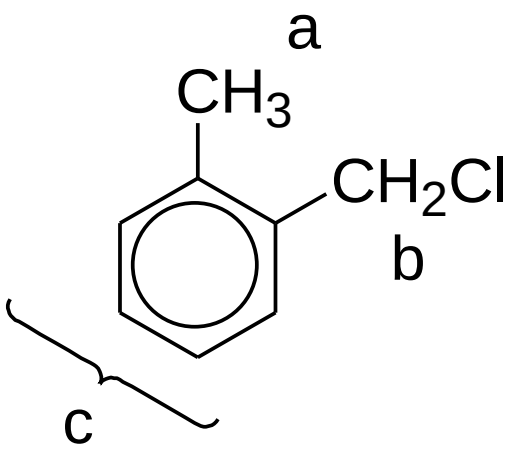

a b
CH3CH2-Br


a b c
CH3CH2CH2-Br


a b a
CH3CHCH3
Cl


b d c a
CH3CHCH2CH3
Br


b a b
Cl-CH2CH2CH2-Cl


a
CH3
CH2Cl
b
c

3. Integration (relative areas under each signal): how many hydrogens of each type.

a b c

$CH_3CH_2CH_2Br$

a 3H

b 2H

c 2H

a : b : c = 3 : 2 : 2

a b a

CH_3CHCH_3

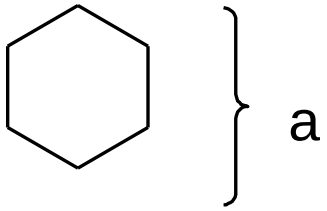
Cl

a 6H

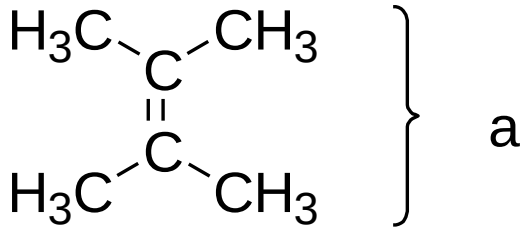
b 1H

a : b = 6 : 1

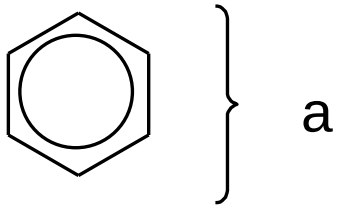
integration



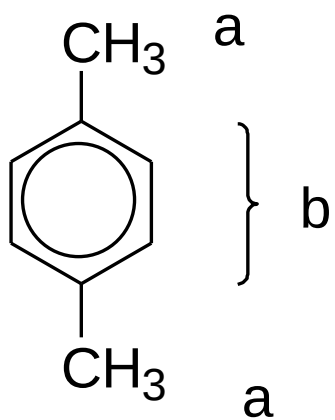
a 12 H



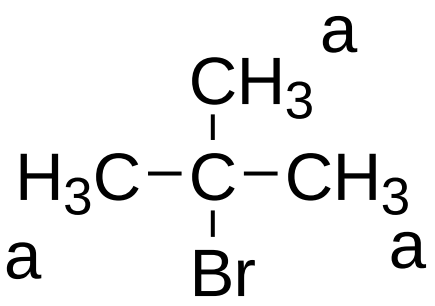
a 12 H



a 6 H



a 6 H
b 4 H



a 9 H

a b

CH3CH2-Br

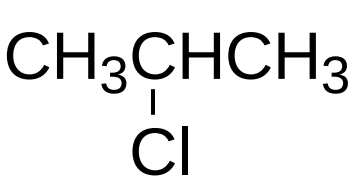
a 3 H
b 2 H

a b c

CH3CH2CH2-Br

a 3 H
b 2 H
c 2 H

a b a



a 6 H
b 1 H

b d c a

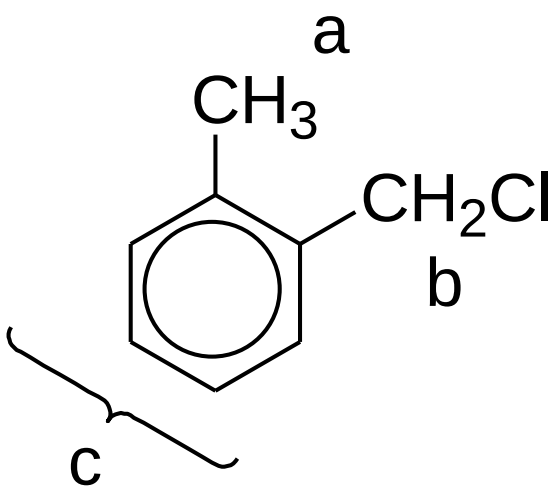
$CH_3\underset{\underset{Br}{|}}{C}HCH_2CH_3$

a 3 H
b 3 H
c 2 H
d 1 H

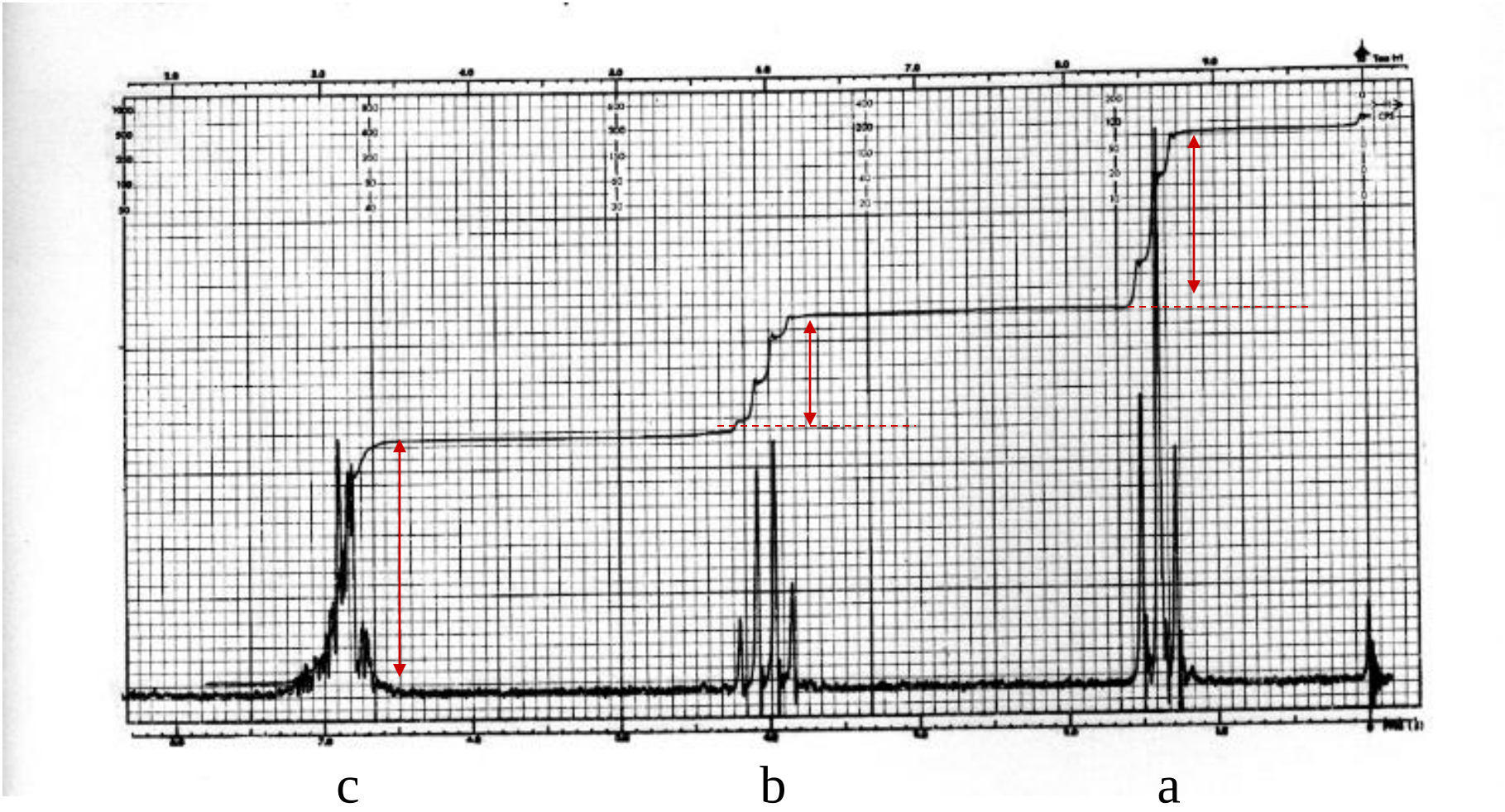
b a b

Cl-$CH_2CH_2CH_2$-Cl

a 2 H
b 4 H

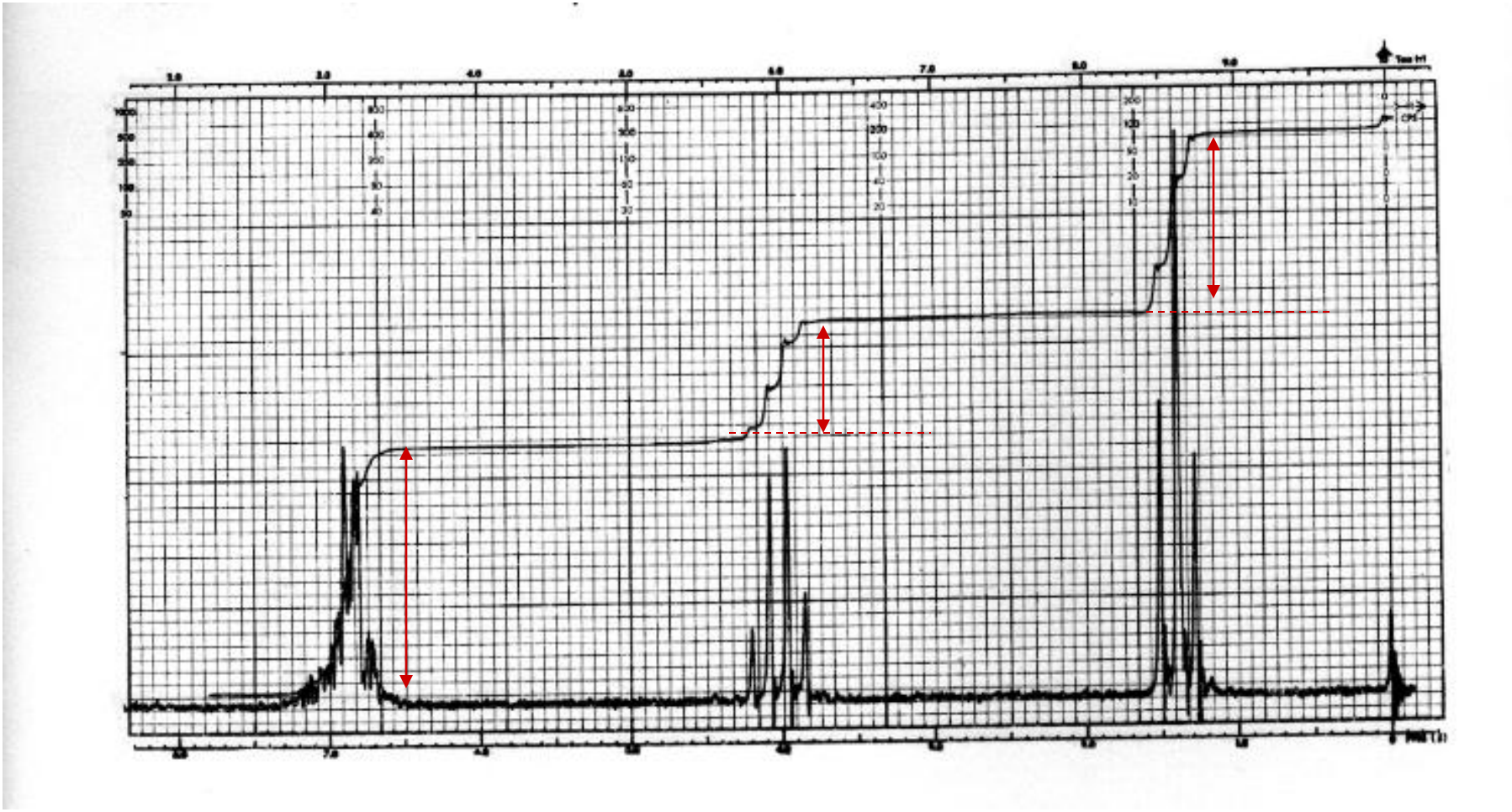


a 3 H
b 2 H
c 4 H



c b a

Integration: measure the height of each “step” in the integration and then calculate the lowest whole number ratio: a:b:c = 24 mm : 16 mm : 32 mm = 1.5 : 1.0 : 2.0 → 3H : 2H : 4H



If the formula is known (C_8H_9OF), add up all of the “steps” and divide by the number of hydrogens = (24 + 16 + 32 mm) / 9H = 8.0 mm / Hydrogen.
a = 24 mm / 8.0 mm/H → 3 H; b = 16 mm/8.0 mm/H → 2H;
c = 32 mm/8.0 mm/H → 4H.

4. Splitting pattern: how many neighboring hydrogens.

In general, n-equivalent neighboring hydrogens will split a ^{1}H signal into an (n + 1) Pascal pattern.

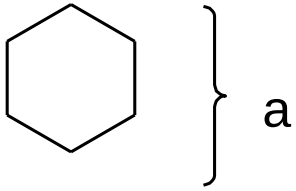
"neighboring" – no more than three bonds away

n	n + 1	Pascal pattern:	
0	1	1	singlet
1	2	1 1	doublet
2	3	1 2 1	triplet
3	4	1 3 3 1	quartet
4	5	1 4 6 4 1	quintet

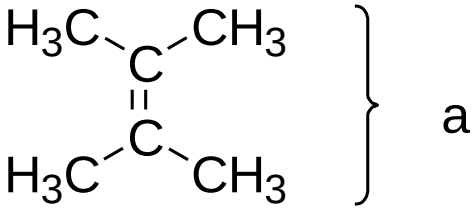
note: n must be equivalent neighboring hydrogens to give rise to a Pascal splitting pattern. If the neighbors are not equivalent, then you will see a complex pattern (aka complex multiplet).

note: the alcohol hydrogen –OH usually does not split neighboring hydrogen signals nor is it split. Normally a singlet of integration 1 between 1 – 5.5 ppm (variable).

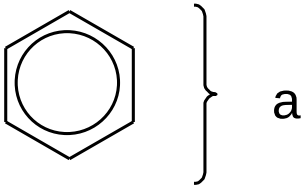
splitting pattern?



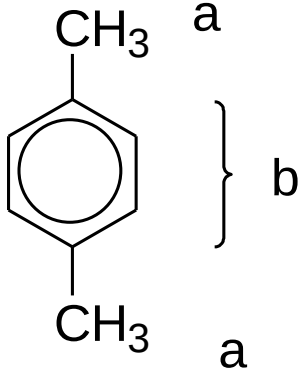
a 12 H singlet



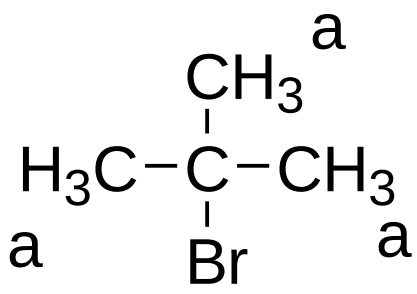
a 12 H singlet



a 6 H singlet



a 6 H singlet
b 4 H singlet



a 9 H singlet

a b

CH_3CH_2-Br

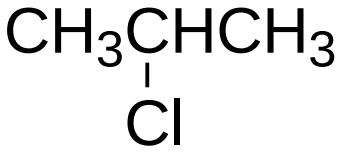
a 3 H triplet
b 2 H quartet

a b c

$CH_3CH_2CH_2$-Br

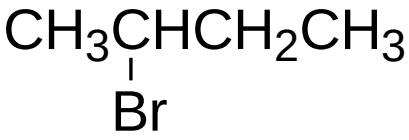
a 3 H triplet
b 2 H complex
c 2 H triplet

a b a



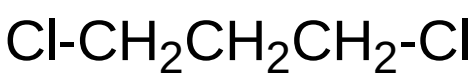
a 6 H doublet
b 1 H septet

b d c a

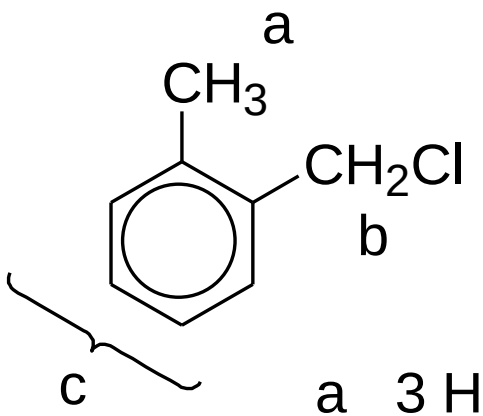


a 3 H triplet
b 3 H doublet
c 2 H complex
d 1 H complex

b a b

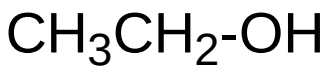


a 2 H quintet
b 4 H triplet



a 3 H singlet
b 2 H singlet
c 4 H ~singlet

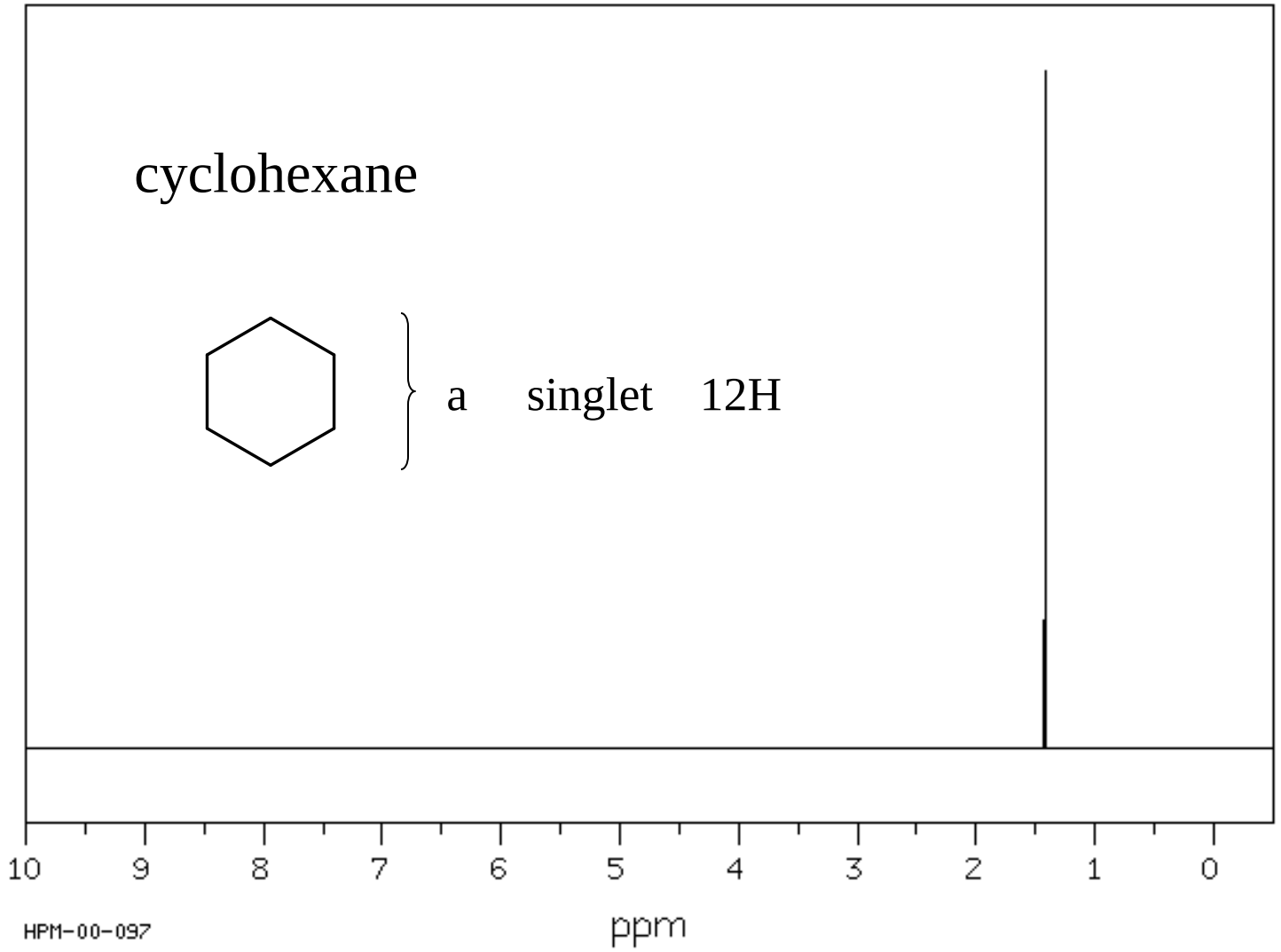
a b c



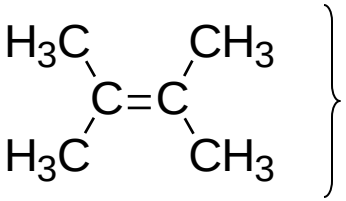
a 3 H triplet
b 2 H quartet
c 1 H singlet

Information from ^{1}H-nmr spectra:

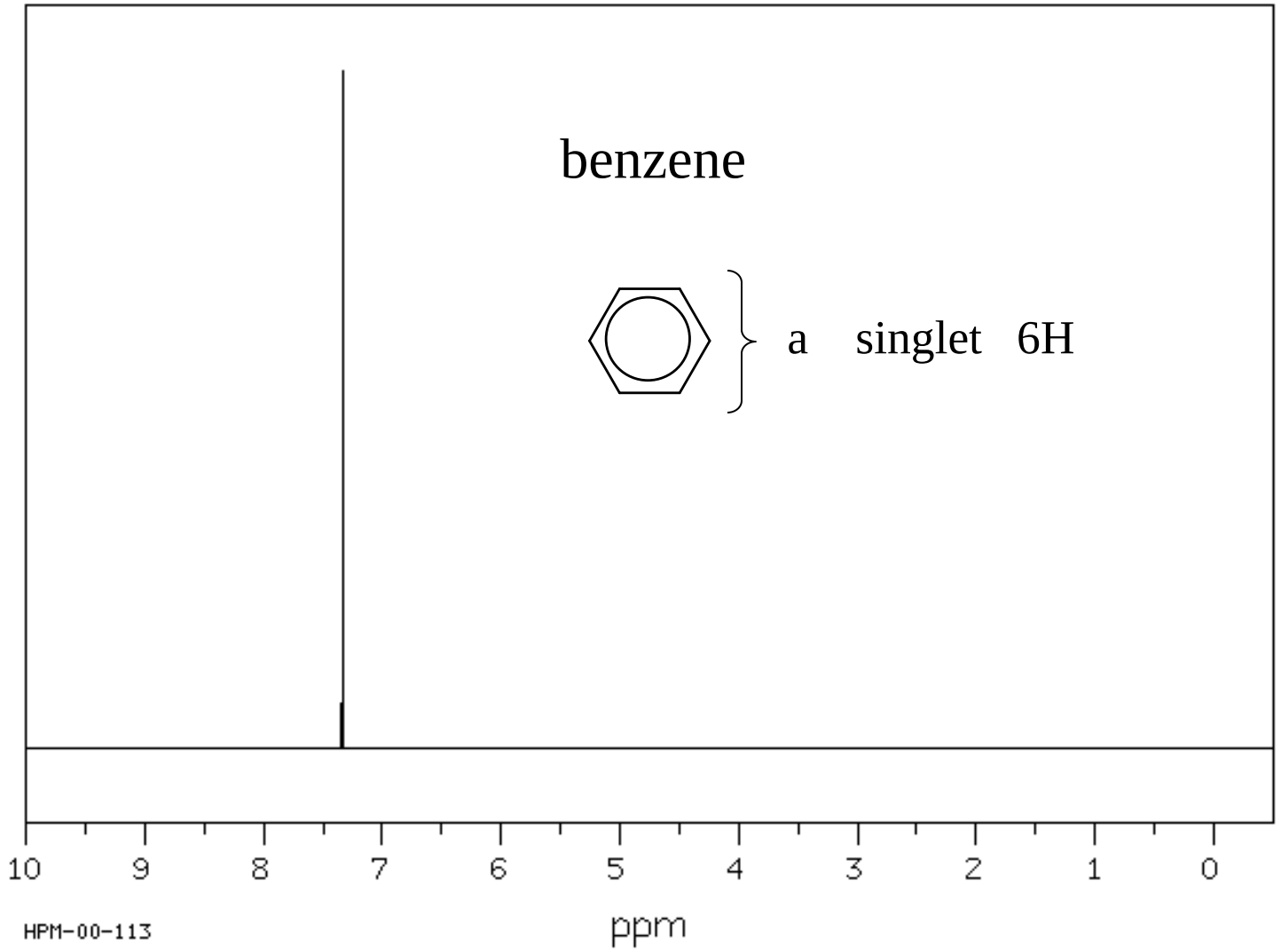
1. **Number of signals: How many different types of hydrogens in the molecule.**
2. **Position of signals (chemical shift): What types of hydrogens.**
3. **Relative areas under signals (integration): How many hydrogens of each type.**
4. **Splitting pattern: How many neighboring hydrogens.**

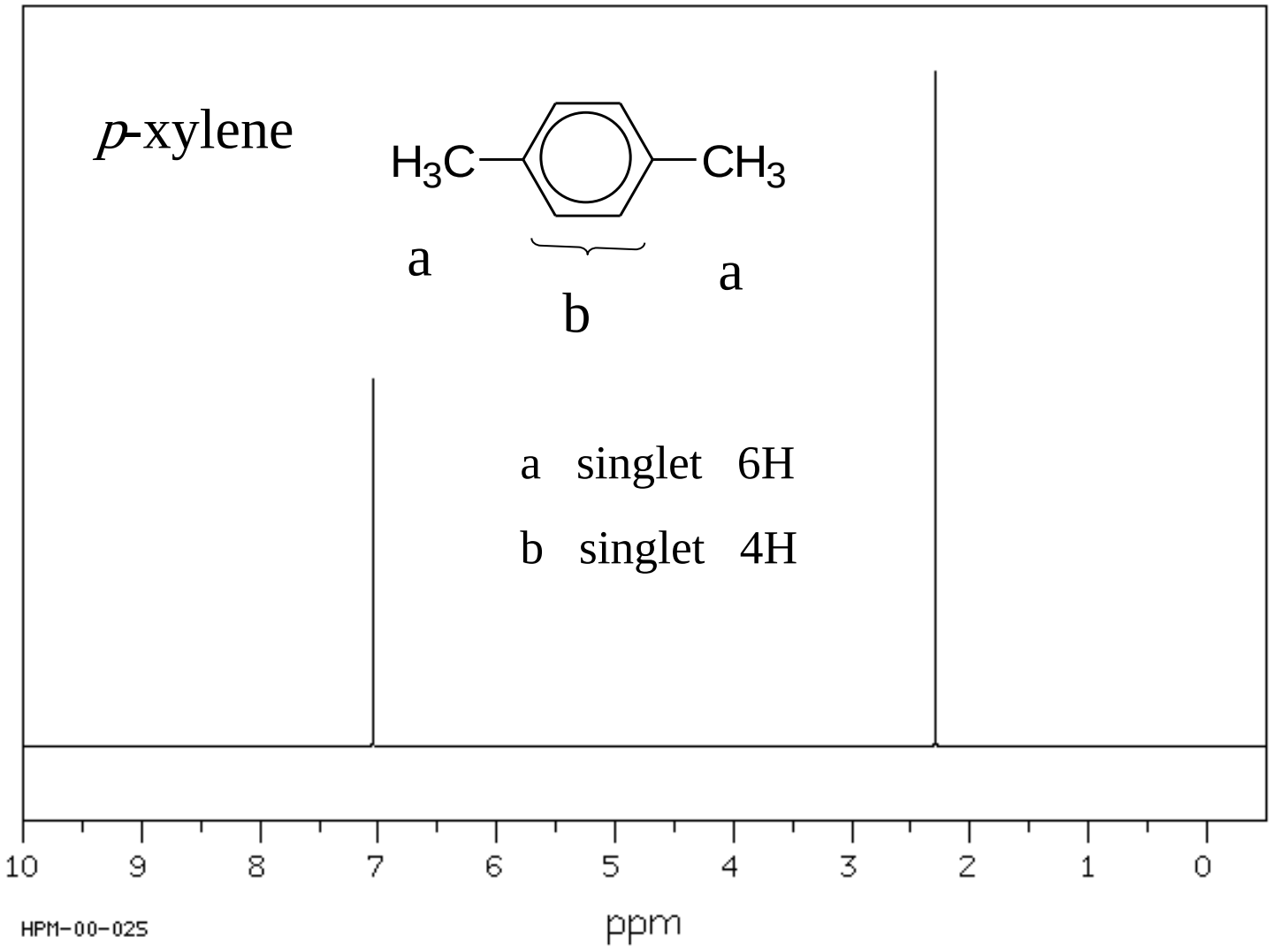

cyclohexane
a singlet 12H
10
9
8
7
6
5
4
3
2
1
0
ppm
HPM-00-097

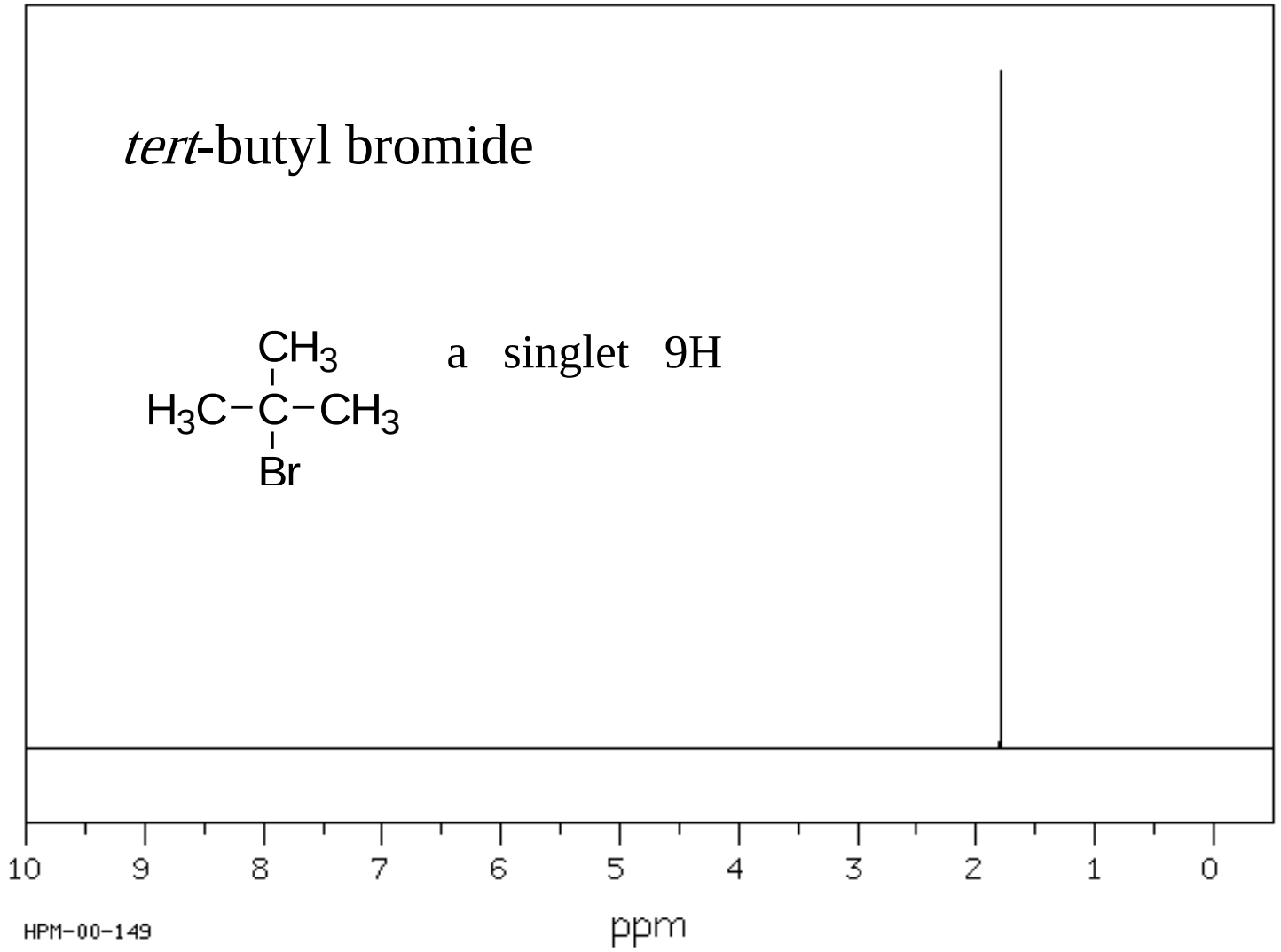
2,3-dimethyl-2-butene



a singlet 12H


benzene
a singlet 6H
10
9
8
7
6
5
4
3
2
1
0
HPM-00-113
ppm


p-xylene
H_3C
CH_3
a
a
b
a singlet 6H
b singlet 4H
10
9
8
7
6
5
4
3
2
1
0
HPM-00-025
ppm


tert-butyl bromide
CH3
H3C−C−CH3
Br
a singlet 9H
10
9
8
7
6
5
4
3
2
1
0
ppm
HPM-00-149

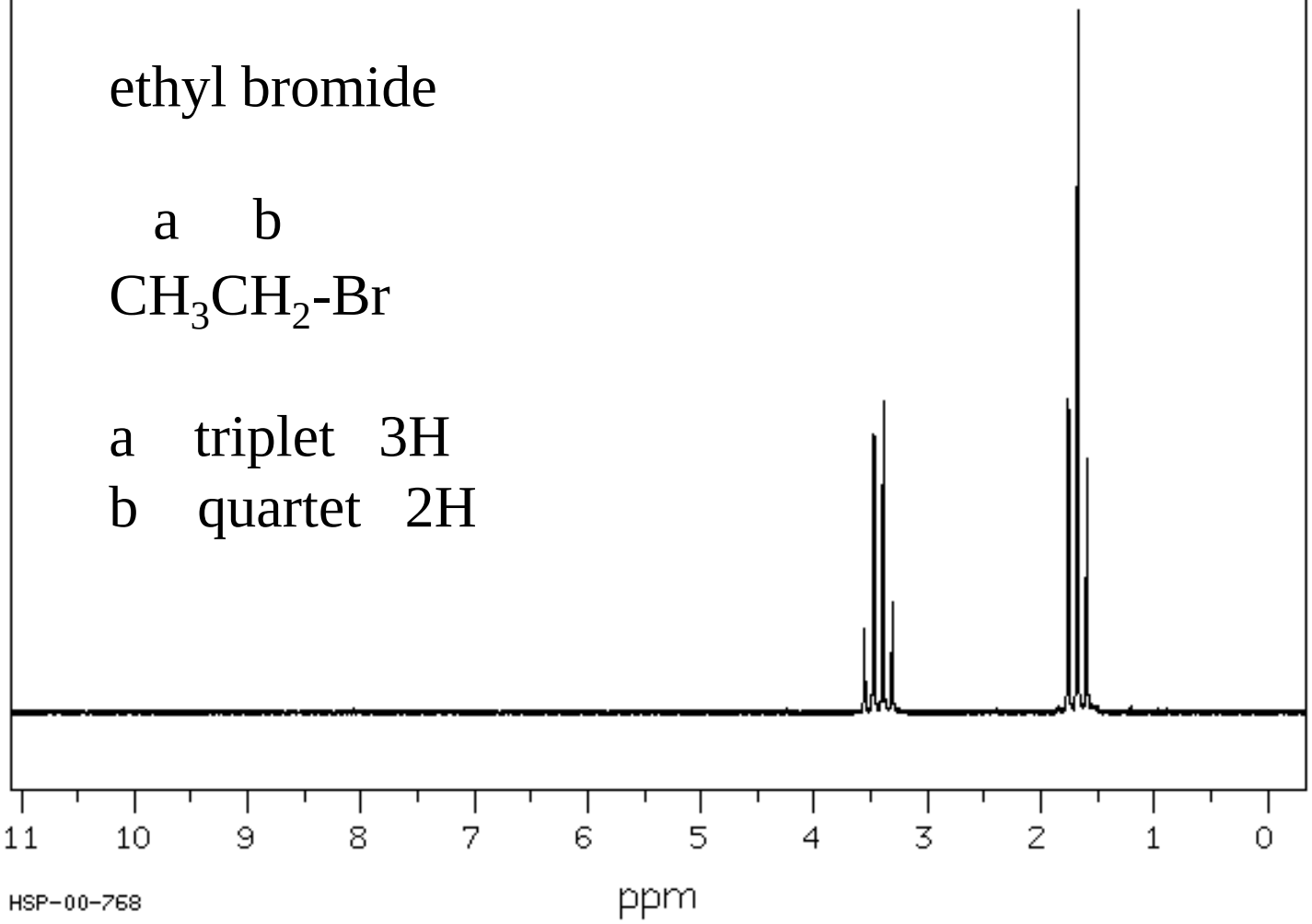
ethyl bromide

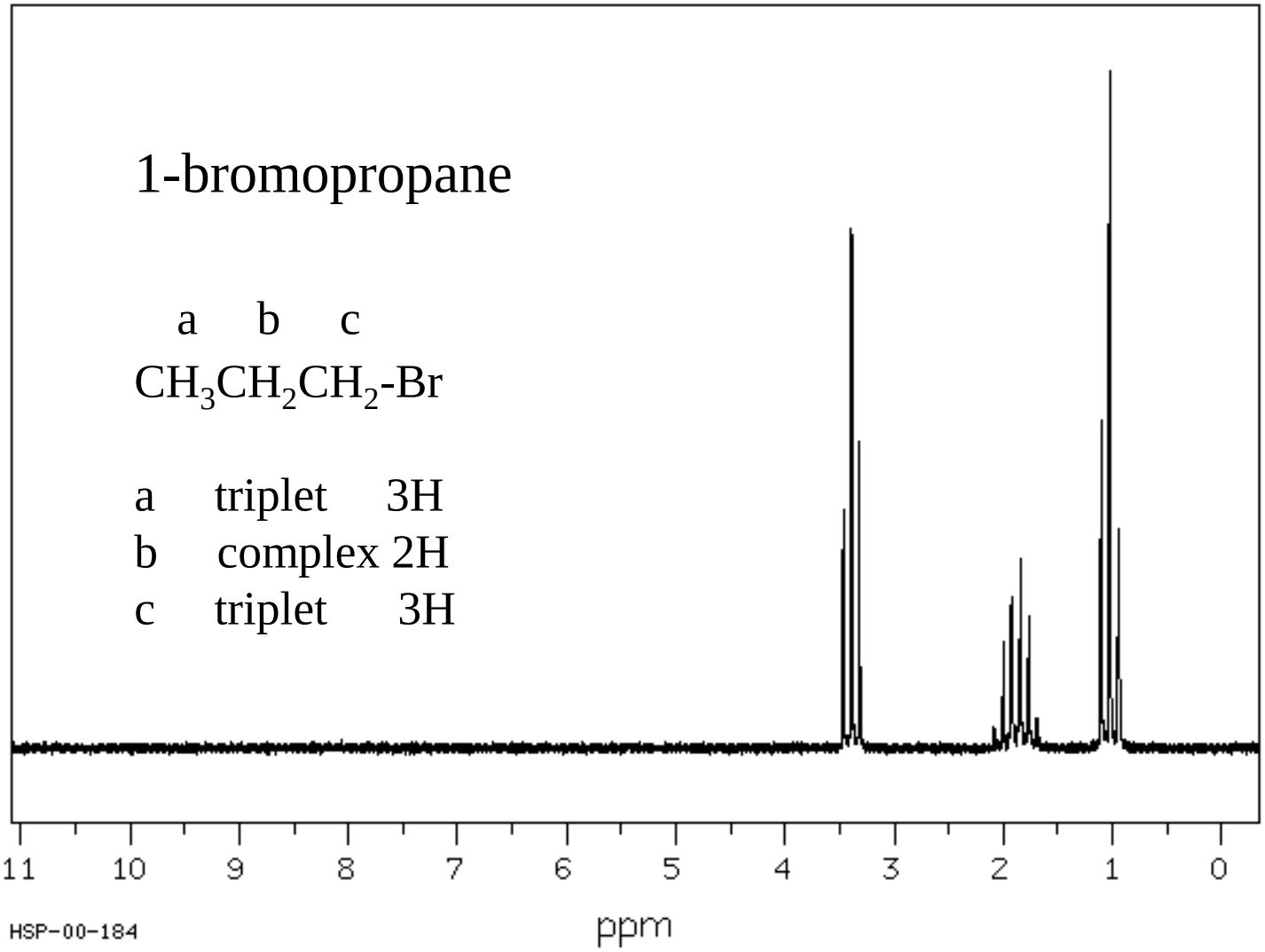
a b

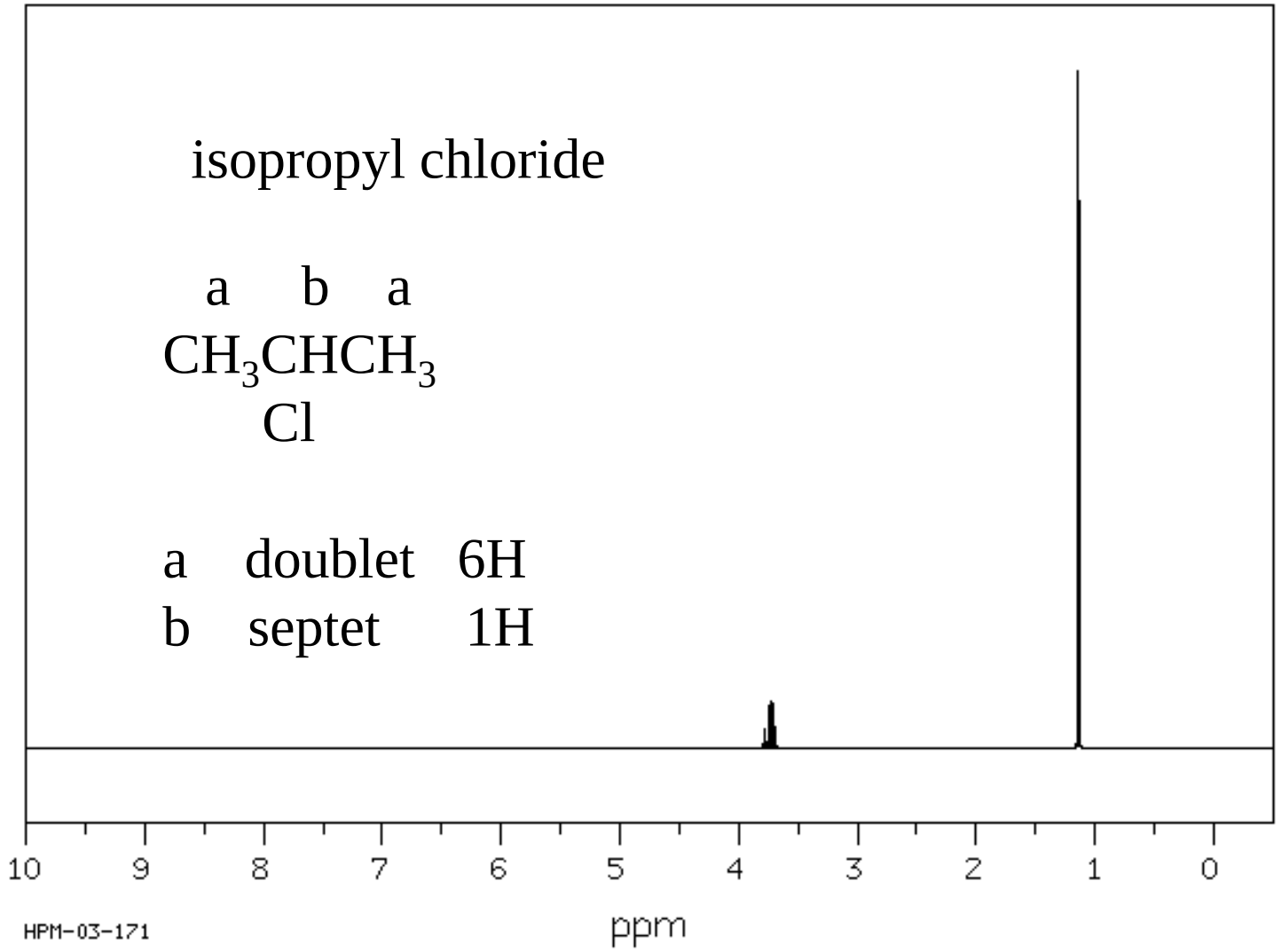
CH_3CH_2-Br

a triplet 3H

b quartet 2H




1-bromopropane
a b c
CH3CH2CH2-Br
a triplet 3H
b complex 2H
c triplet 3H
11
10
9
8
7
6
5
4
3
2
1
0
HSP-00-184
ppm


isopropyl chloride
a b a
CH3CHCH3
Cl
a doublet 6H
b septet 1H
10 9 8 7 6 5 4 3 2 1 0
ppm
HPM-03-171

2-bromobutane

b d c a

$CH_3CHCH_2CH_3$

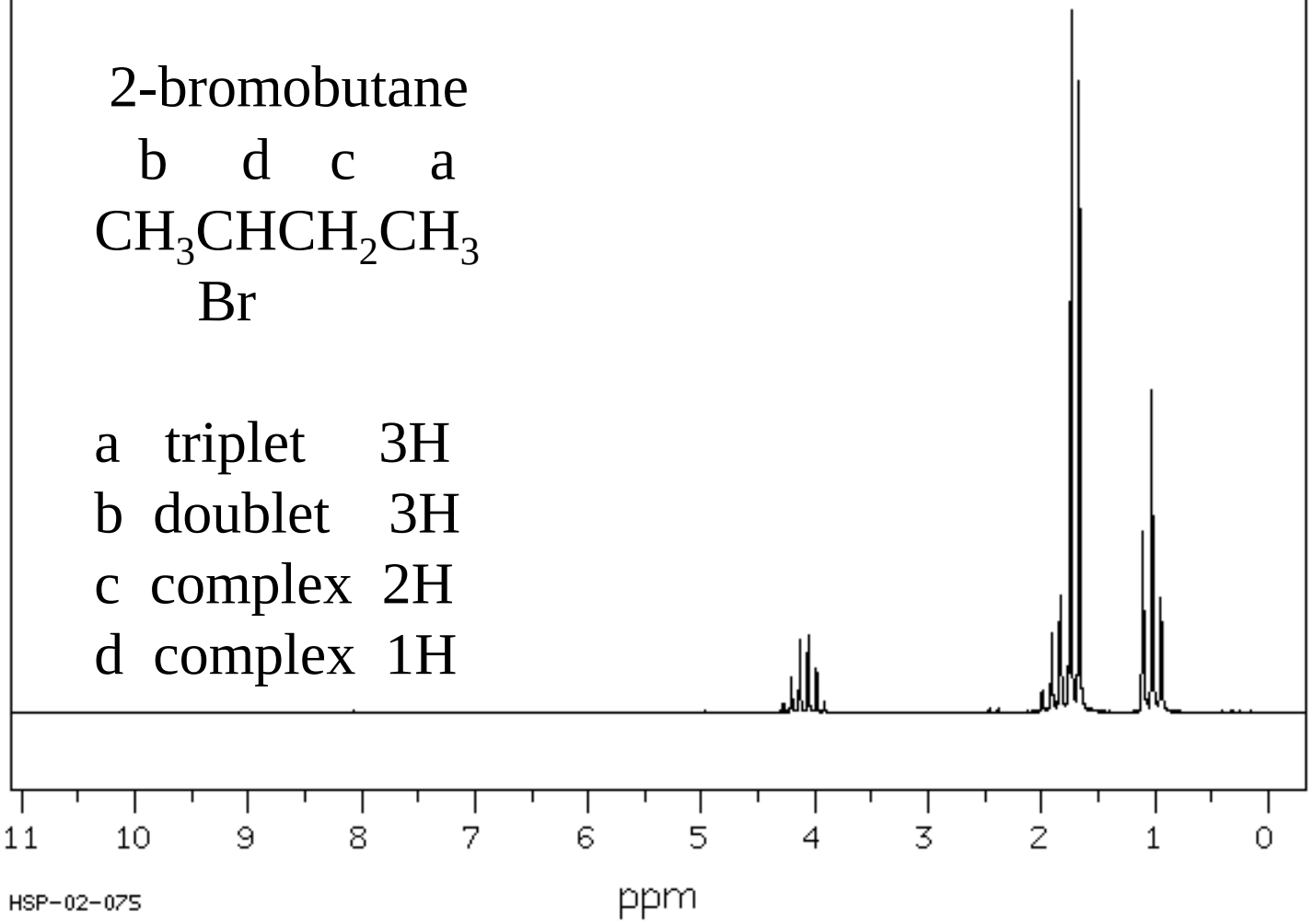
Br

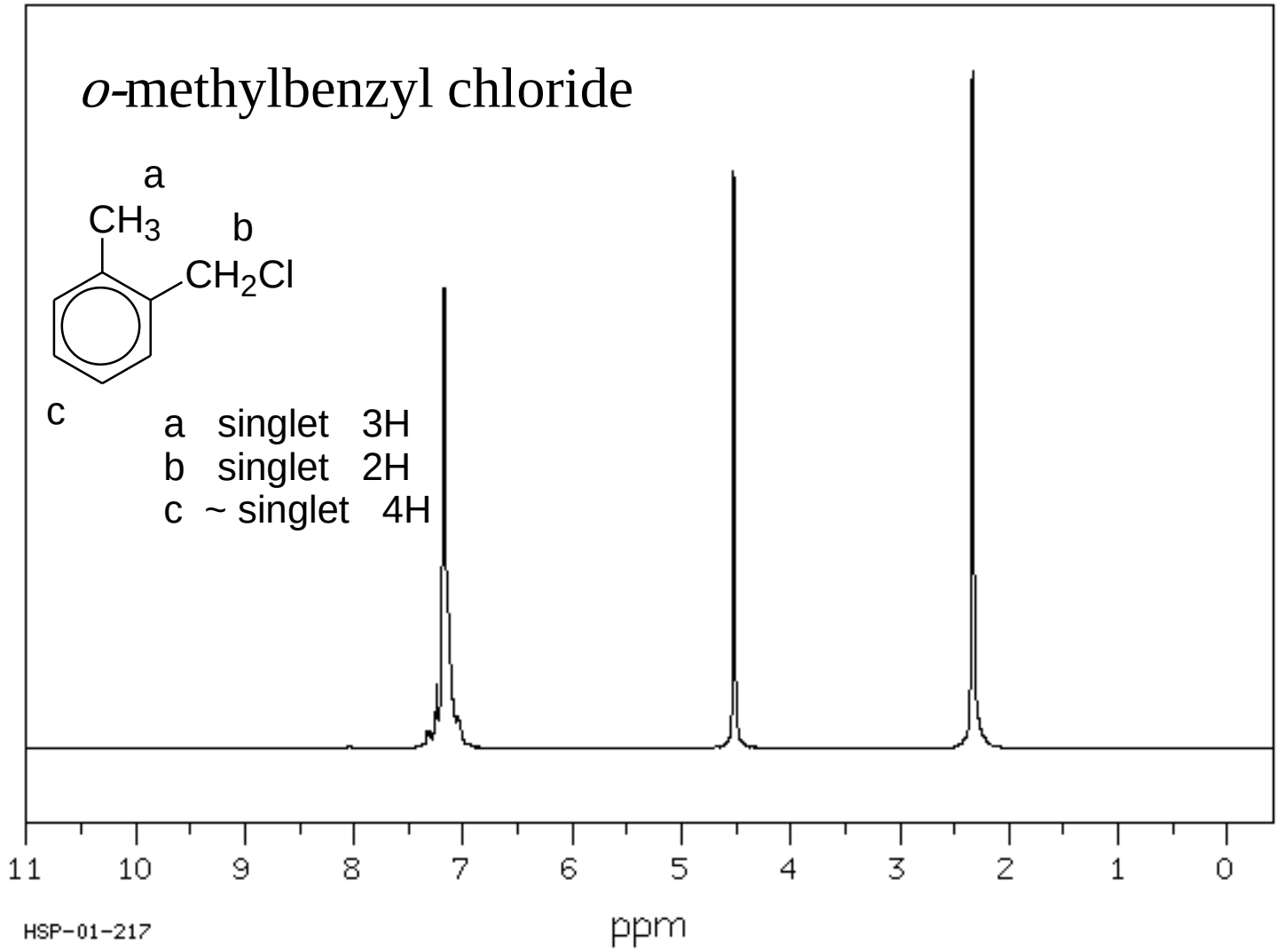
a triplet 3H

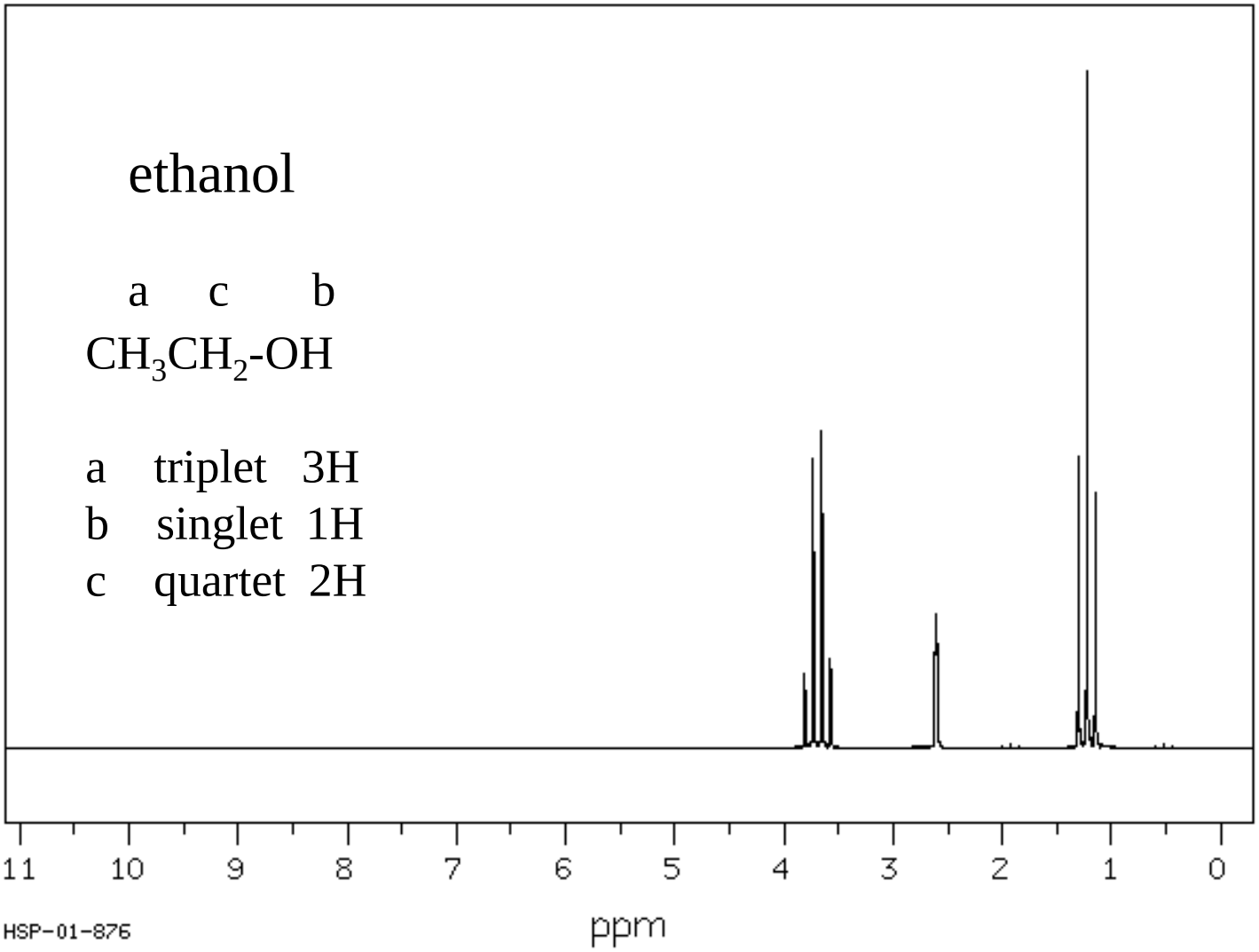
b doublet 3H

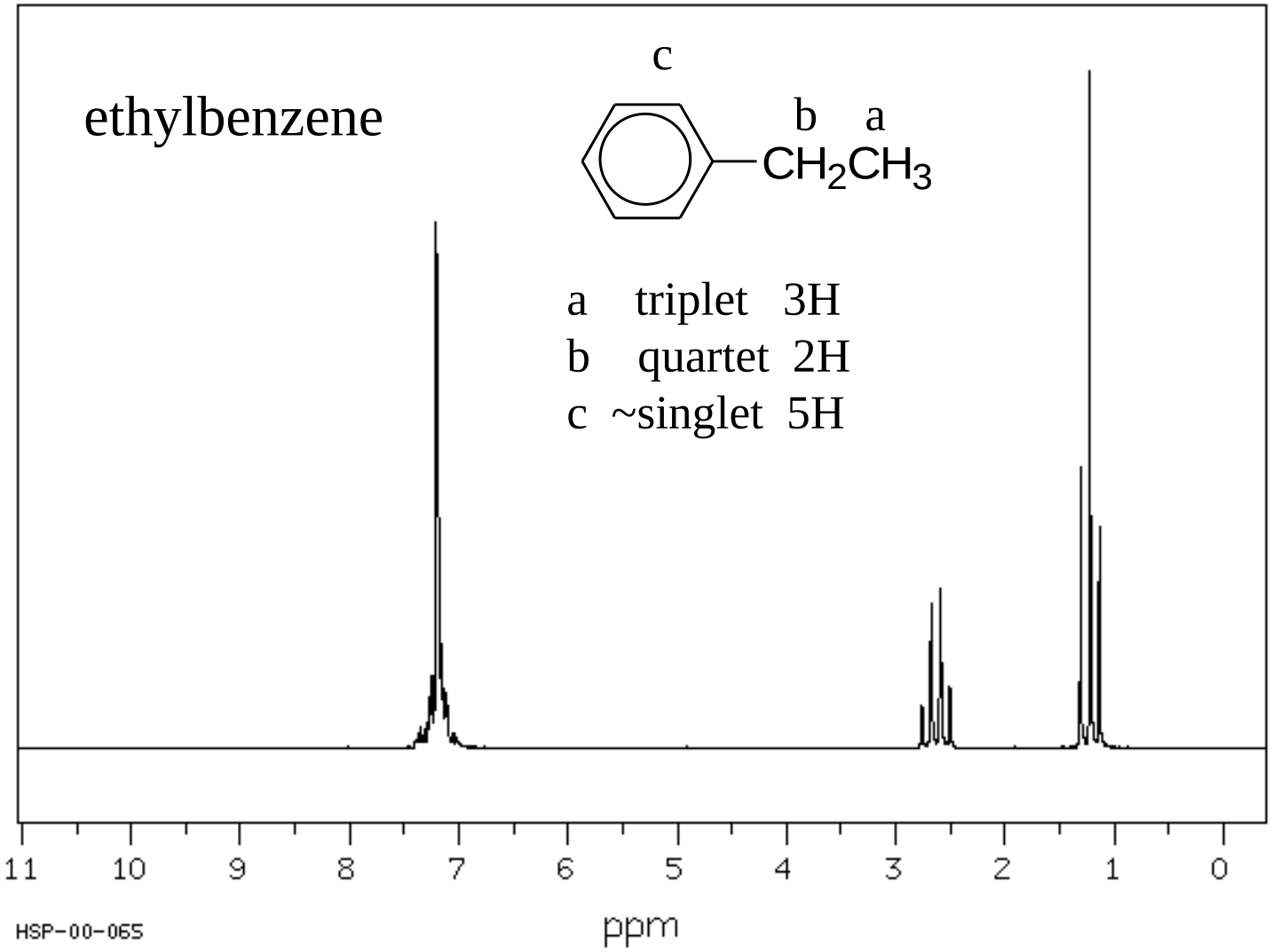
c complex 2H

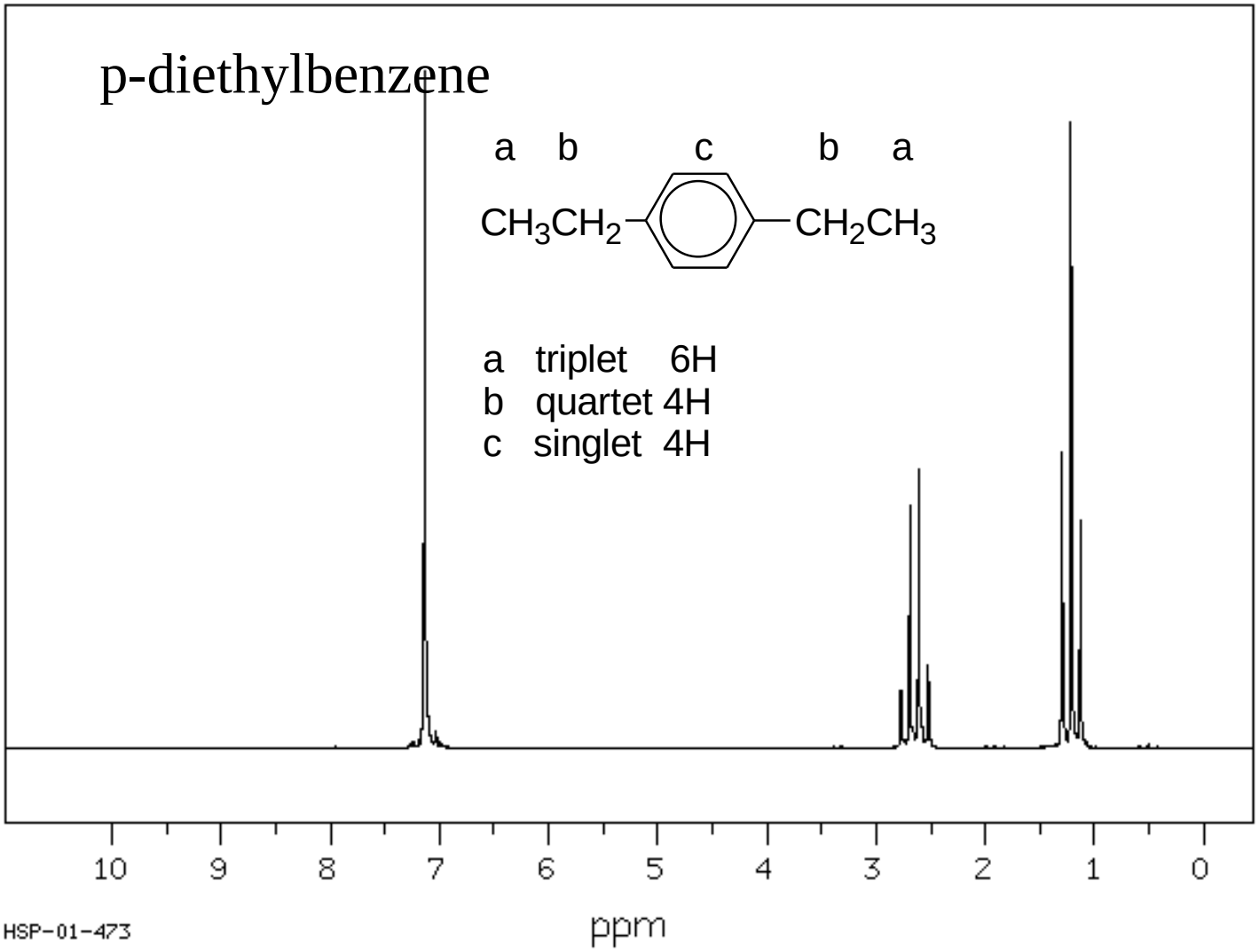
d complex 1H

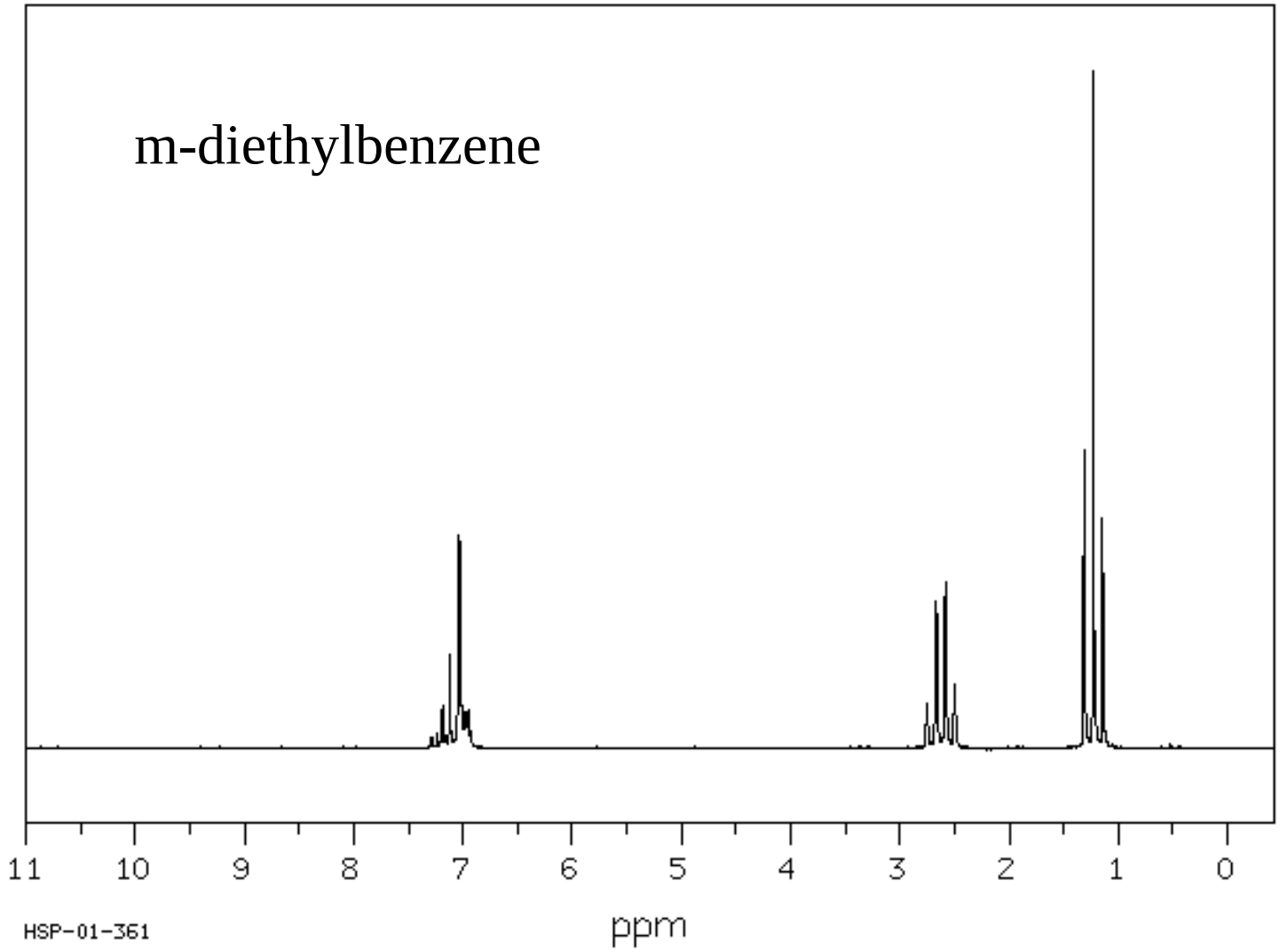


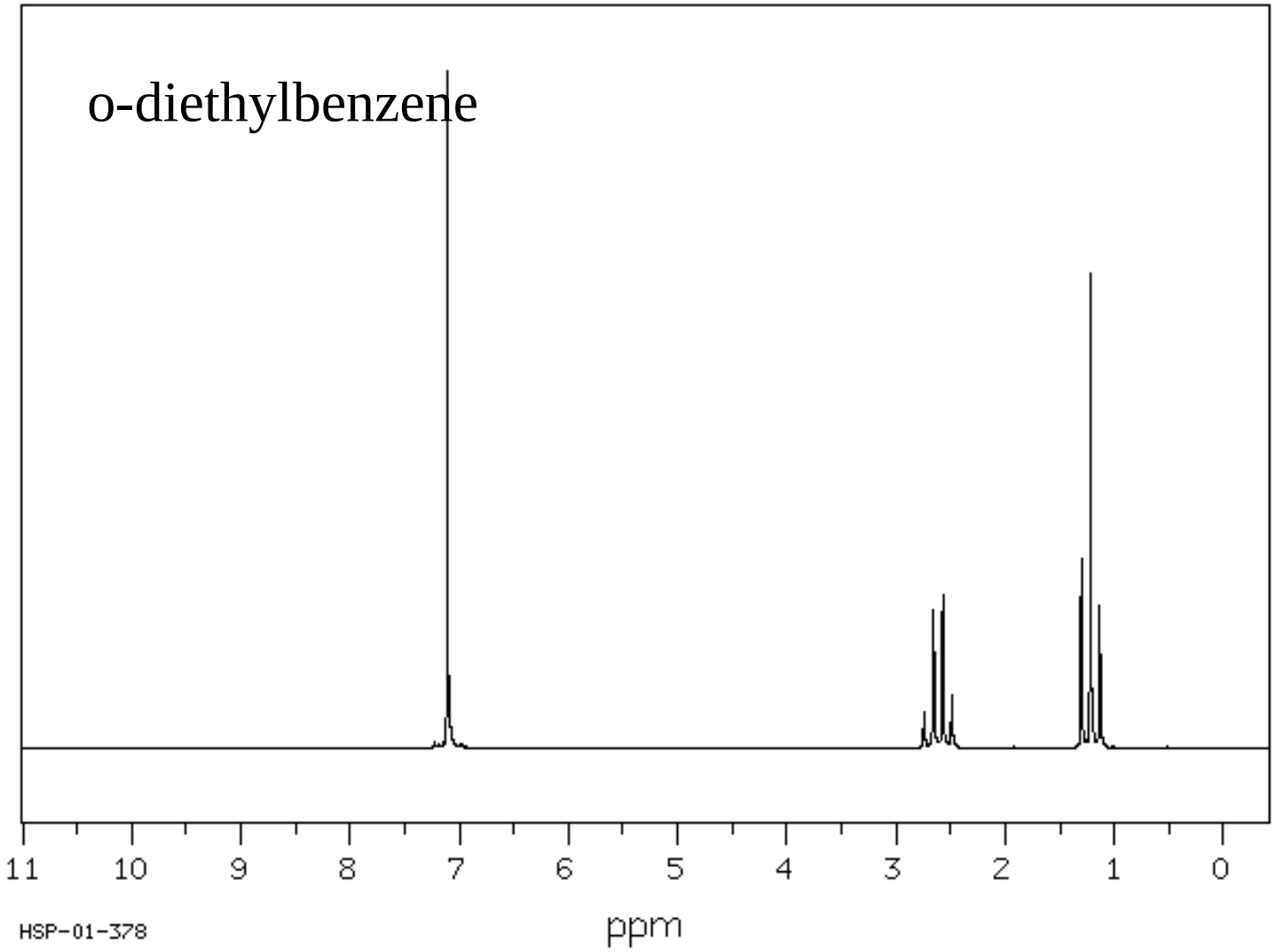

o-methylbenzyl chloride
a
CH3
b
CH2Cl
c
a singlet 3H
b singlet 2H
c ~ singlet 4H
11
10
9
8
7
6
5
4
3
2
1
0
ppm
HSP-01-217

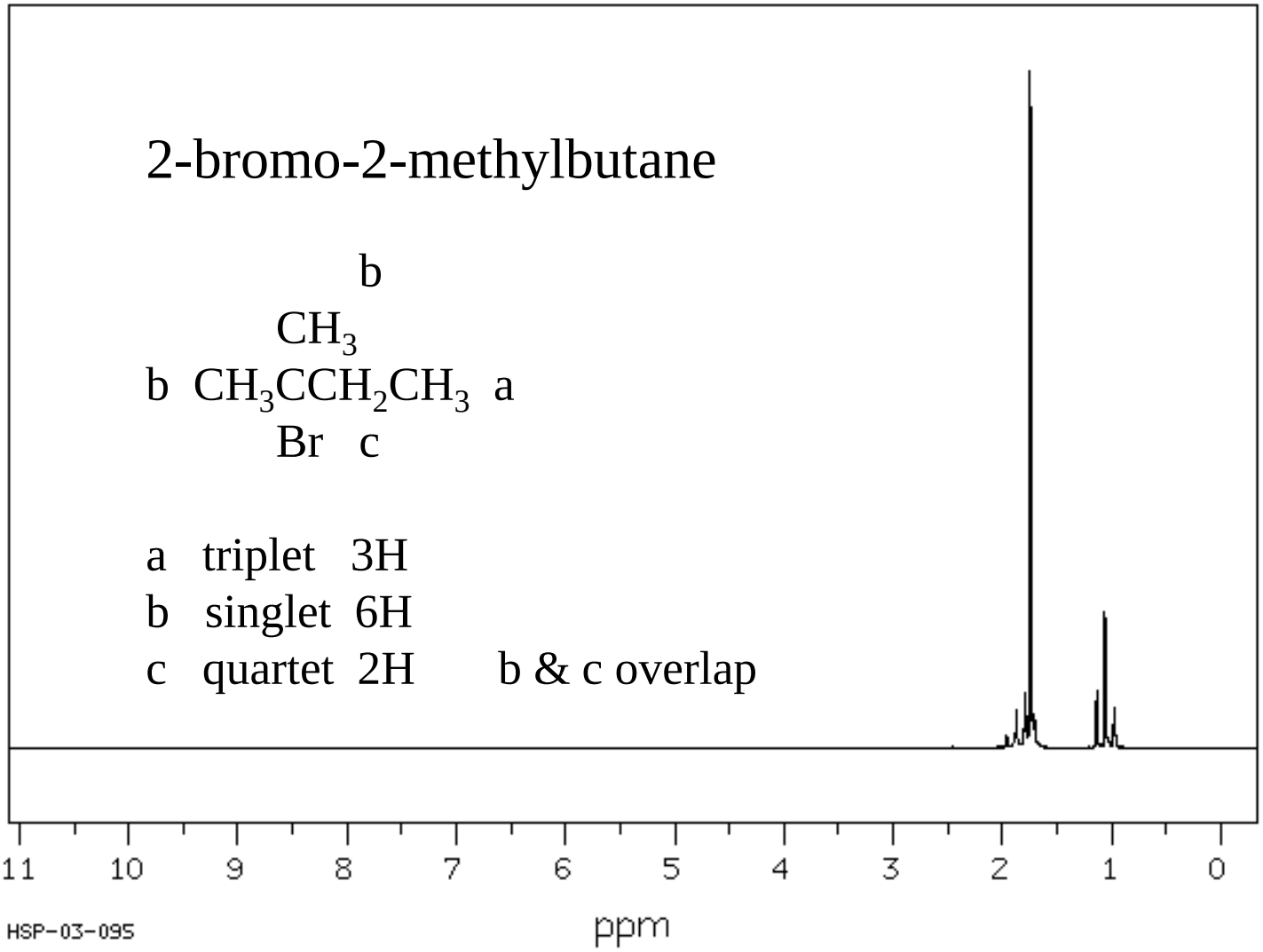

ethanol
a c b
CH3CH2-OH
a triplet 3H
b singlet 1H
c quartet 2H
11 10 9 8 7 6 5 4 3 2 1 0
HSP-01-876
ppm

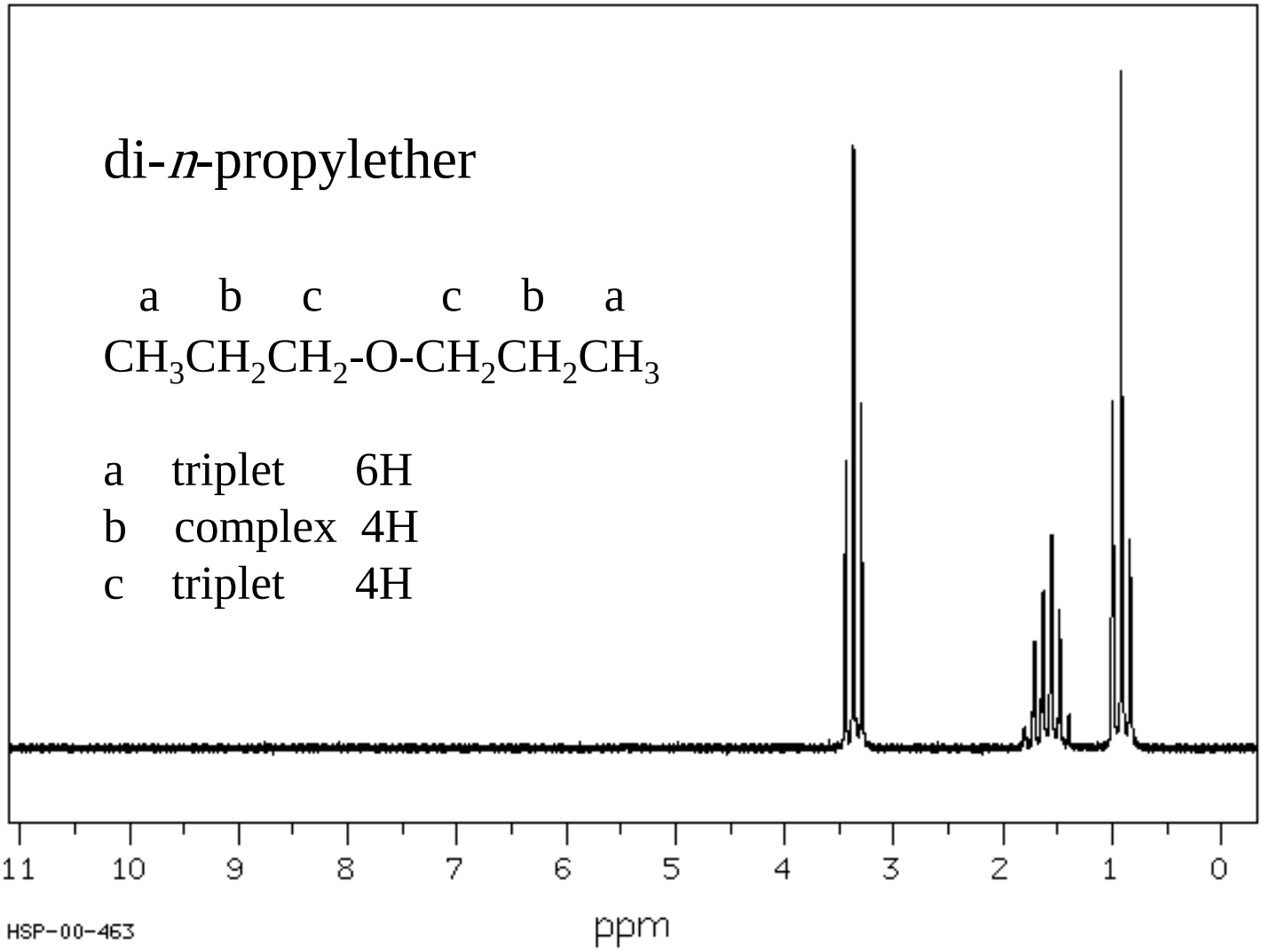

ethylbenzene
c
b a
CH2CH3
a triplet 3H
b quartet 2H
c ~singlet 5H
11
10
9
8
7
6
5
4
3
2
1
0
HSP-00-065
ppm

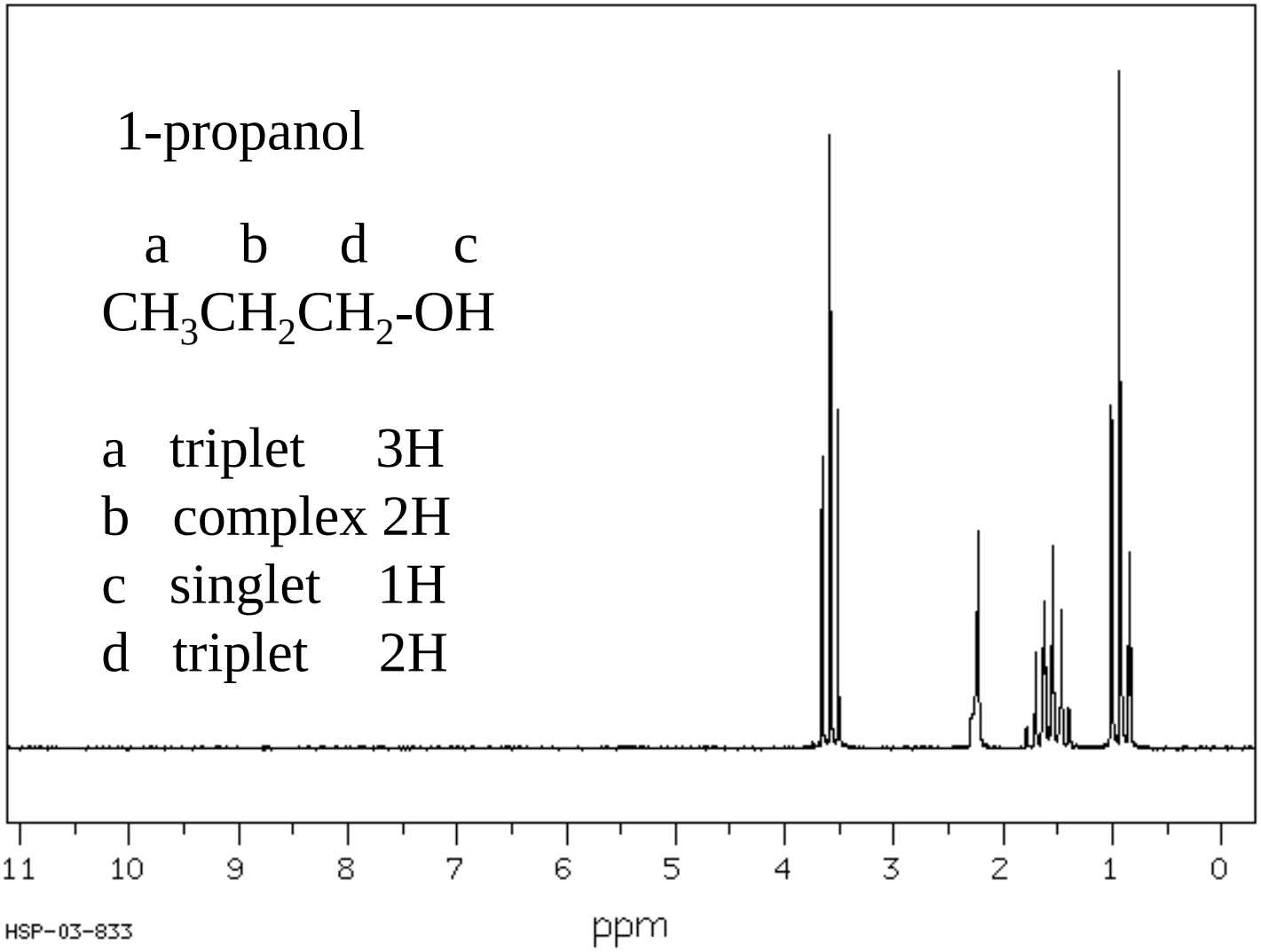

p-diethylbenzene
a b c b a
CH3CH2
CH2CH3
a triplet 6H
b quartet 4H
c singlet 4H
10 9 8 7 6 5 4 3 2 1 0
ppm
HSP-01-473


m-diethylbenzene
11
10
9
8
7
6
5
4
3
2
1
0
HSP-01-361
ppm

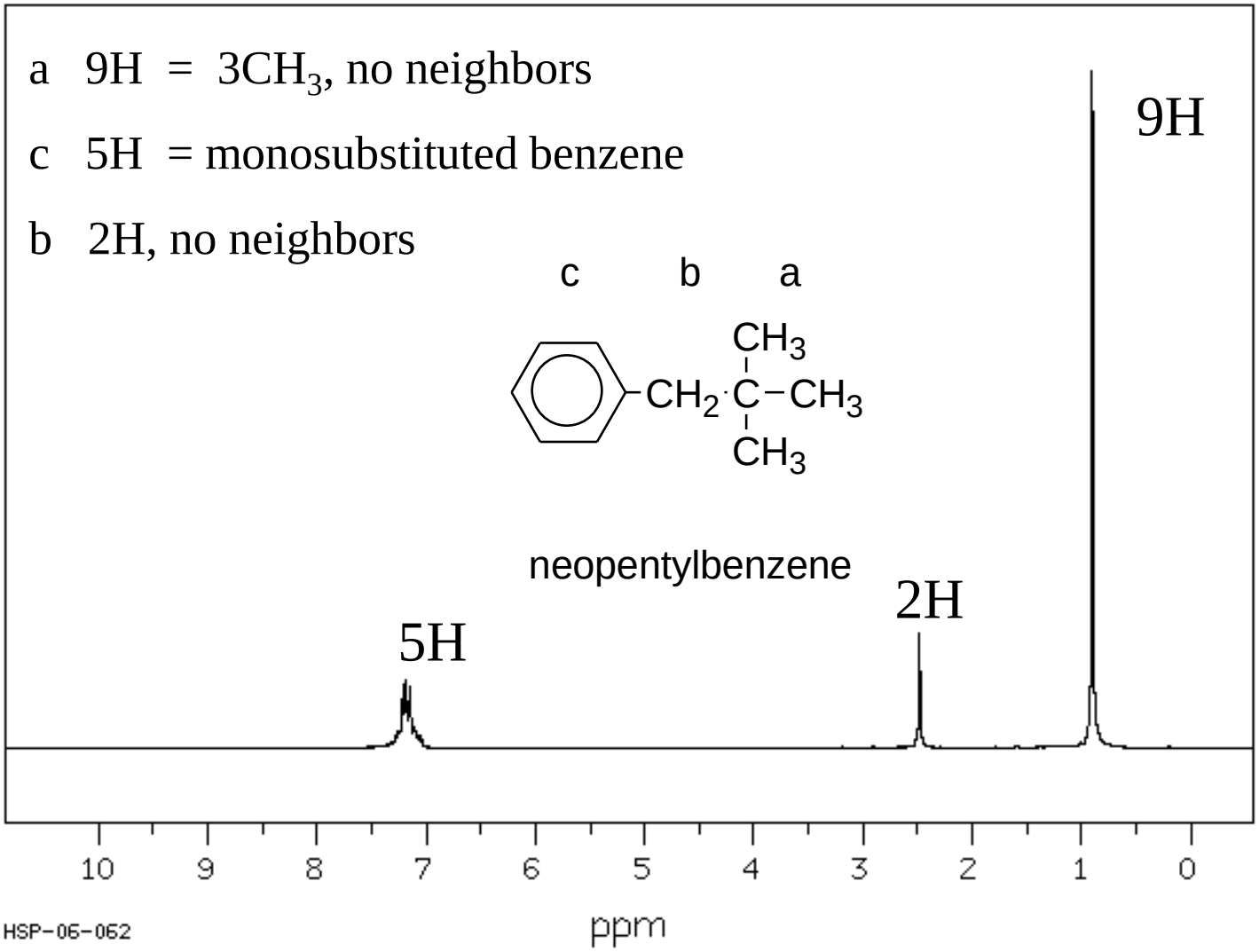

o-diethylbenzene
11
10
9
8
7
6
5
4
3
2
1
0
HSP-01-378
ppm


2-bromo-2-methylbutane
b
CH3
b CH3CCH2CH3 a
Br c
a triplet 3H
b singlet 6H
c quartet 2H b & c overlap
11 10 9 8 7 6 5 4 3 2 1 0
HSP-03-095
ppm


di-*n*-propylether
a b c c b a
$CH_3CH_2CH_2$-O-$CH_2CH_2CH_3$
a triplet 6H
b complex 4H
c triplet 4H
11 10 9 8 7 6 5 4 3 2 1 0
ppm
HSP-00-463


1-propanol
a b d c
CH3CH2CH2-OH
a triplet 3H
b complex 2H
c singlet 1H
d triplet 2H
11
10
9
8
7
6
5
4
3
2
1
0
HSP-03-833
ppm

$C_{11}H_{16}$

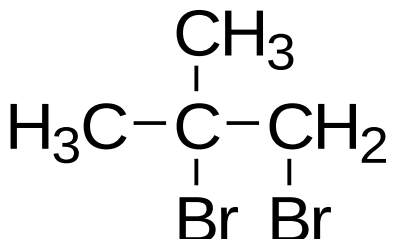

a 9H = 3CH3, no neighbors
c 5H = monosubstituted benzene
b 2H, no neighbors
c
b
a
CH3
CH2
C
CH3
CH3
neopentylbenzene
9H
2H
5H
10
9
8
7
6
5
4
3
2
1
0
ppm
HSP-06-062

$C_4H_8Br_2$

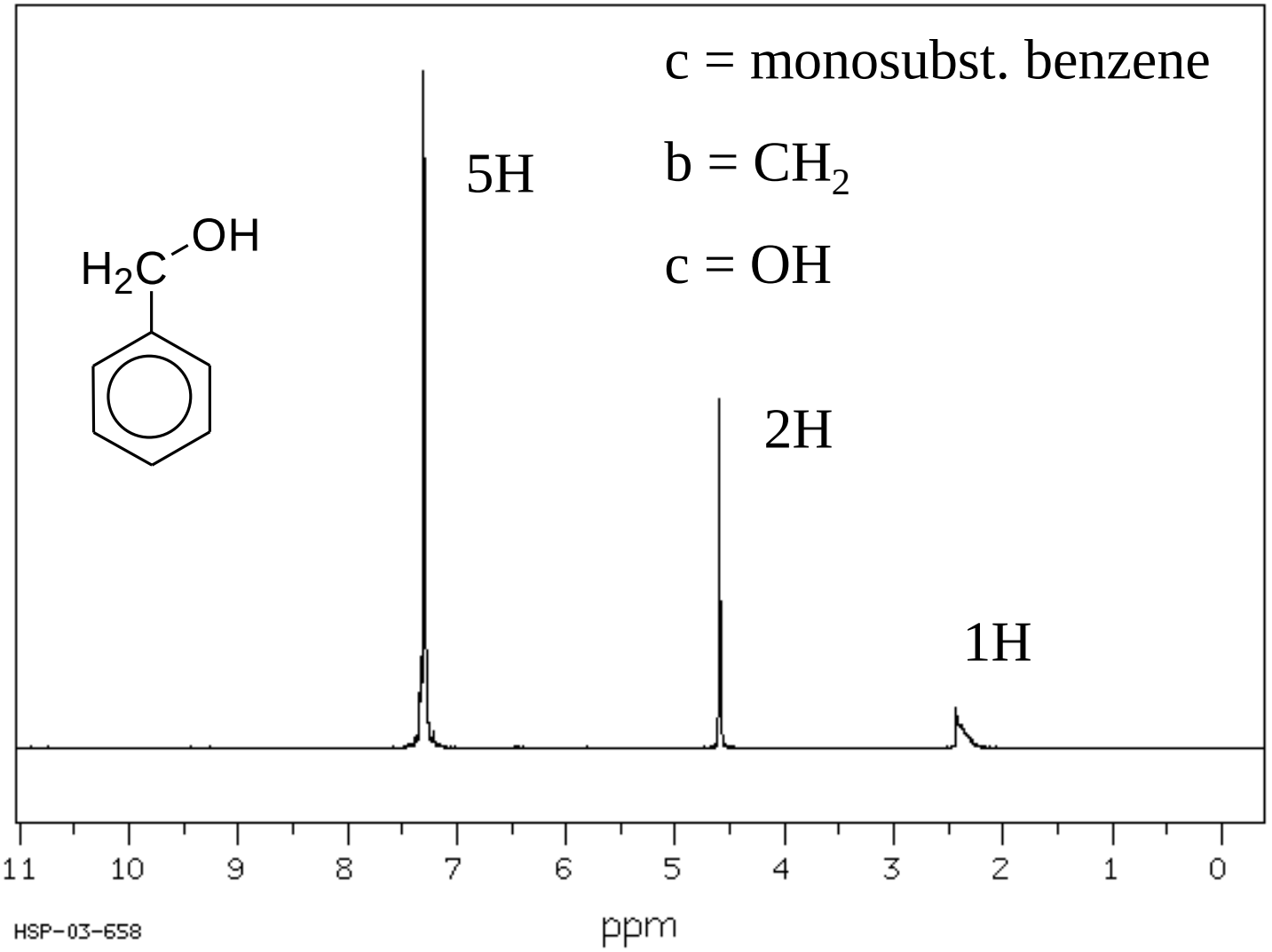
a = 6H, two CH_3 with no neighbors

$(CH_3)_2C$—

b = CH_2, no neighbors & shifted downfield due to Br



C_7H_8O

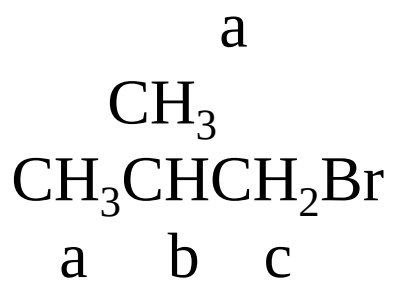

c = monosubst. benzene
b = CH2
c = OH
5H
2H
1H
H2C
OH
11
10
9
8
7
6
5
4
3
2
1
0
ppm
HSP-03-658

C_4H_9Br

a	doublet	1.04 ppm	6H
b	complex	1.95 ppm	1H
c	doublet	3.33 ppm	2H

a = two equivalent CH_3's with one neighboring H (b?)

c = CH_2 with one neighbor H (also b)



a	6H	doublet
b	1H	complex
c	2H	doublet

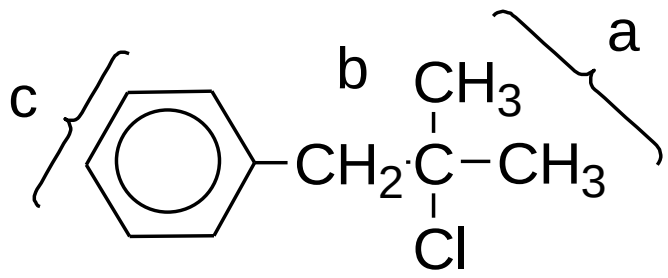
$C_{10}H_{13}Cl$

a singlet 1.57 ppm 6H
b singlet 3.07 ppm 2H
c singlet 7.27 ppm 5H

a = two-equilalent CH_3's with no neighbors

c = monosubstituted benzene ring

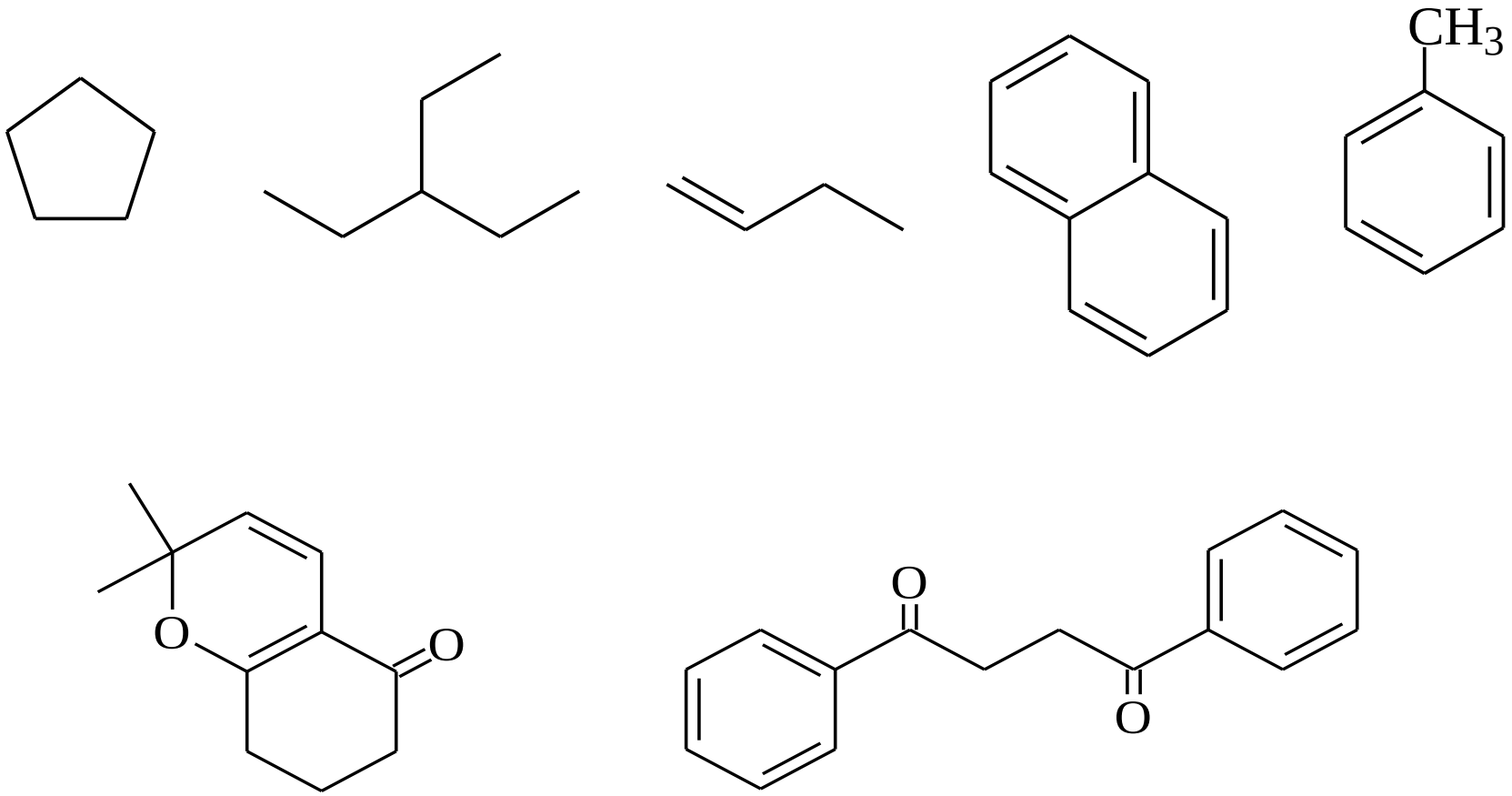
b = CH_2



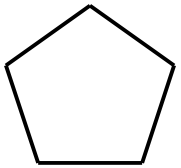
a singlet 6H
b singlet 2H
c singlet 5H

Chemical Equivalence

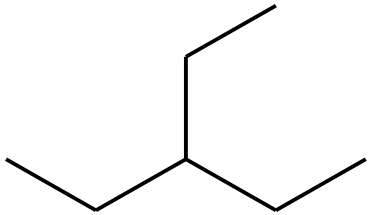
How many signals in ^{1}H NMR spectrum?



Number of Equivalent Protons

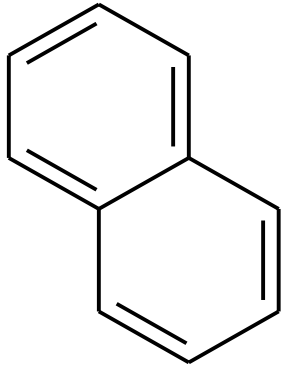


1

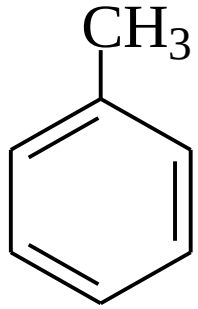


3

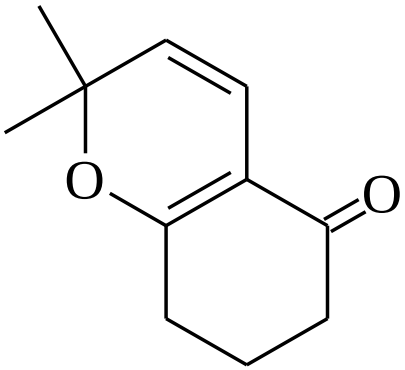
5



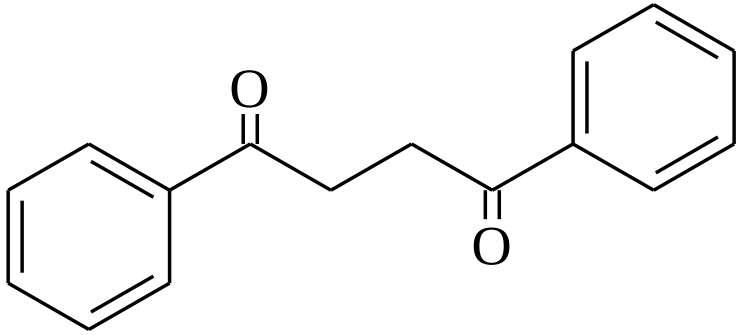
2



4



6

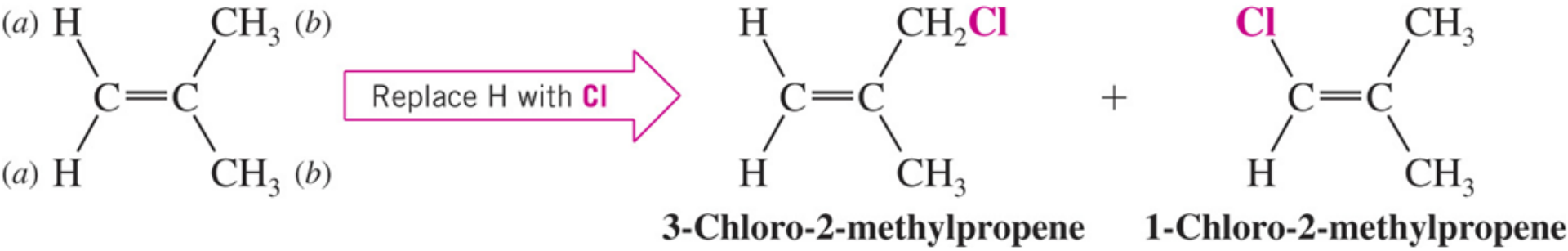


4

Homotopic H's

– **Homotopic Hydrogens**

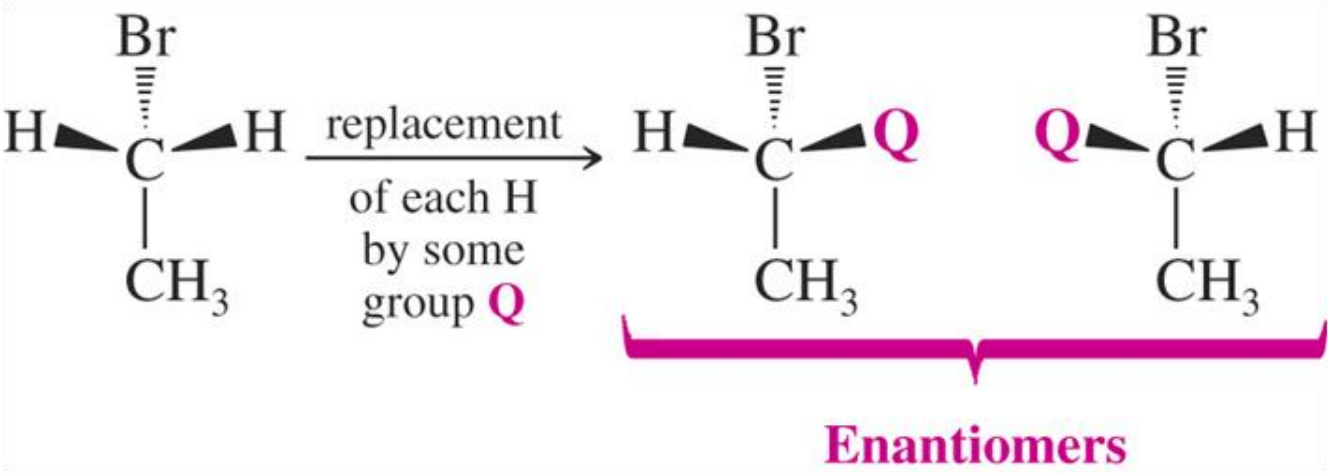
- **Hydrogens are chemically equivalent or homotopic if replacing each one in turn by the same group would lead to an identical compound**



3-Chloro-2-methylpropene **1-Chloro-2-methylpropene**

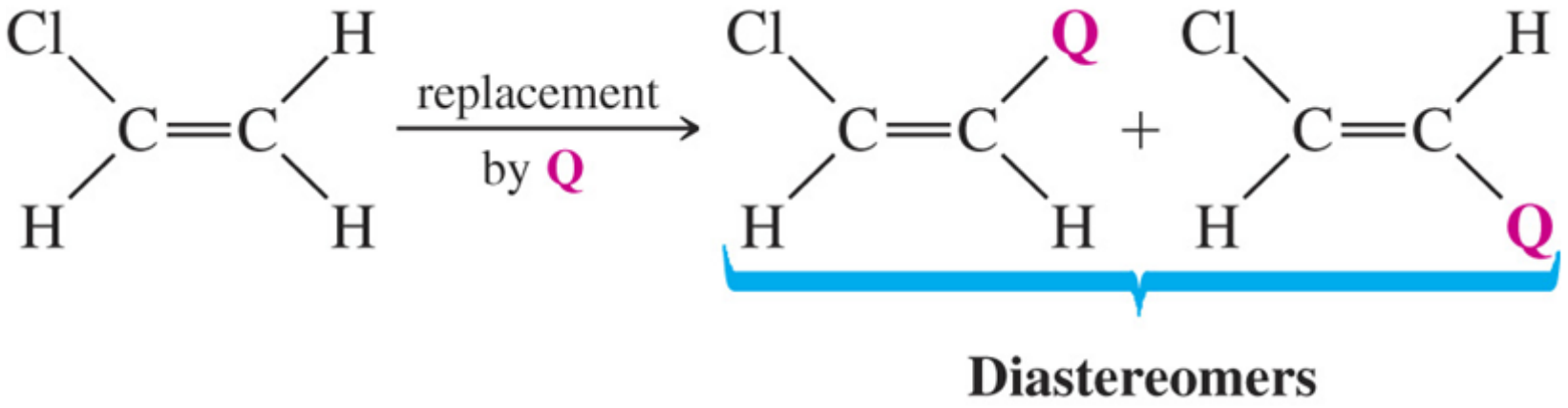
Enantiotopic H's

- **If replacement of each of two hydrogens by some group leads to enantiomers, those hydrogens are enantiotopic**

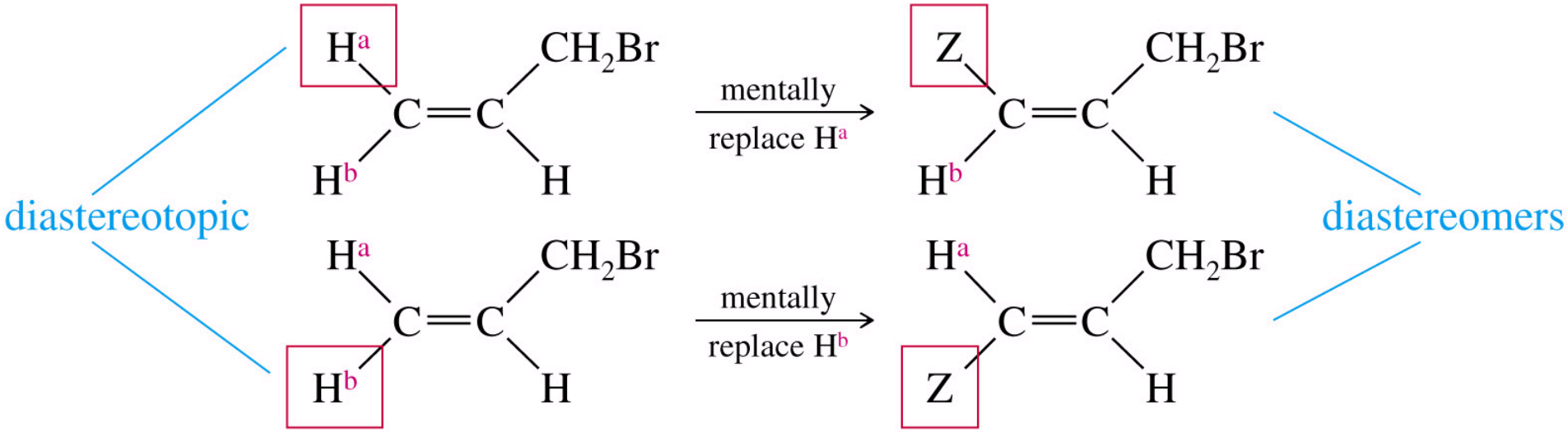


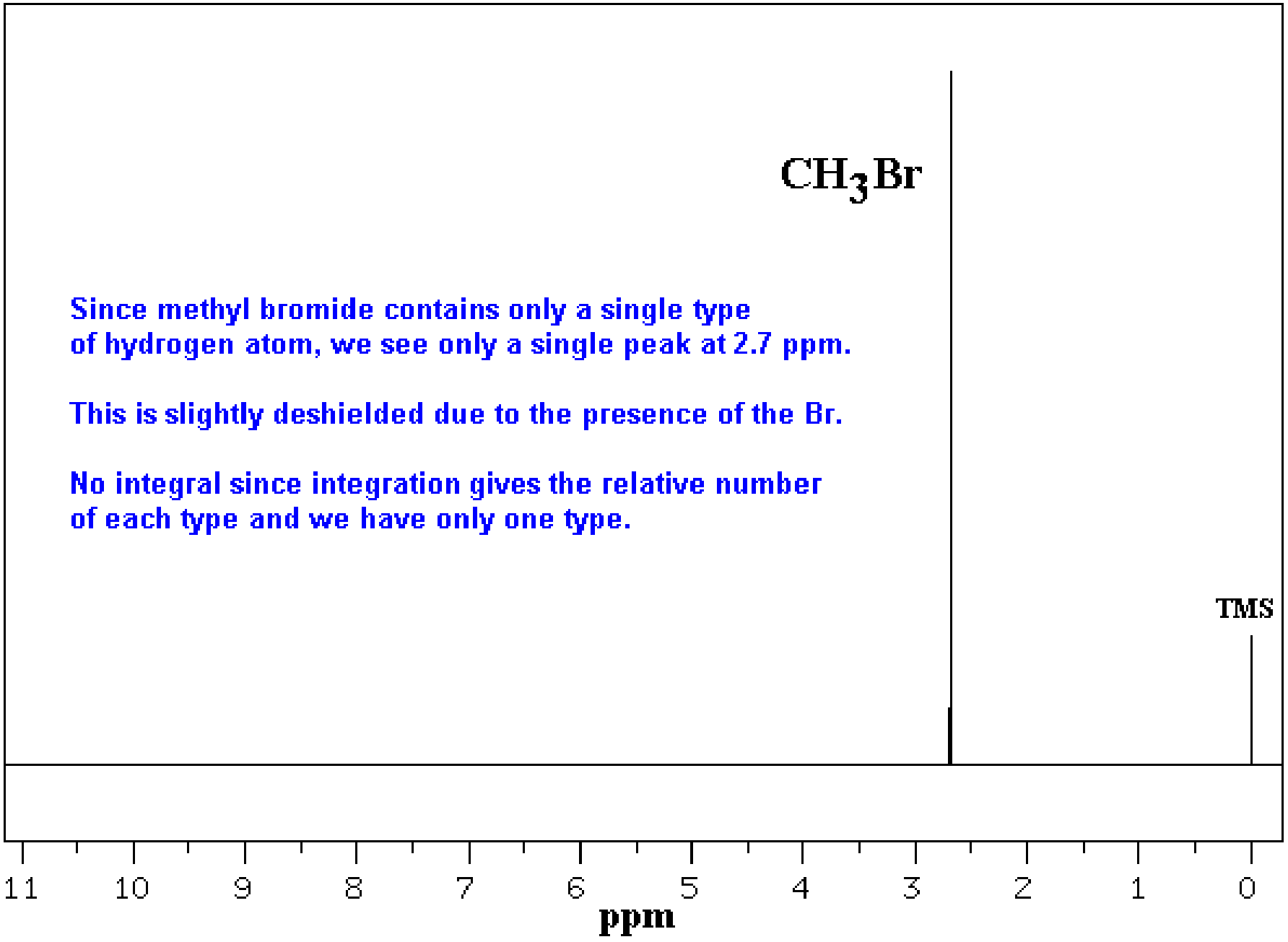
Diastereotopic H's

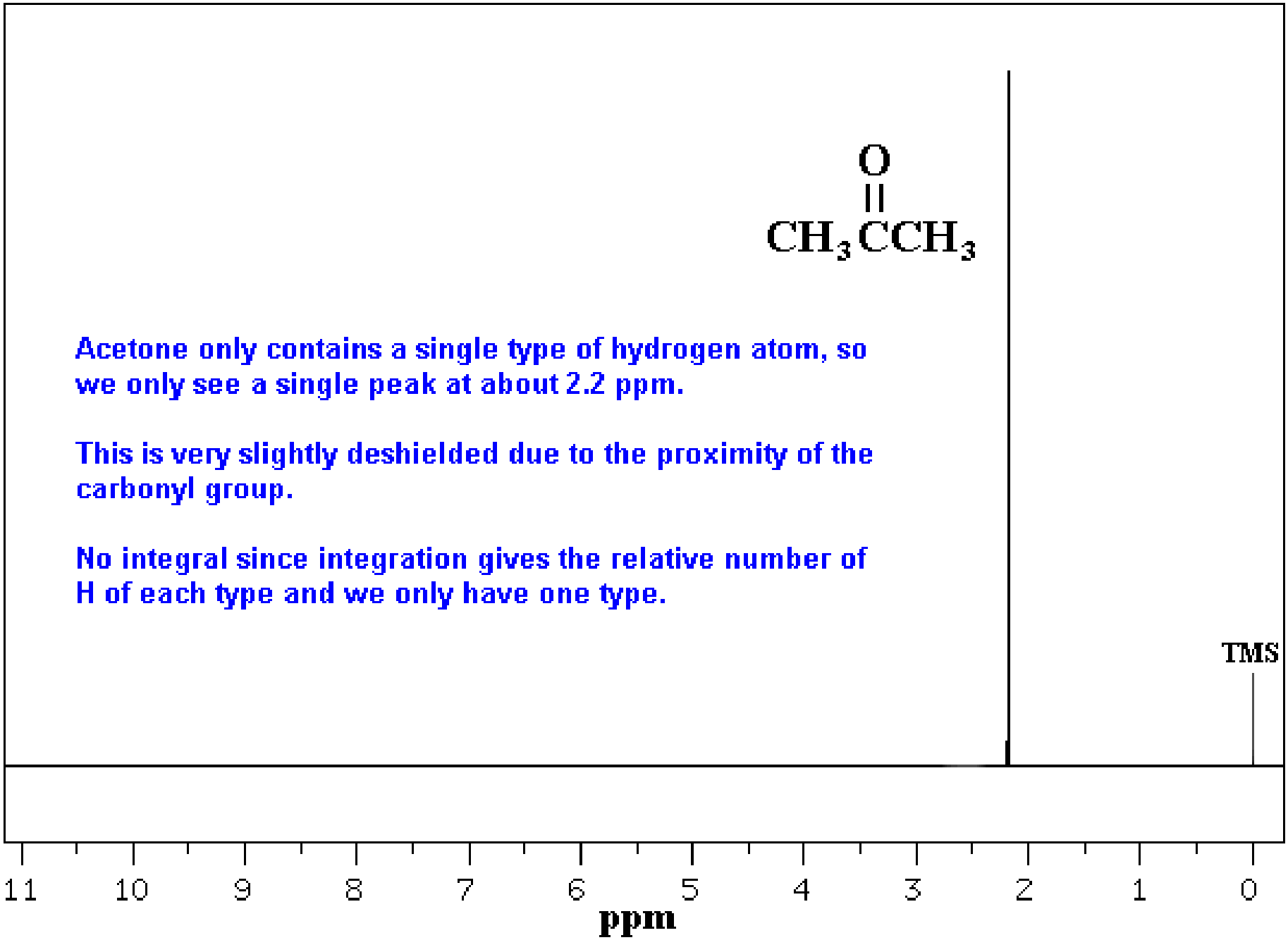
- **If replacement of each of two hydrogens by some group leads to diastereomers, the hydrogens are diastereotopic**
  - **Diastereotopic hydrogens have different chemical shifts and will give different signals**

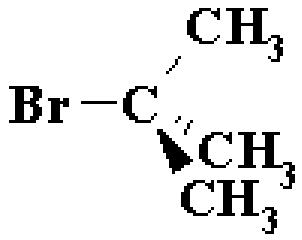


Vinyl Protons




CH_3Br
Since methyl bromide contains only a single type of hydrogen atom, we see only a single peak at 2.7 ppm.
This is slightly deshielded due to the presence of the Br.
No integral since integration gives the relative number of each type and we have only one type.
TMS
11
10
9
8
7
6
5
4
3
2
1
0
ppm

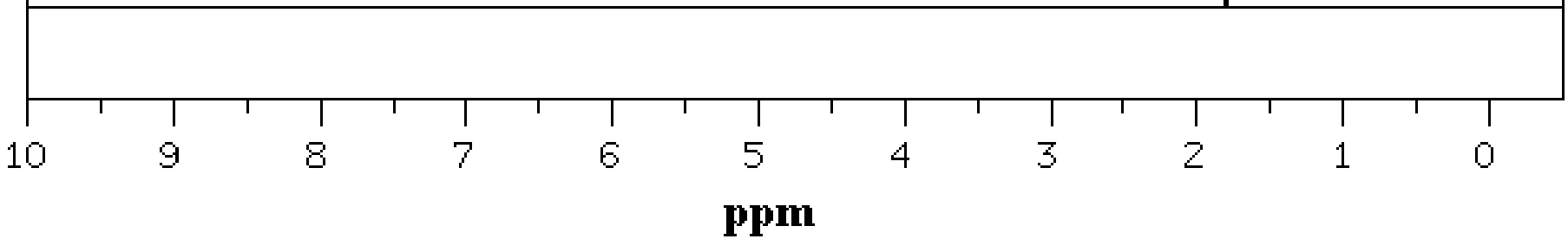

O
CH3CCH3
Acetone only contains a single type of hydrogen atom, so we only see a single peak at about 2.2 ppm.
This is very slightly deshielded due to the proximity of the carbonyl group.
No integral since integration gives the relative number of H of each type and we only have one type.
TMS
11
10
9
8
7
6
5
4
3
2
1
0
ppm

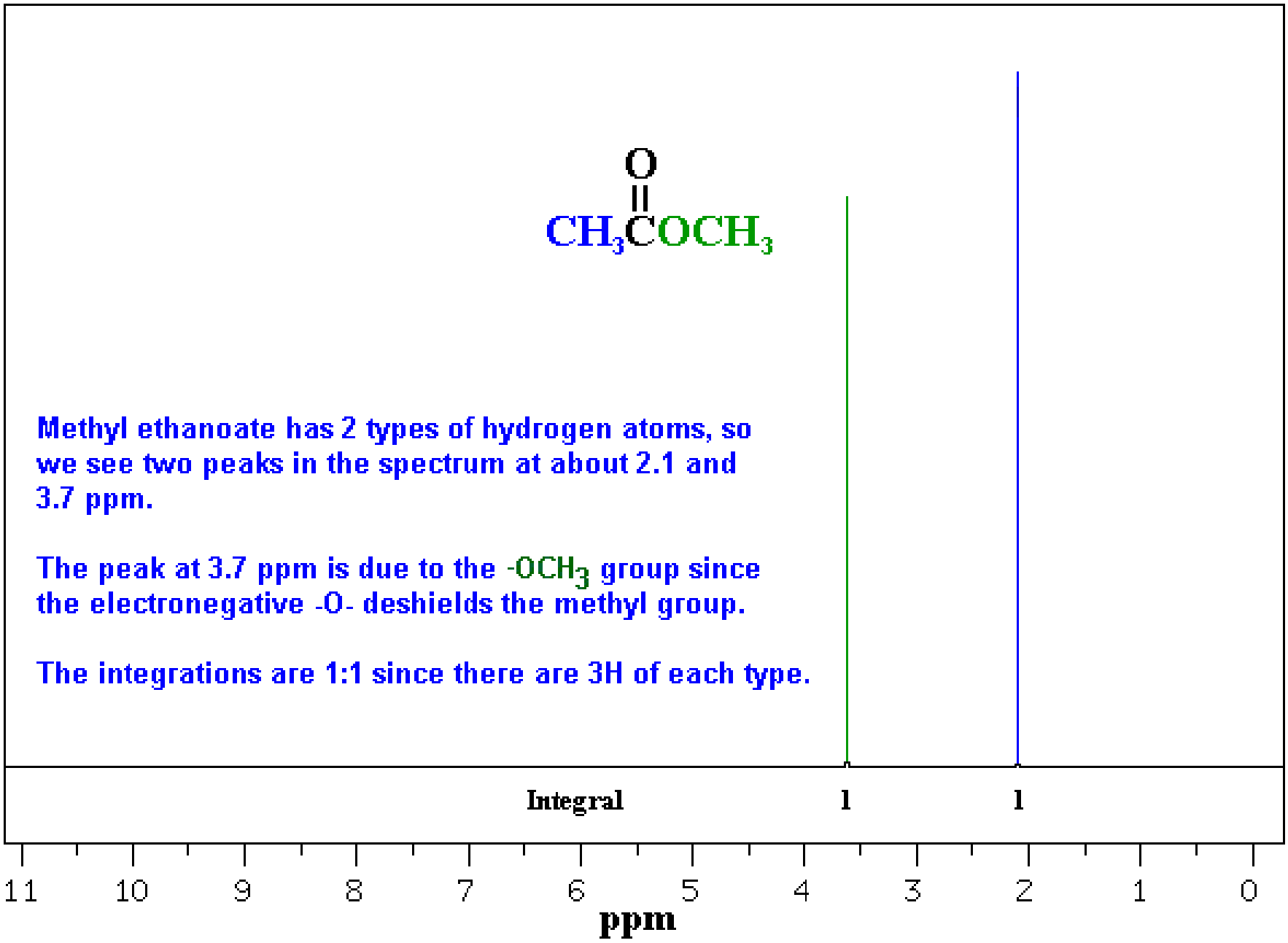


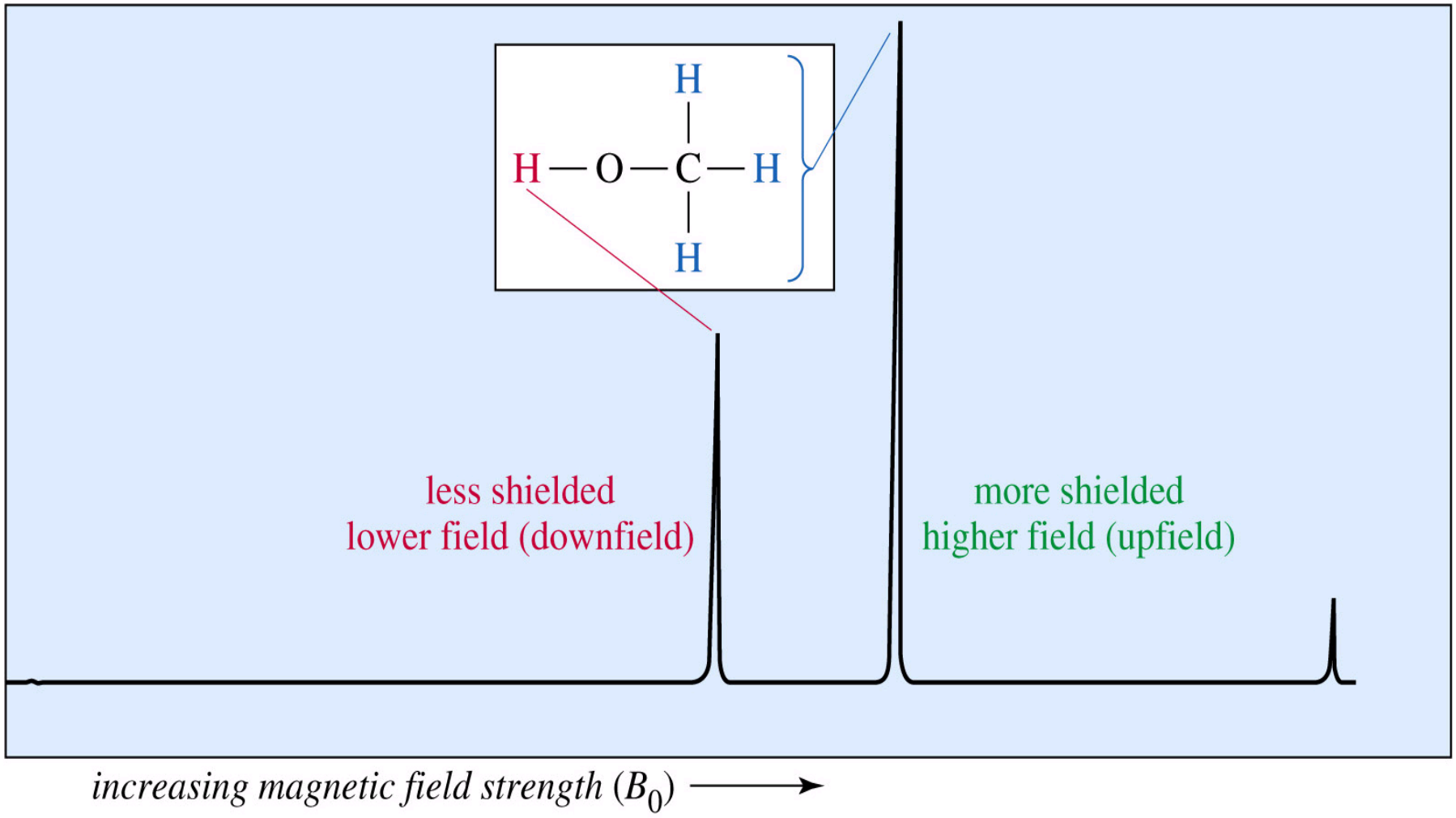
Since t-butyl bromide contains only a single type of hydrogen atom, we see only a single peak at 1.8 ppm.

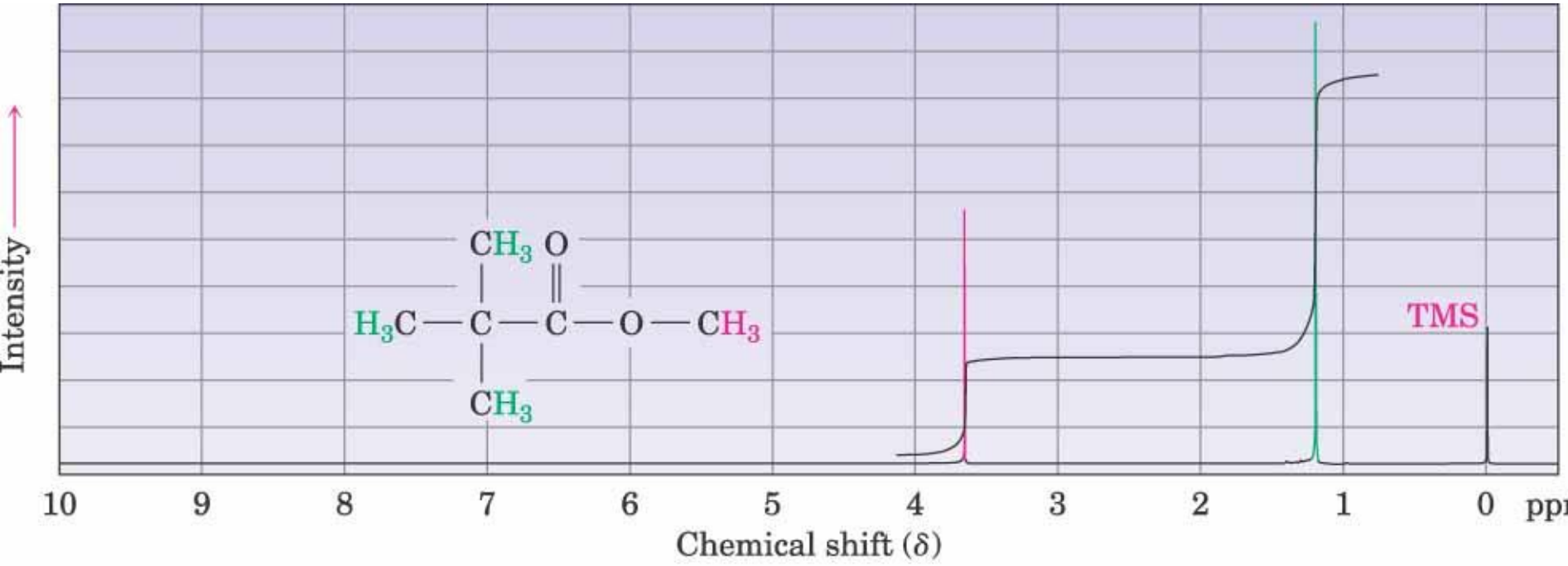
Since the Br atom is further away from the H atoms than methyl bromide, there is less deshielding than in methyl bromide.

No integral since integration gives the relative number of each type, and we have only one type.



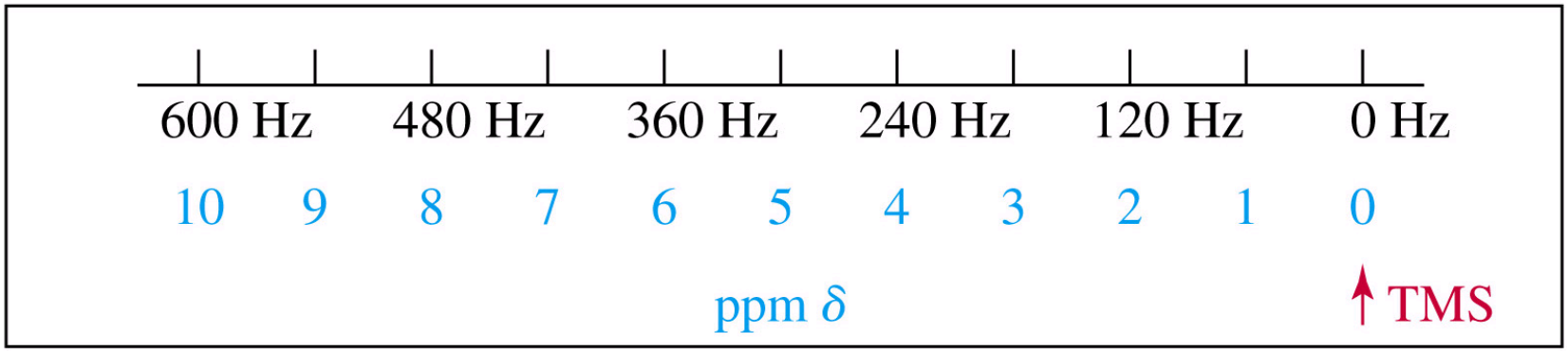

O
CH3COCH3
Methyl ethanoate has 2 types of hydrogen atoms, so we see two peaks in the spectrum at about 2.1 and 3.7 ppm.
The peak at 3.7 ppm is due to the -OCH3 group since the electronegative -O- deshields the methyl group.
The integrations are 1:1 since there are 3H of each type.
Integral
1
1
11
10
9
8
7
6
5
4
3
2
1
0
ppm


H
H — O — C — H
H
less shielded
lower field (downfield)
more shielded
higher field (upfield)
increasing magnetic field strength (B_0) ⟶

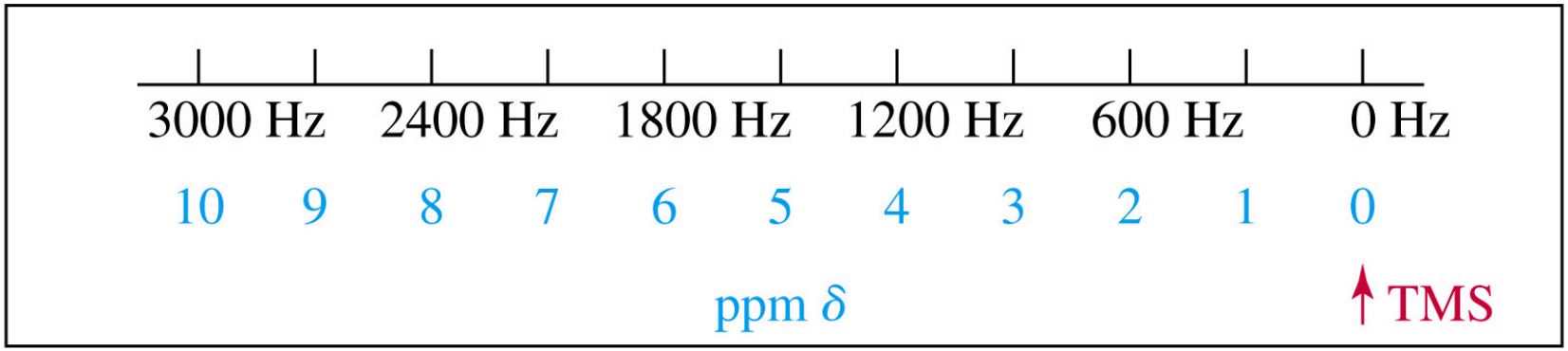


The δ Scale

$$\text{chemical shift, ppm } \delta = \frac{\text{shift downfield from TMS (in Hz)}}{\text{spectrometer frequency (in MHz)}}$$



60 MHz

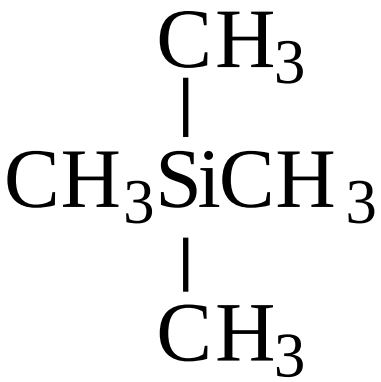


300 MHz

Tetramethylsilane (TMS)

Arbitrarily assigned a chemical shi

of δ 0.00



TMS

Chemical Shift Ranges, ppm

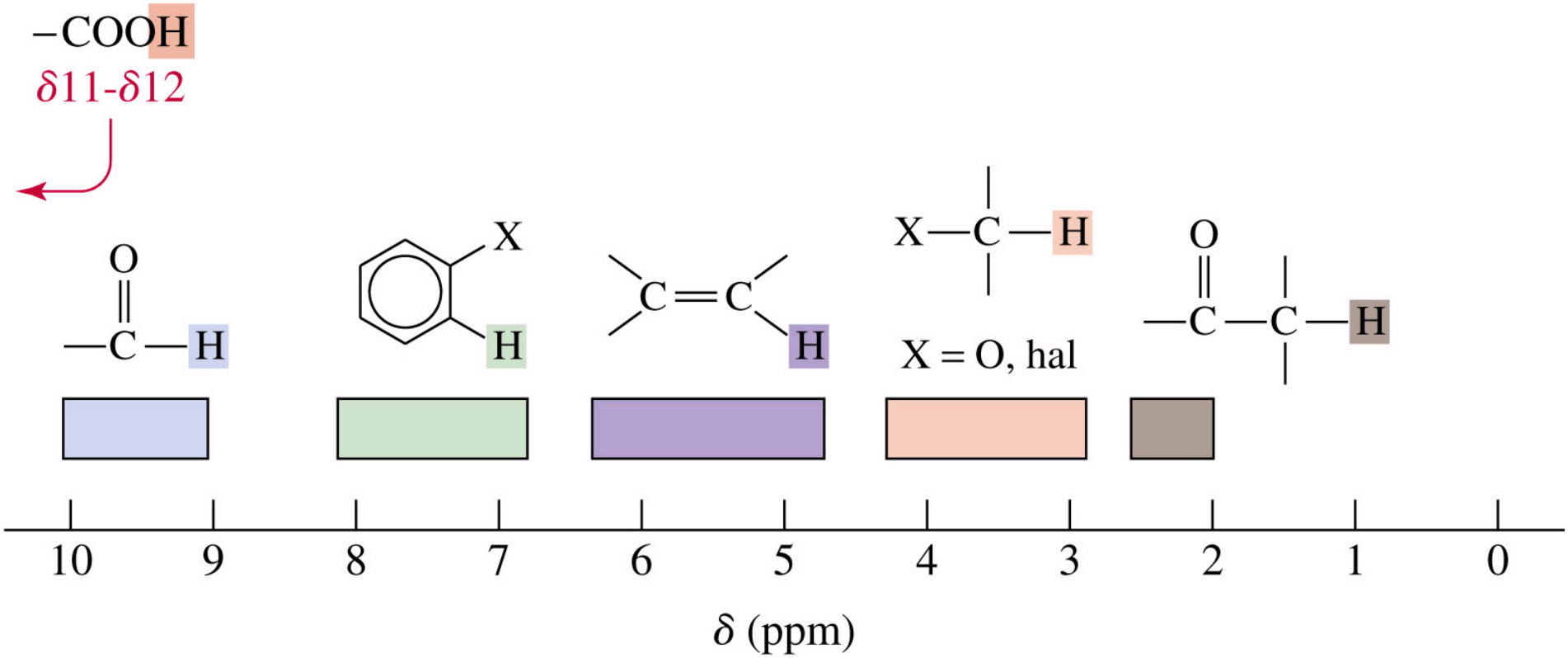
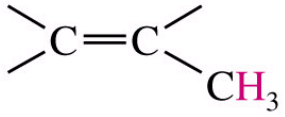
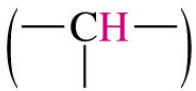
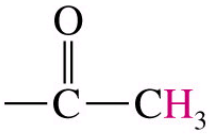
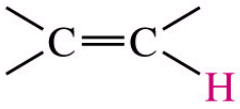
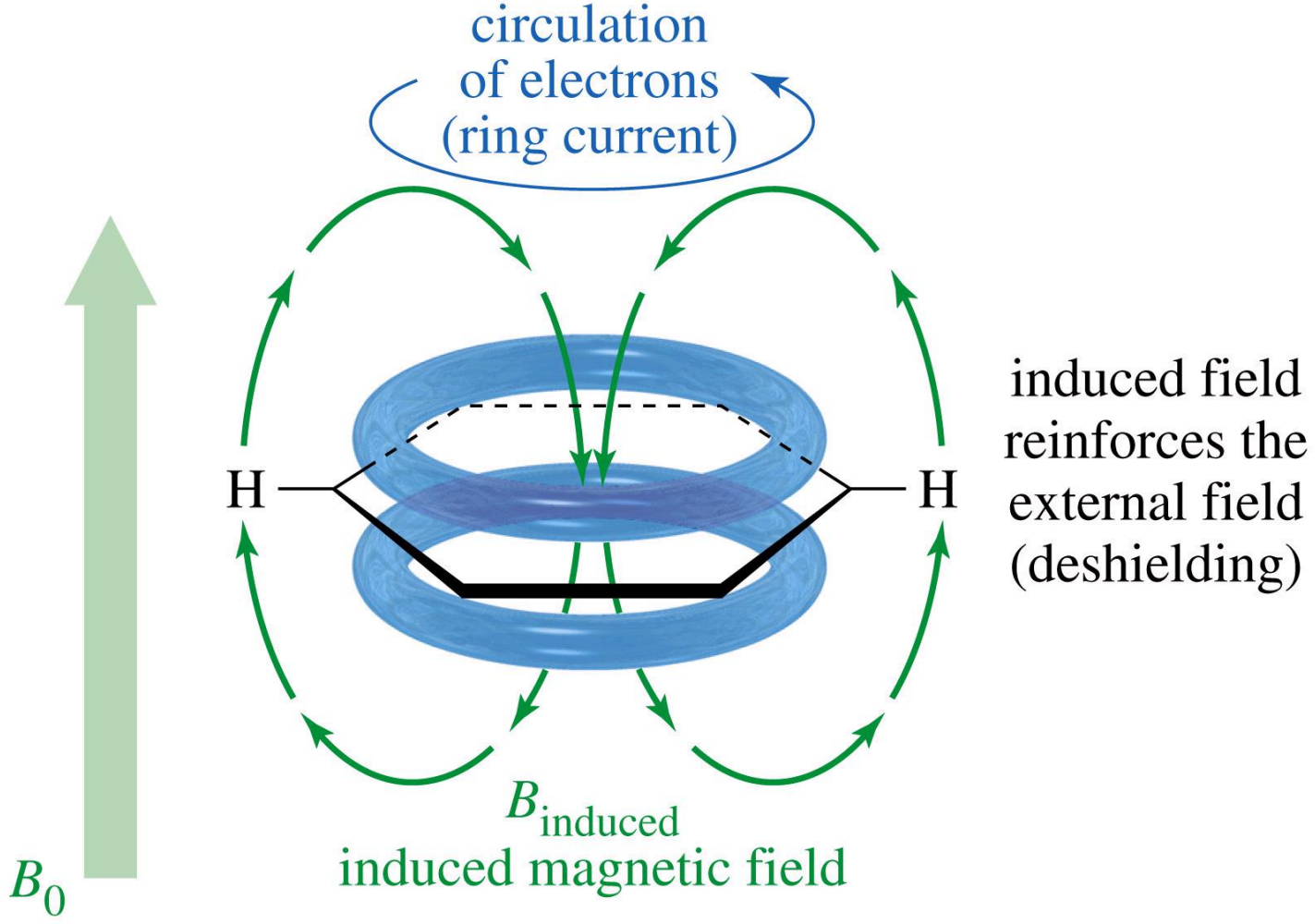


TABLE 13-3 Typical Values of Chemical Shifts

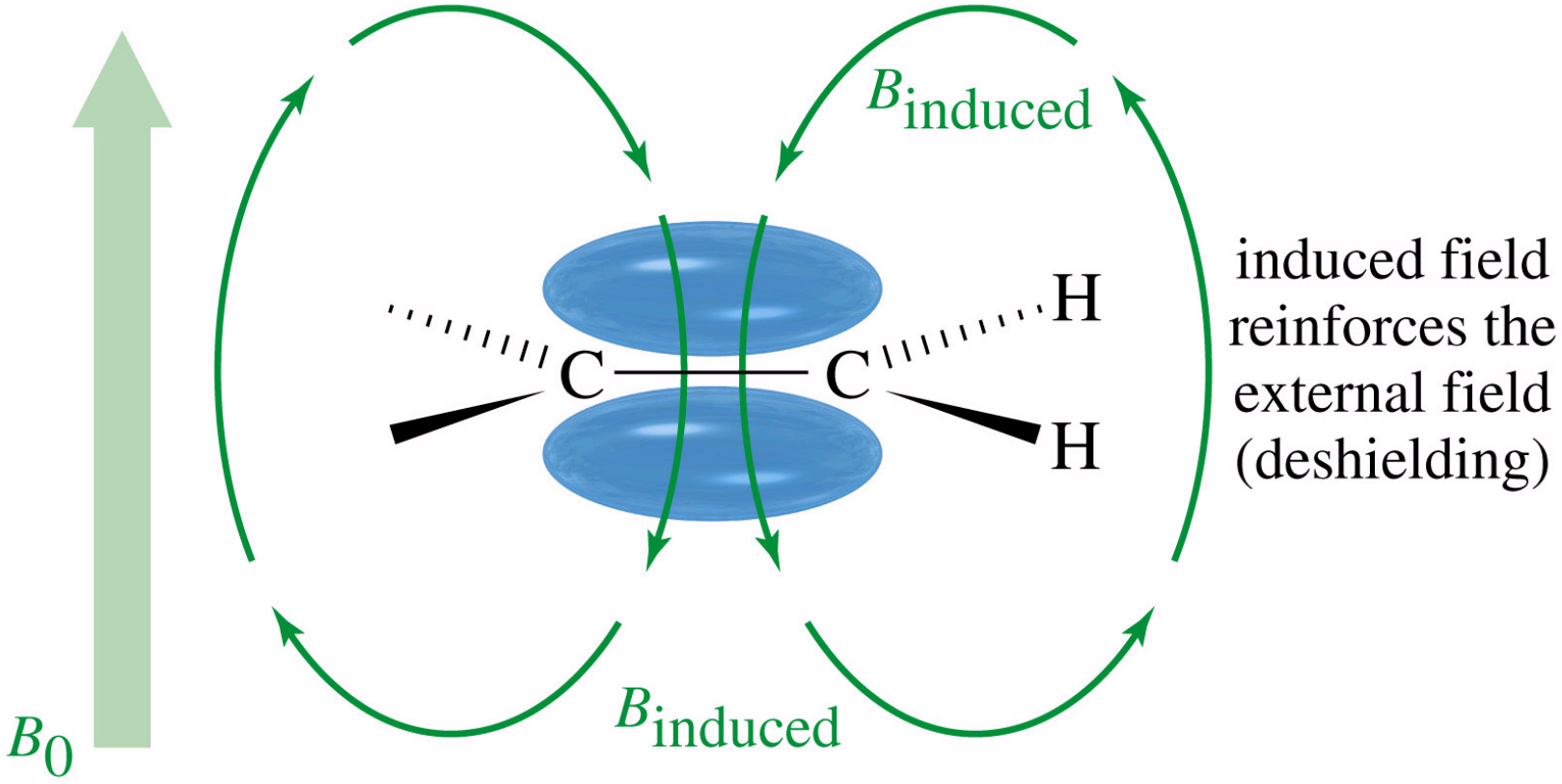
Type of Proton	Approximate δ	Type of Proton	Approximate δ
alkane ($-CH_3$)	0.9		1.7
alkane ($-CH_2-$)	1.3	Ph—H	7.2
alkane 	1.4	Ph—CH_3	2.3
	2.1	R—CHO	9–10
—C≡C—H	2.5	R—COOH	10–12
R—CH_2—X (X = halogen, O)	3–4	R—OH	variable, about 2–5
	5–6	Ar—OH	variable, about 4–7
		R—NH_2	variable, about 1.5–4

Note: These values are approximate, as all chemical shifts are affected by neighboring substituents. The numbers given here assume that alkyl groups are the only other substituents present. A more complete table of chemical shifts appears in Appendix 1.

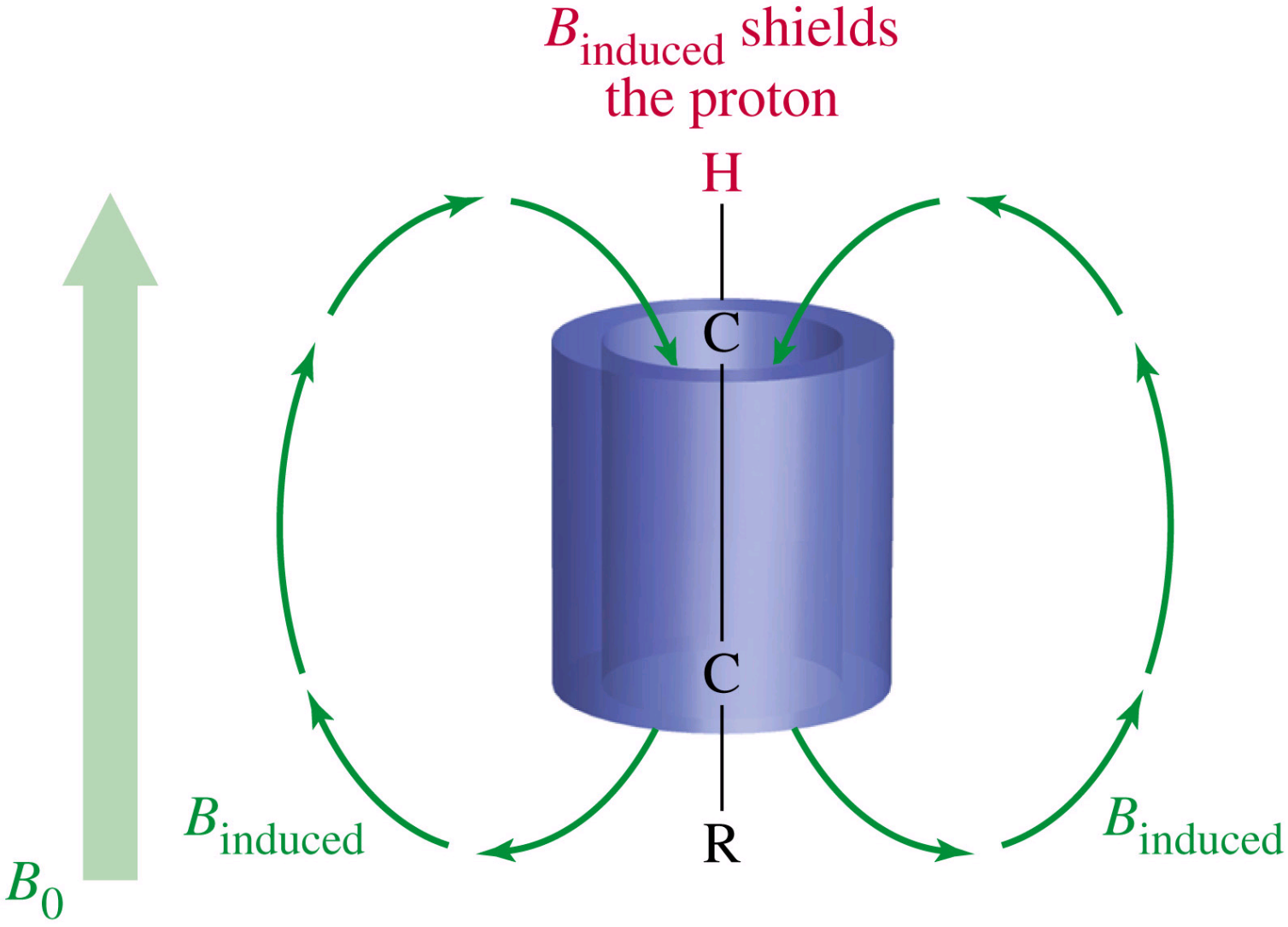
Diamagnetic Anisotropy
Shielding and Deshielding



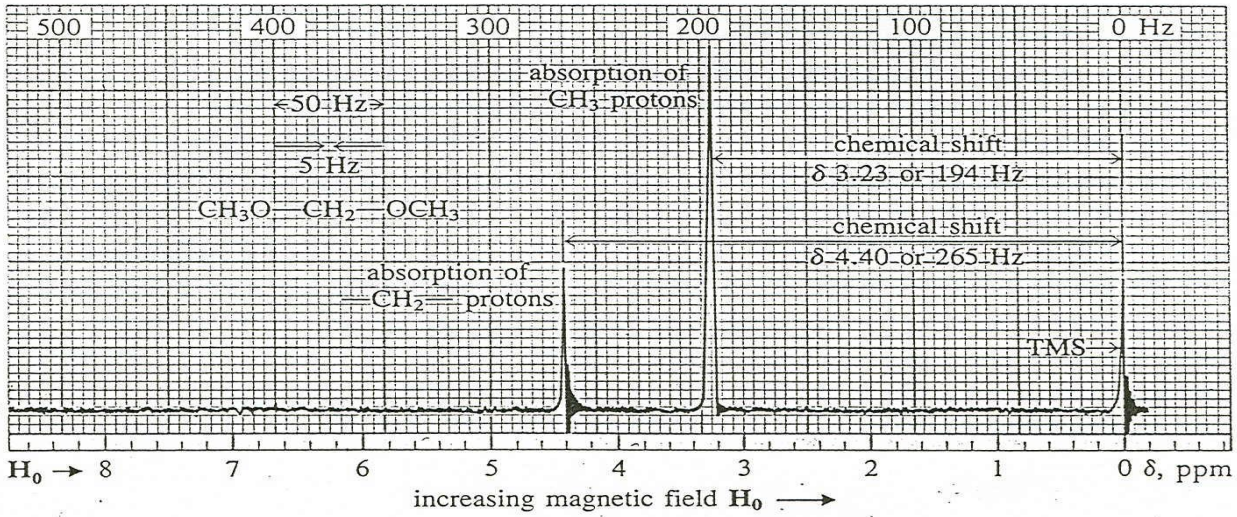
Deshielding in Alkenes

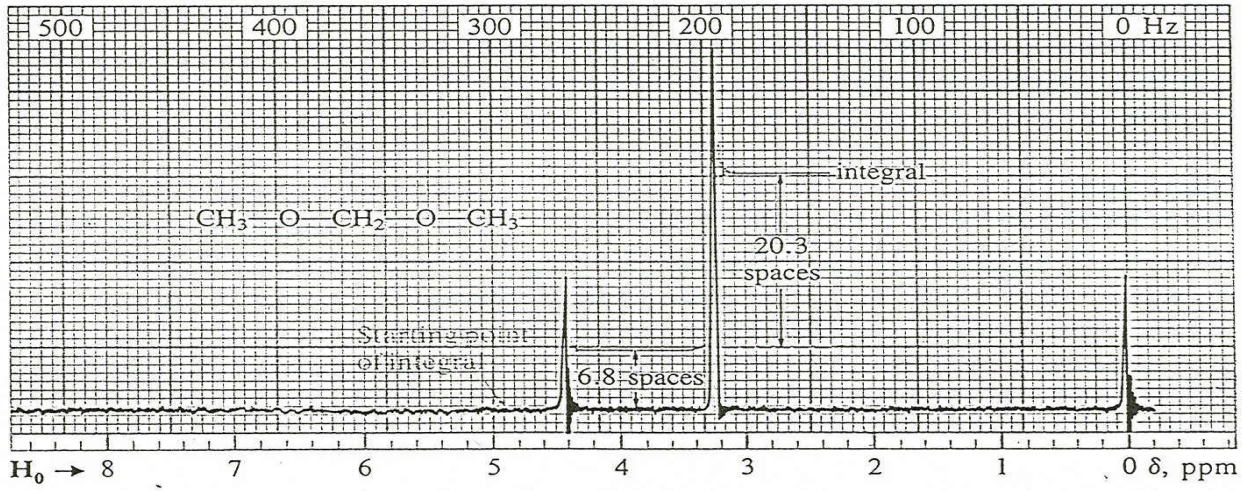


Shielding in Alkynes



NMR spectrum of dimethoxymethane without integral (top) and with integral (bottom) (Figs. 13.2 and 13.3)





Integration

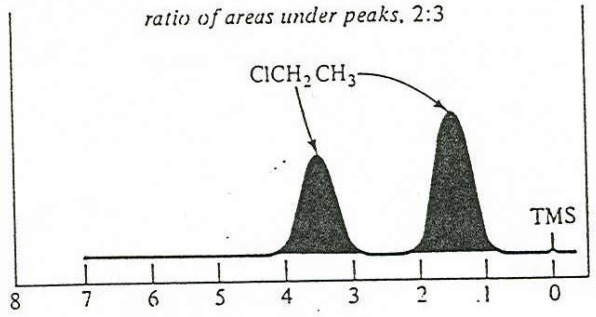
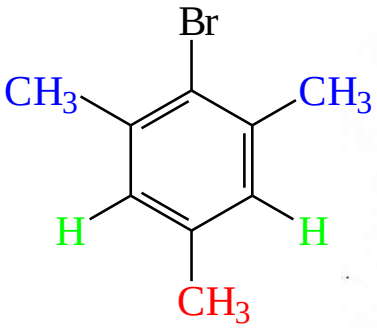


FIGURE 8.29



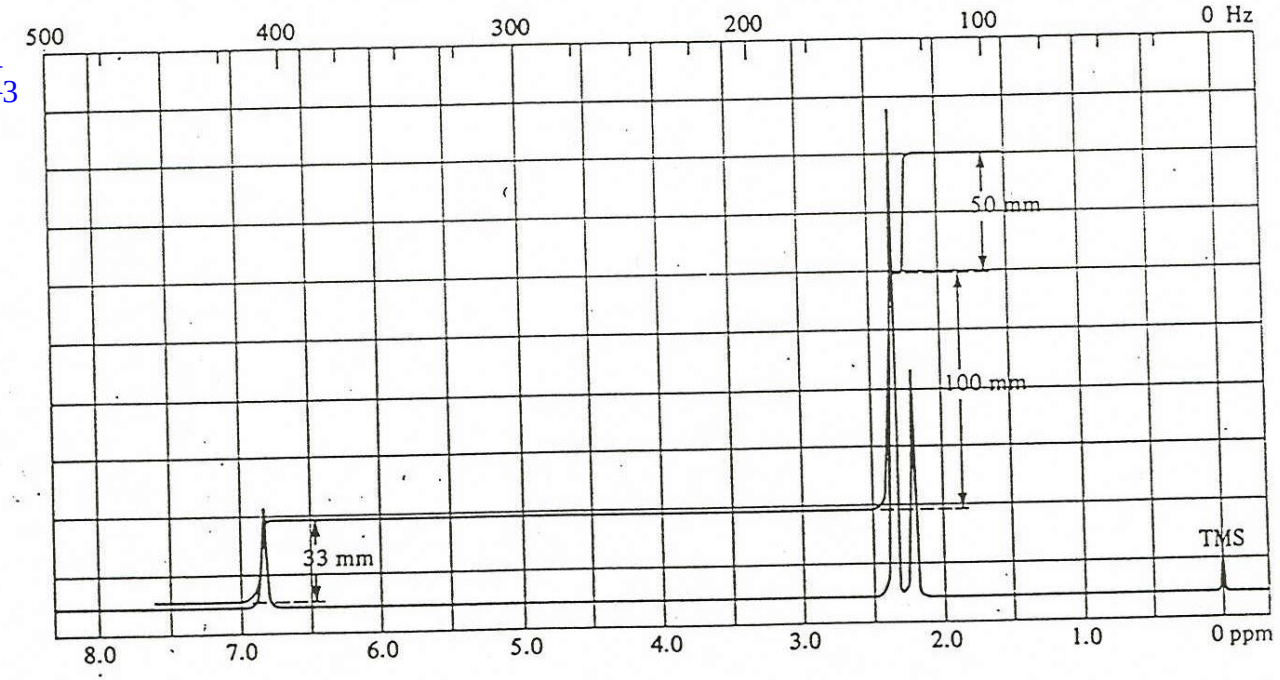
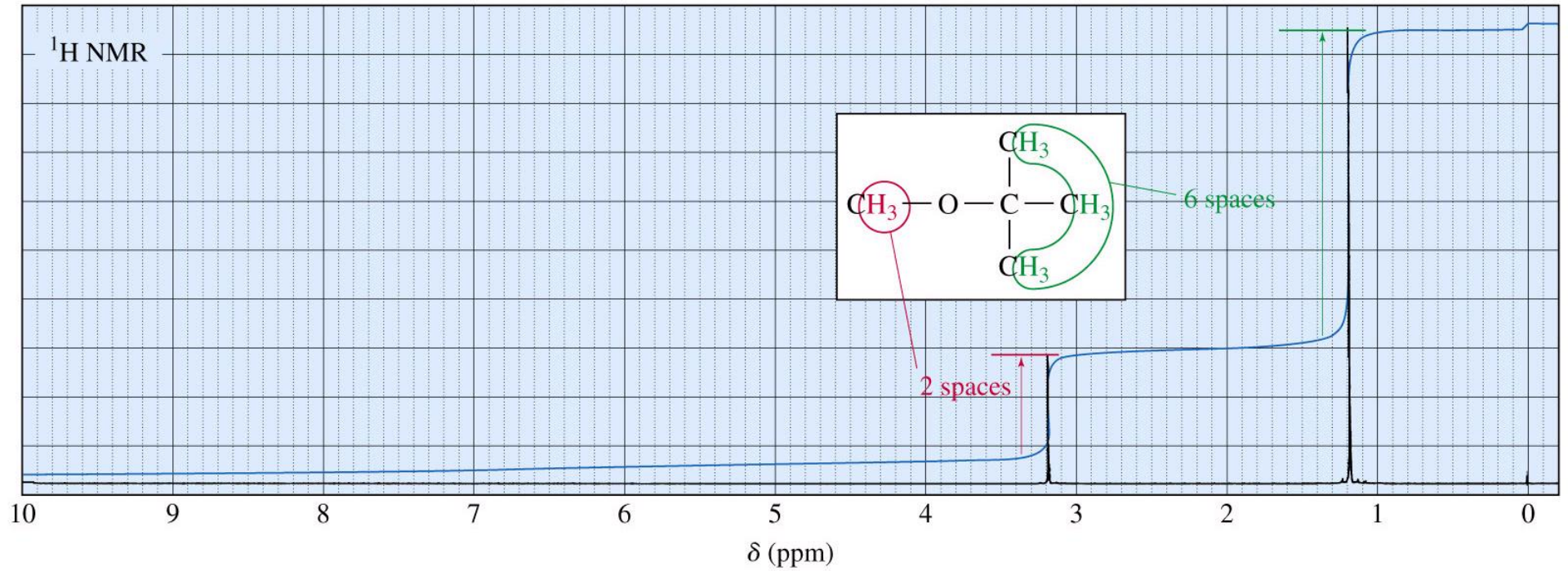
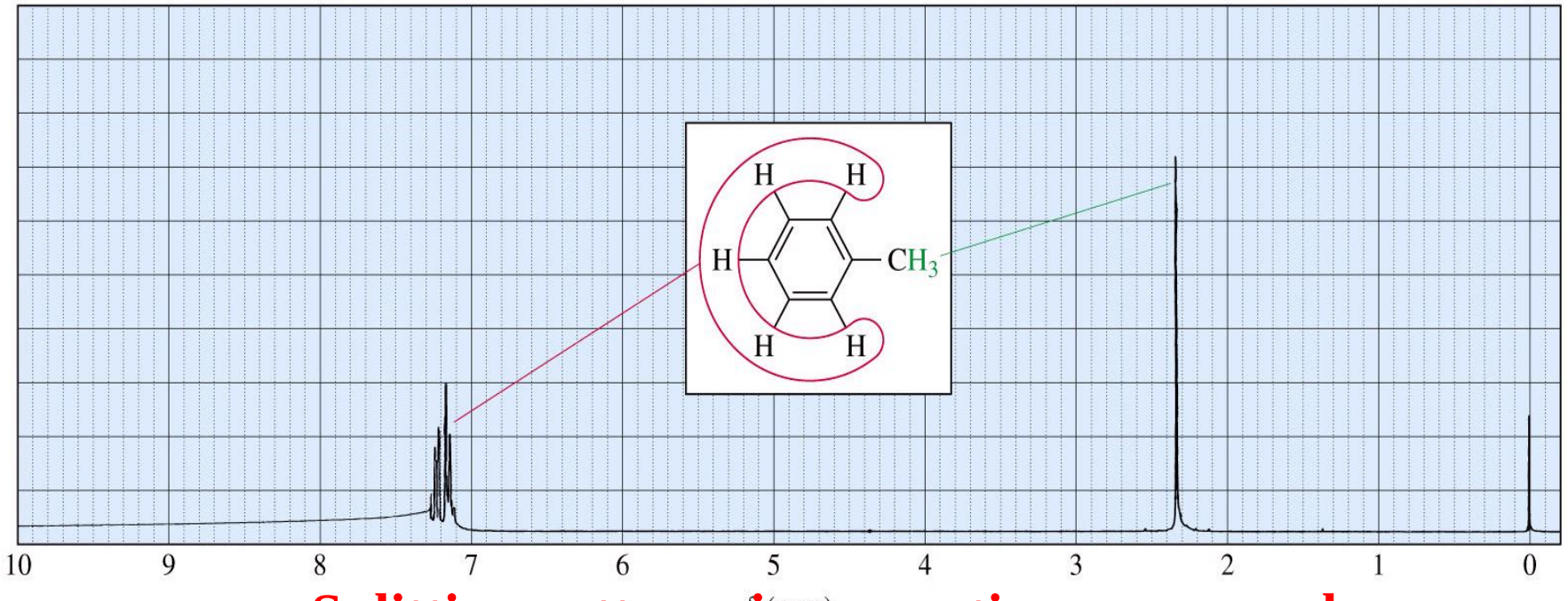


FIGURE 8.30

Methyl *t*-butyl ether (MTBE)



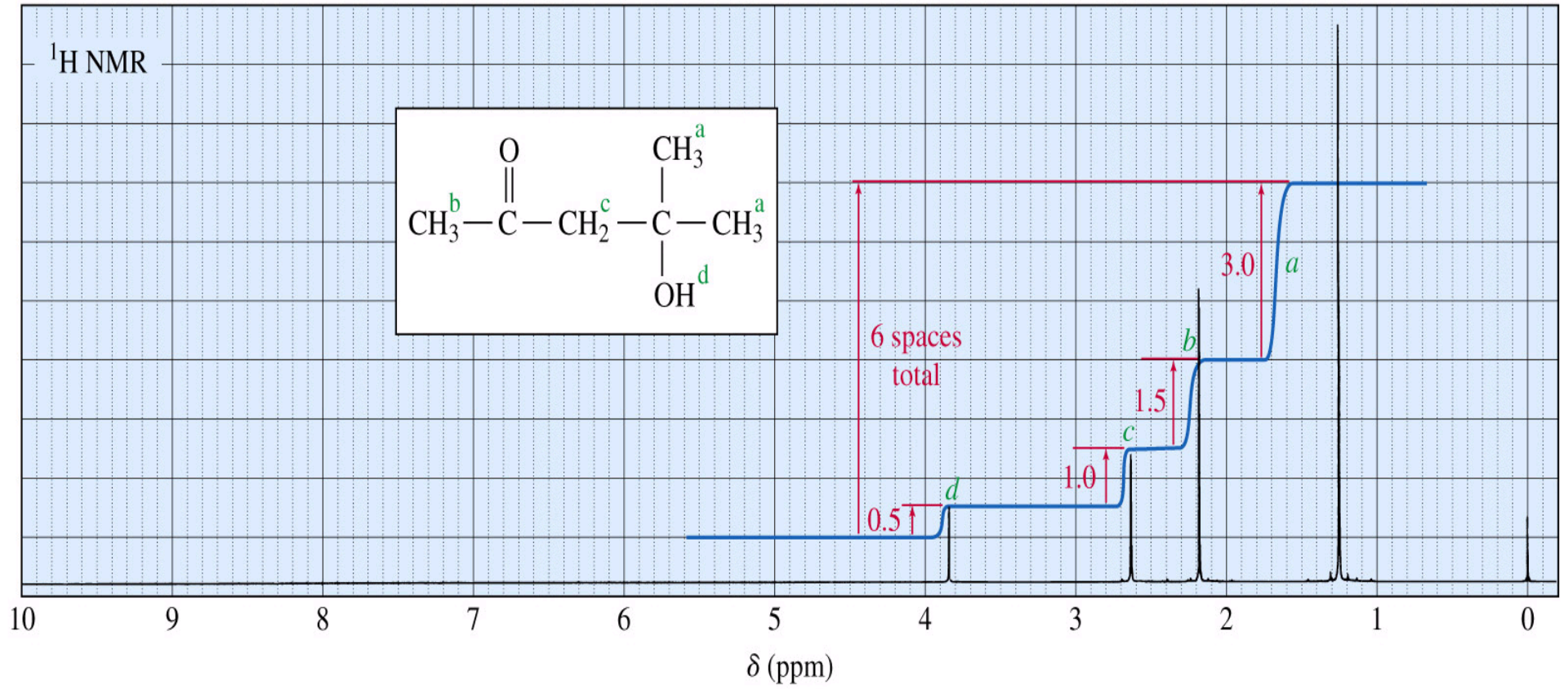
Toluene at Higher Field



Splitting patterns in aromatic groups can be confusing

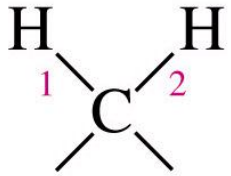
A monosubstituted aromatic ring can appear as an apparent singlet or a complex pattern of peaks

Integral Trace



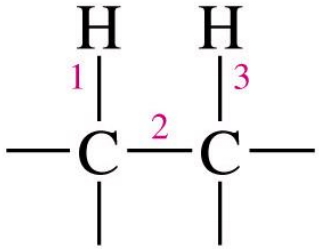
Spin-Spin Splitting

Bonded to the same carbon: two bonds between protons



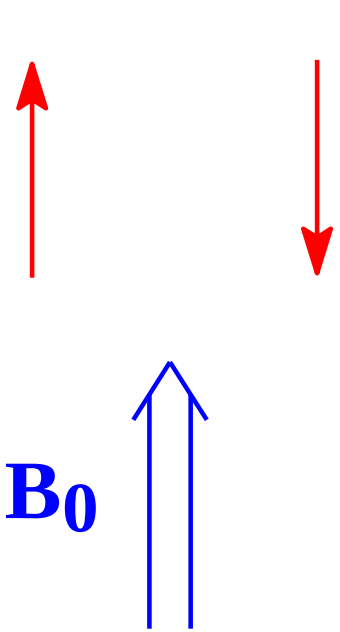
spin-spin splitting is normally observed
(if nonequivalent)

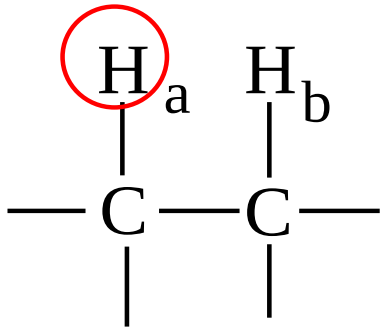
Bonded to adjacent carbons: three bonds between protons



spin-spin splitting is normally observed
(this is the most common case)

The Doublet in ^{1}H NMR



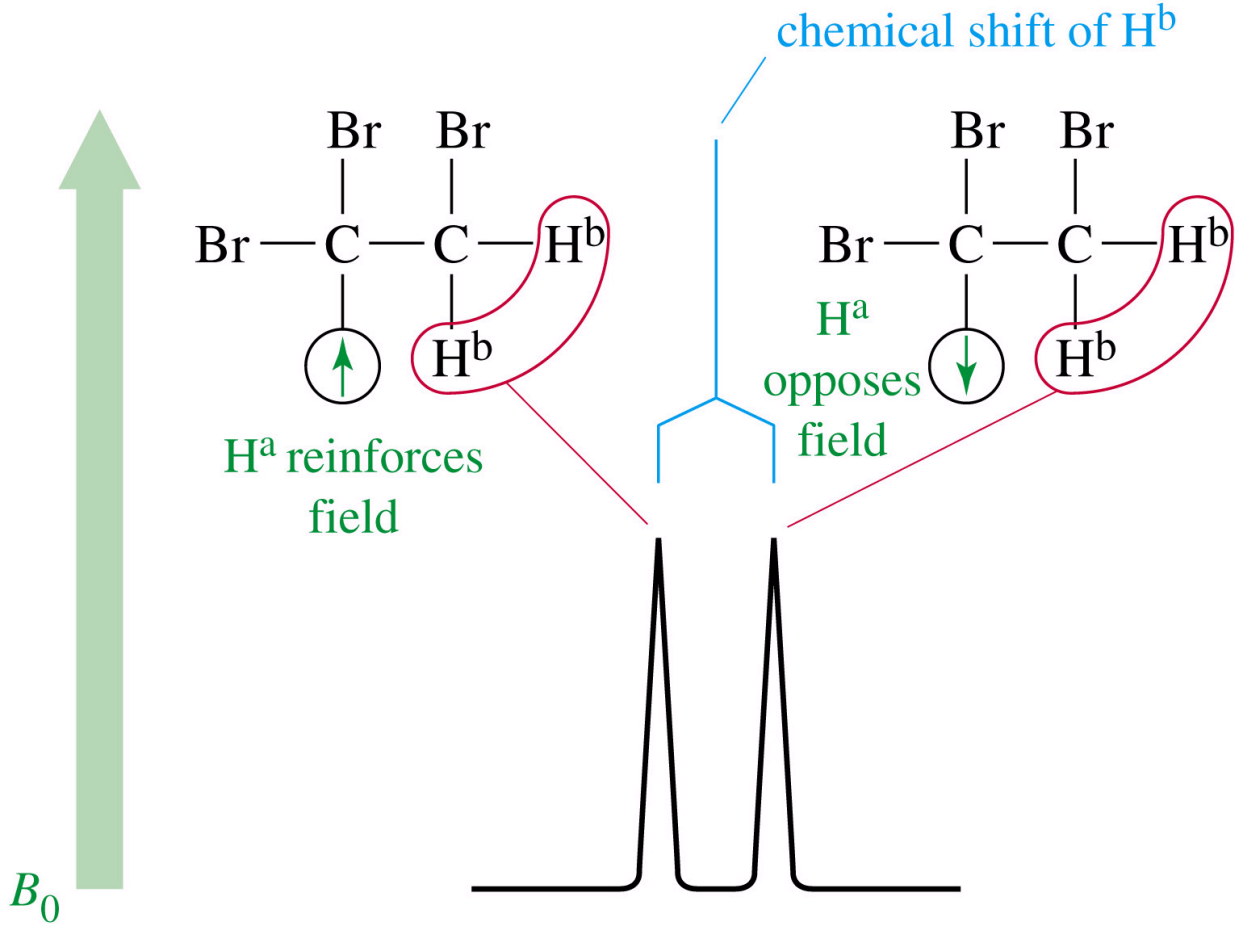


H_a is coupled to H_b

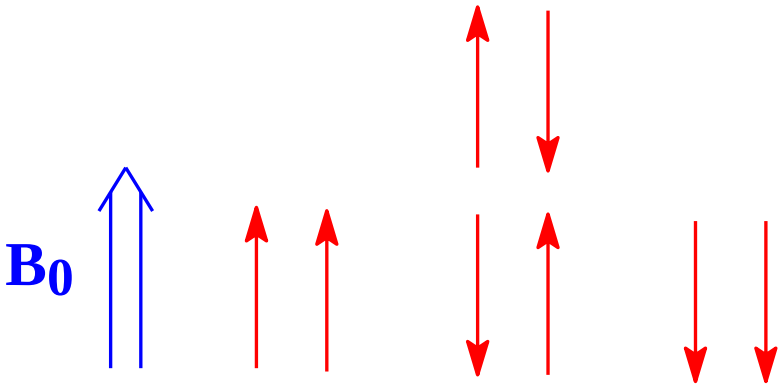
H_b is parallel or anti-parallel to B_0

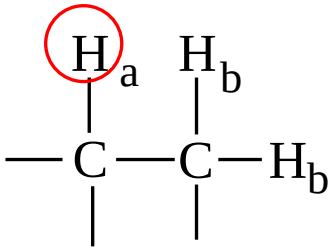
∴ H_a splits into a 1:1 doublet peak

H_b in 1,1,2-Tribromoethane



The Triplet in ^{1}H NMR



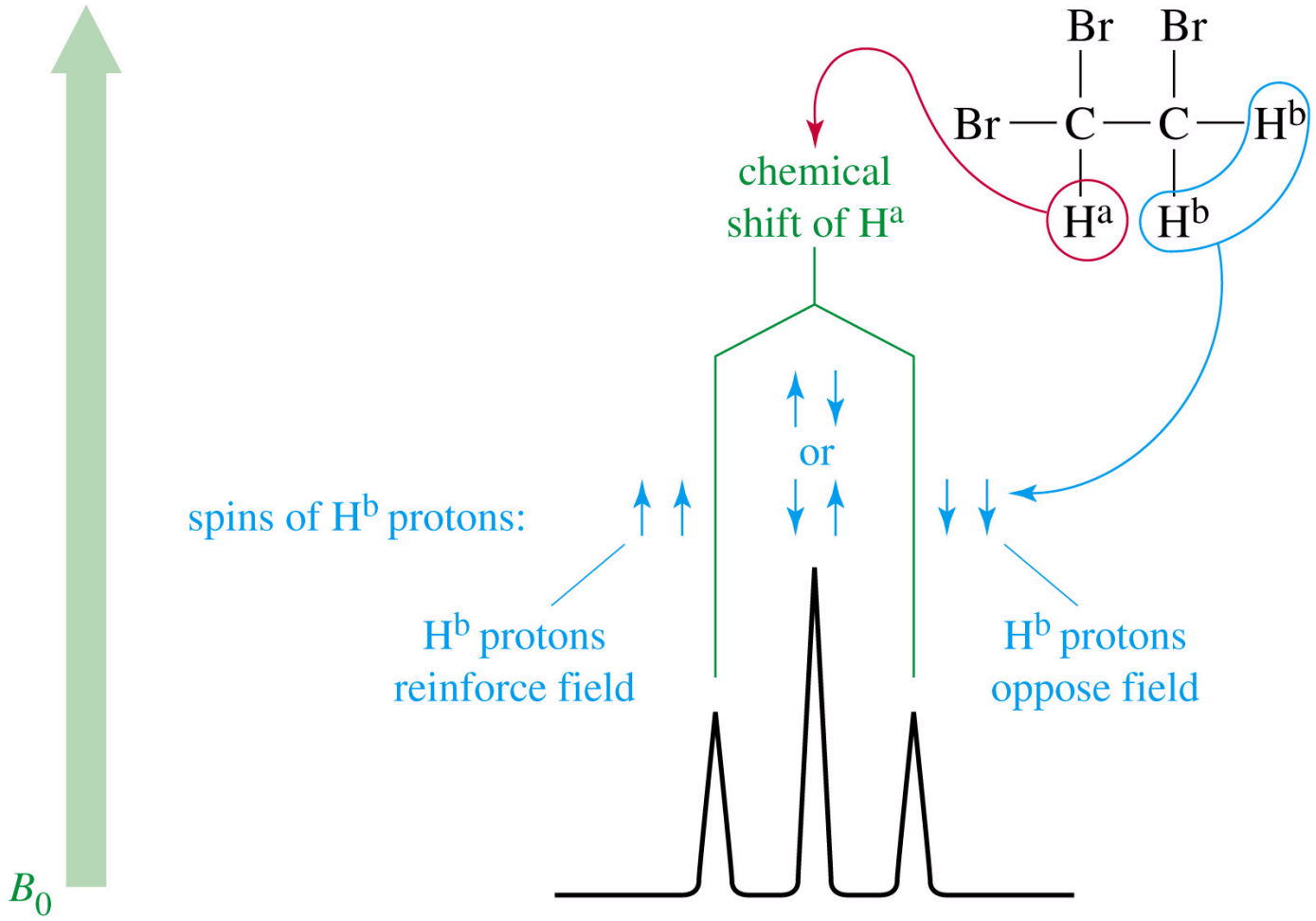


H_a is coupled to H_b and H_b

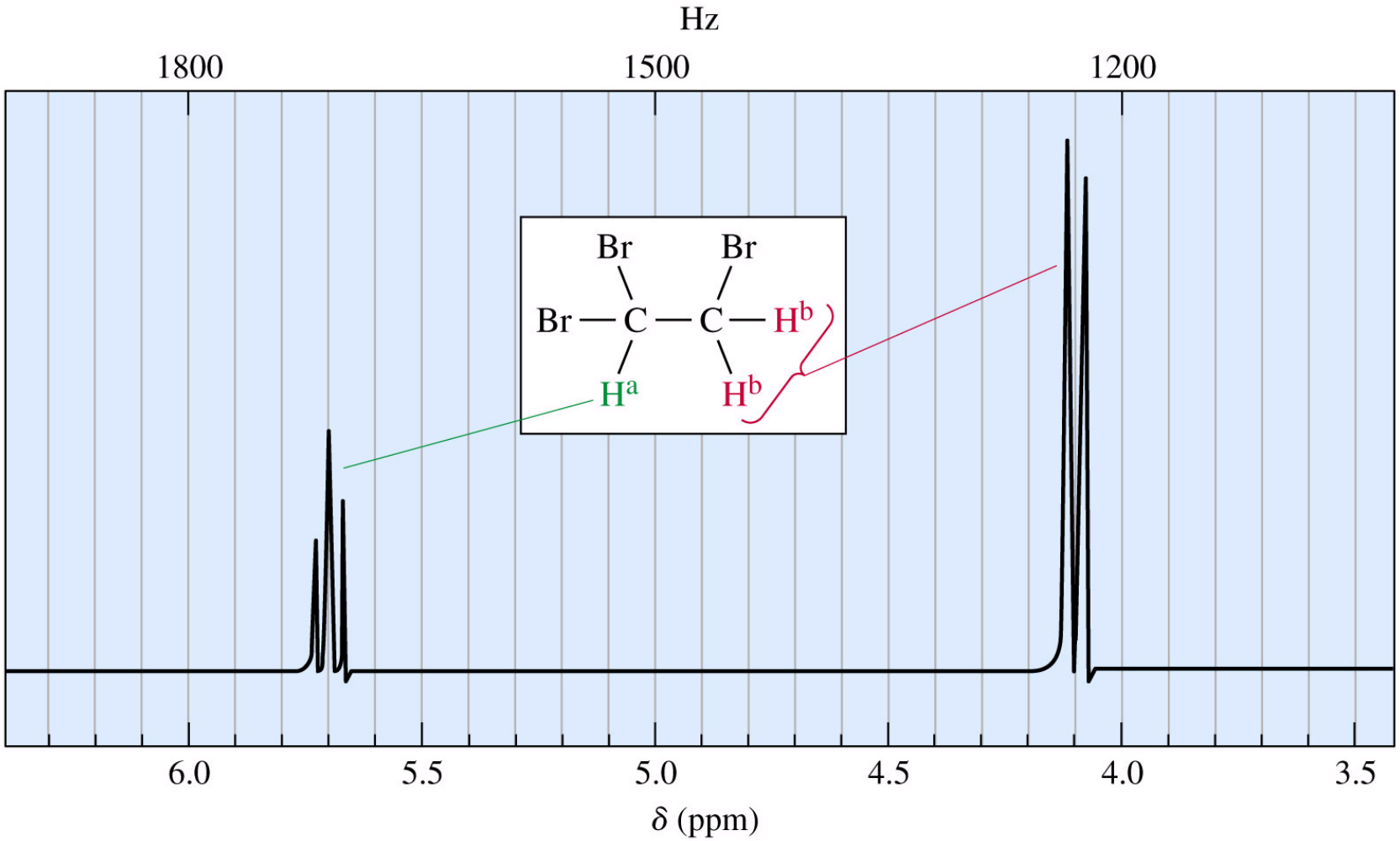
H_b can both be parallel, anti-paralle
or one parallel and one anti-paralle

∴ H_a splits into a 1:2:1 triplet peak

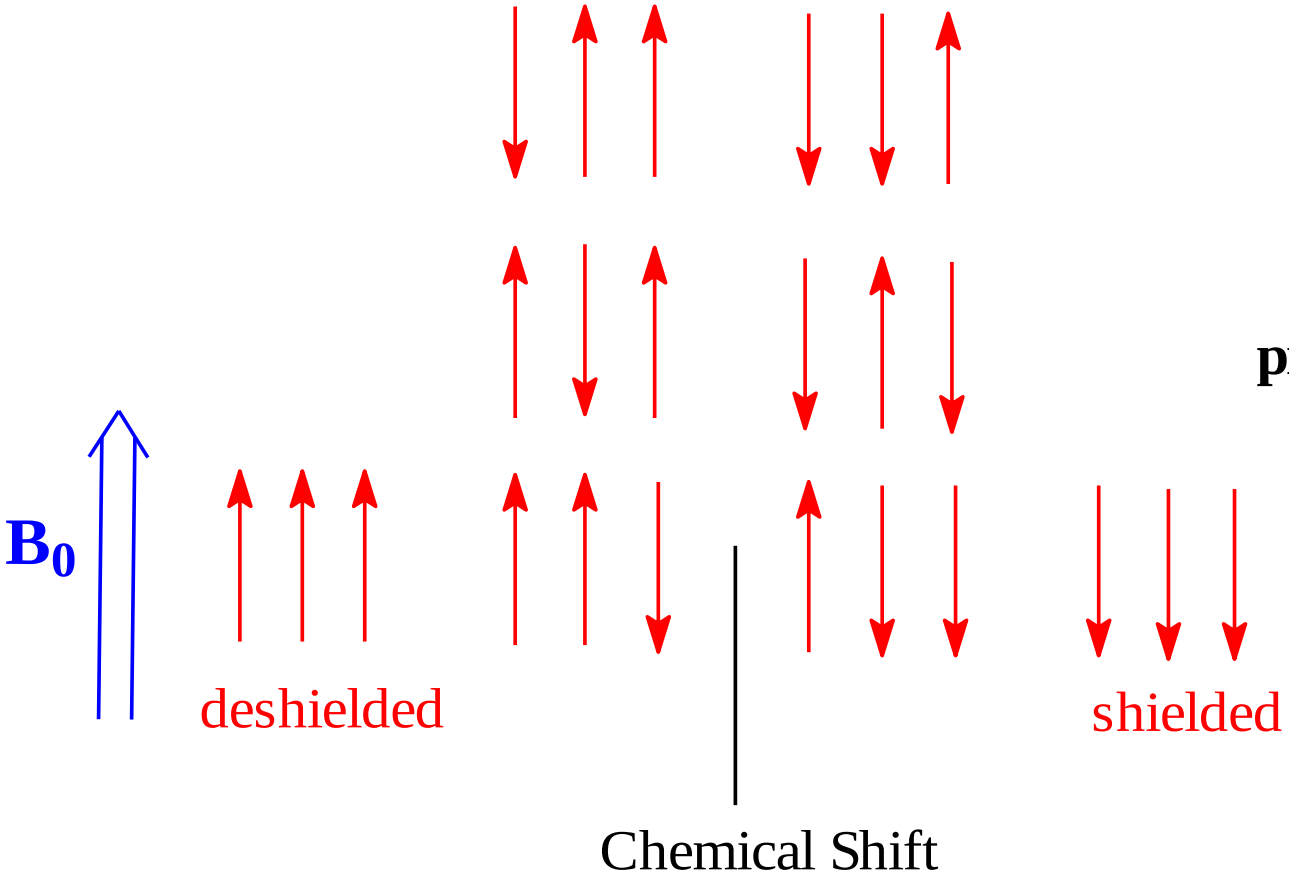
H_a in 1,1,2-Tribromoethane

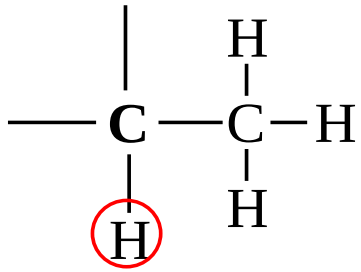


1,1,2-Tribromoethane



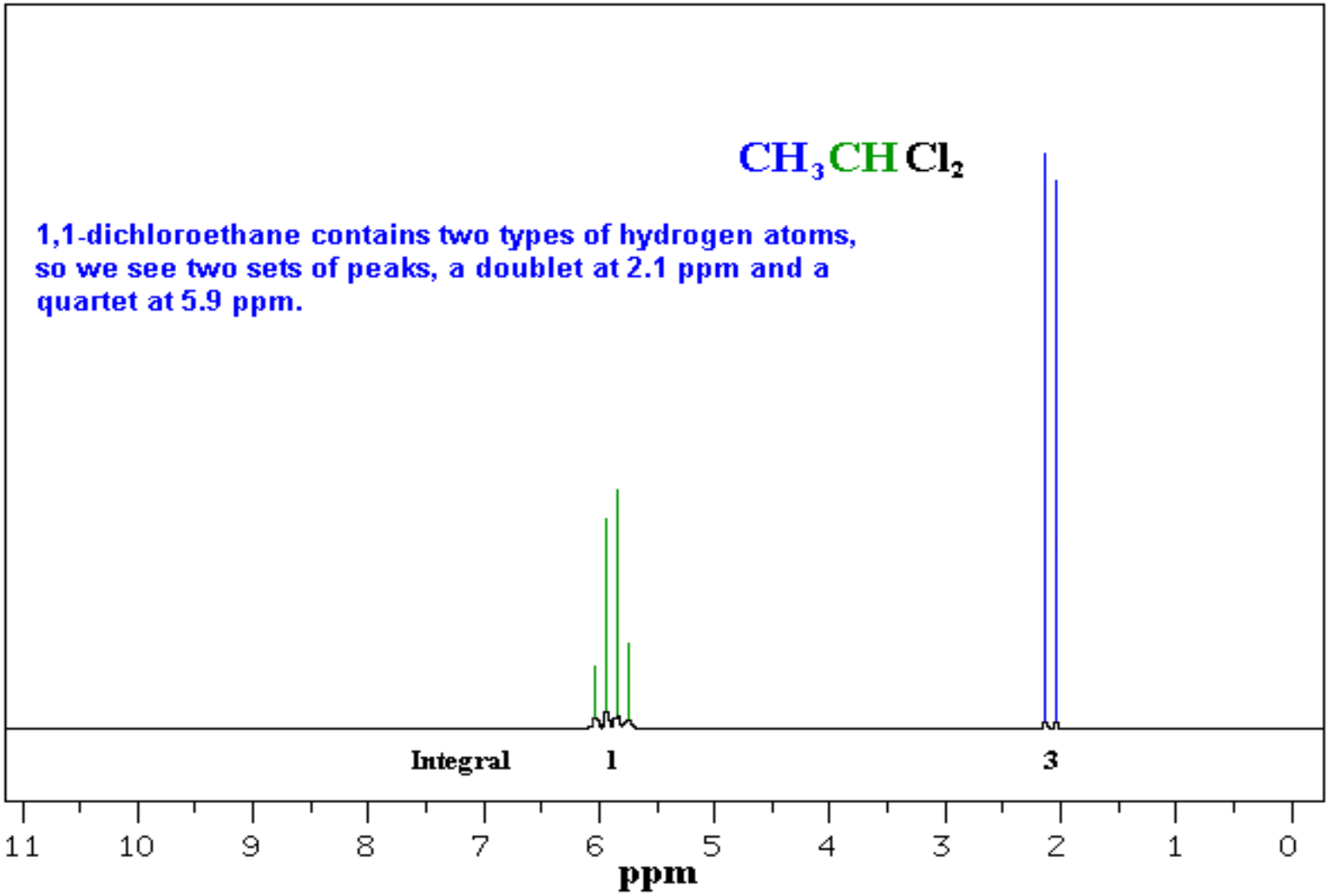
The Quartet in ^{1}HMR



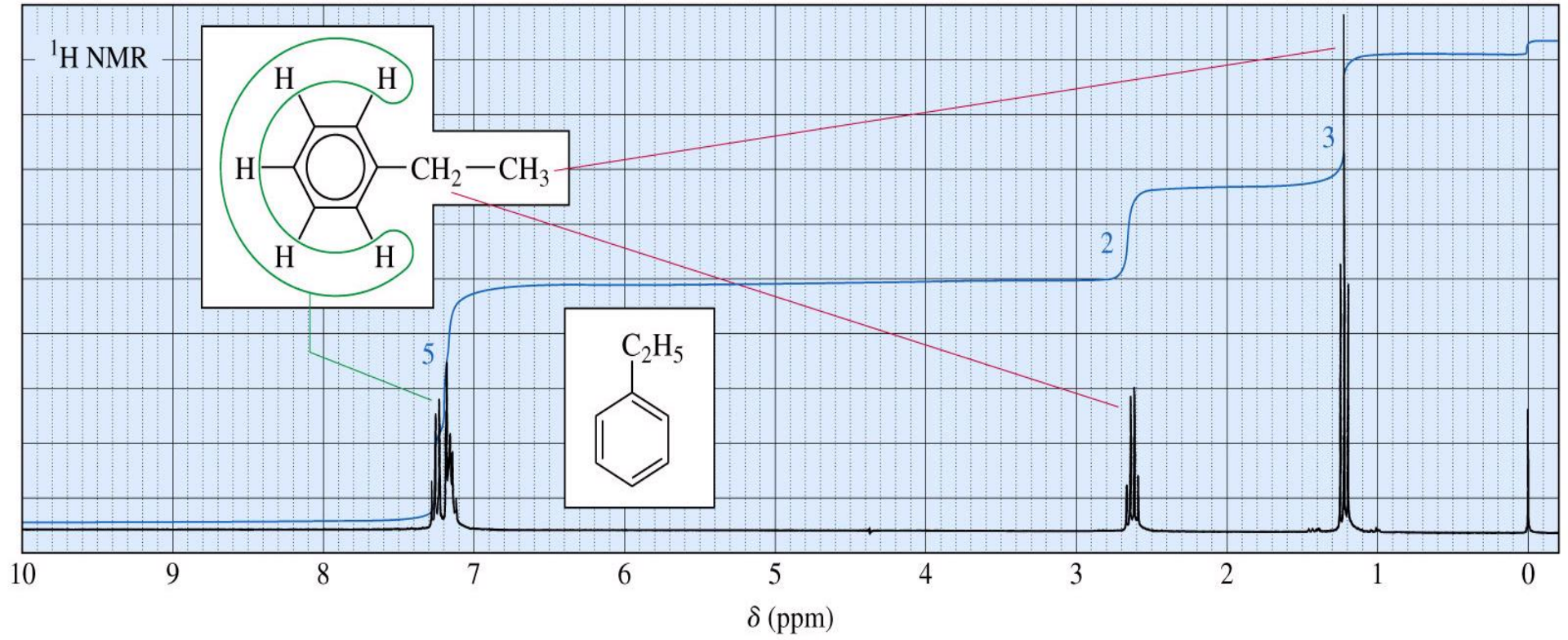


proton splits into n+1
quartet 1:3:3:1
n = # adjacent H's

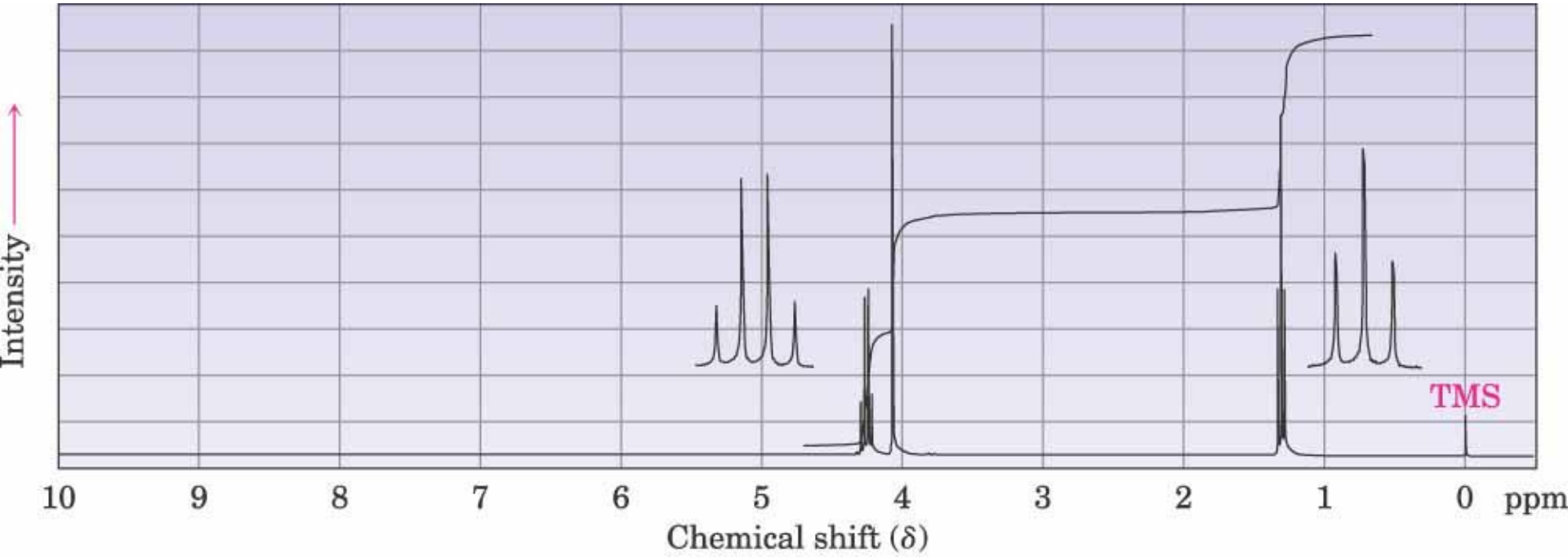
1,1-Dichloroethane



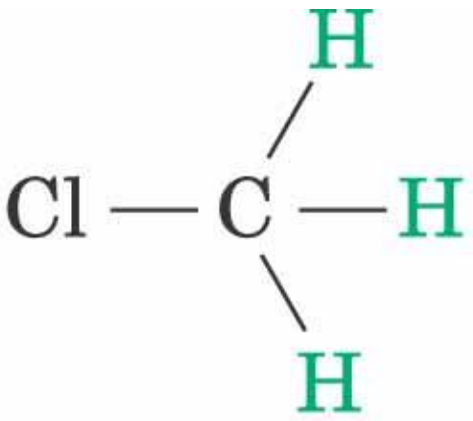
Ethyl benzene



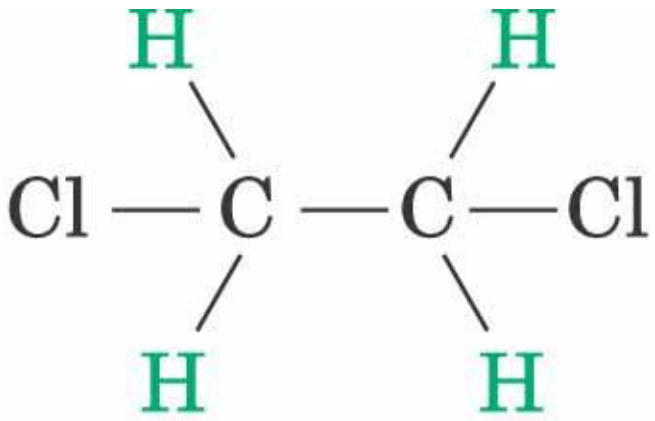
$CH_3CH_2OCH_3$



Equivalent Protons do not Couple



Three C–H protons are chemically equivalent; no splitting occurs.



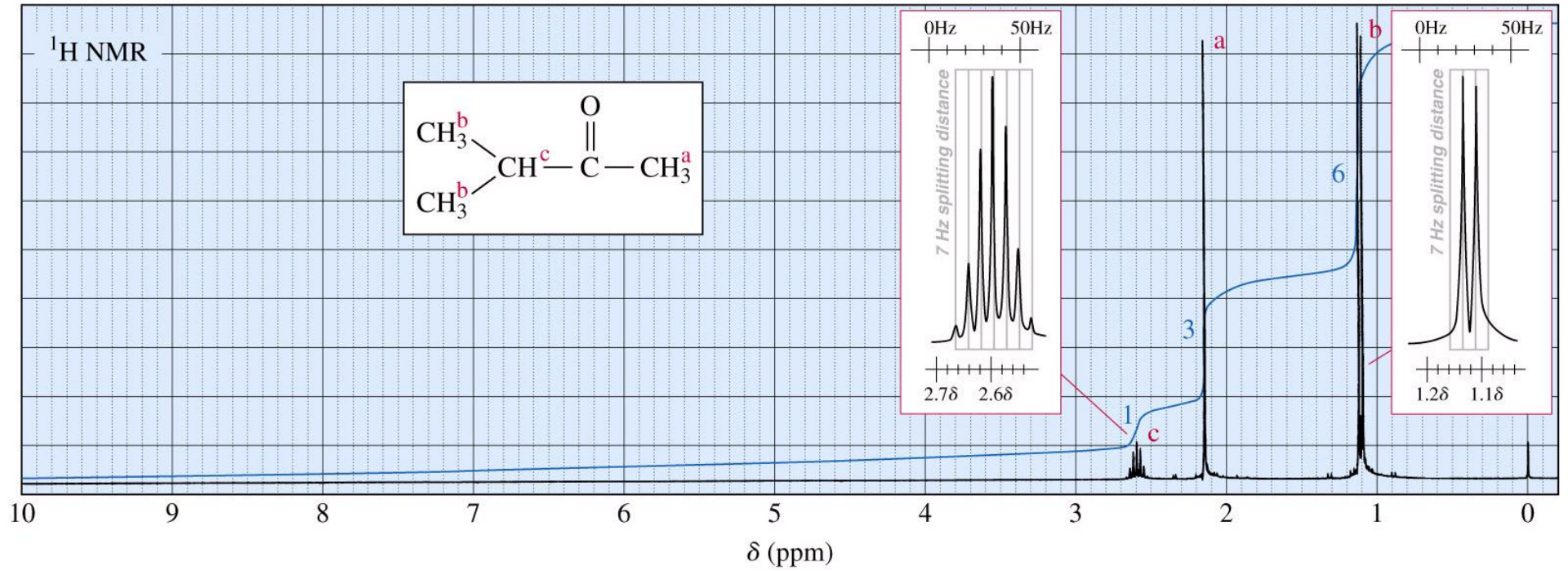
Four C–H protons are chemically equivalent; no splitting occurs.

Pascal's Triangle

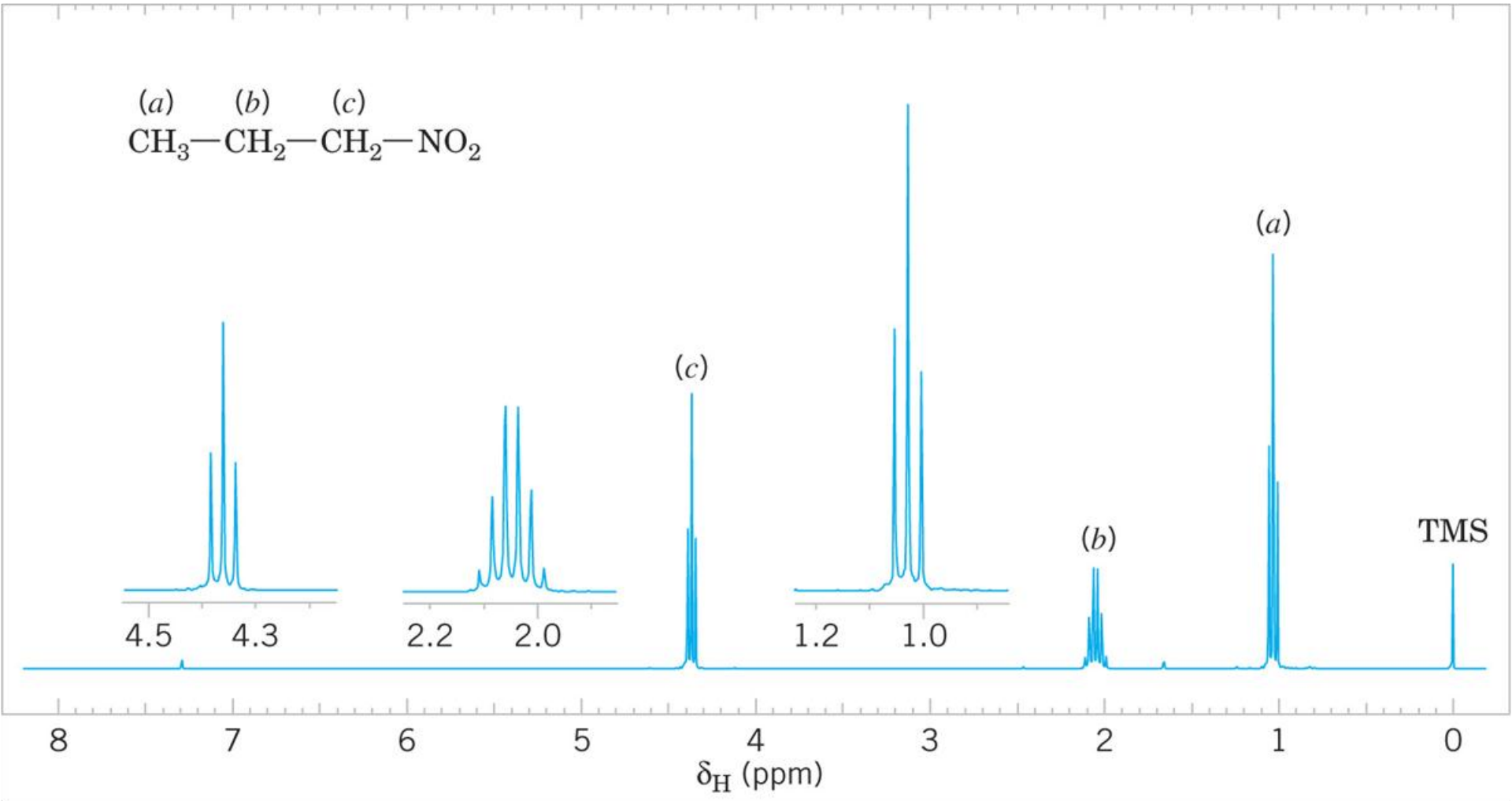
TABLE 13.4 Some Common Spin Multiplicities

Number of equivalent adjacent protons	Type of multiplet observed	Ratio of intensities
0	Singlet	1
1	Doublet	1:1
2	Triplet	1:2:1
3	Quartet	1:3:3:1
4	Quintet	1:4:6:4:1
6	Septet	1:6:15:20:15:6:1

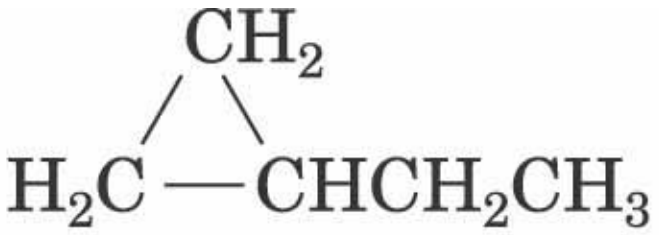
Methyl Isopropyl Ketone



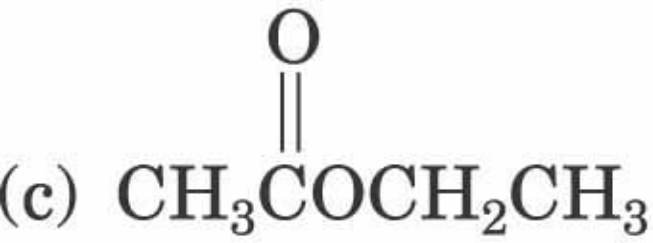
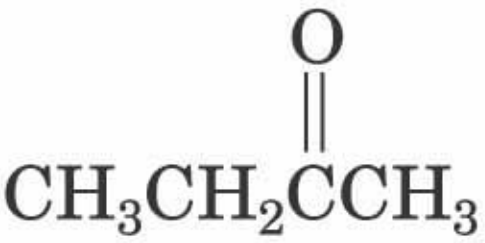
1-Nitropropane

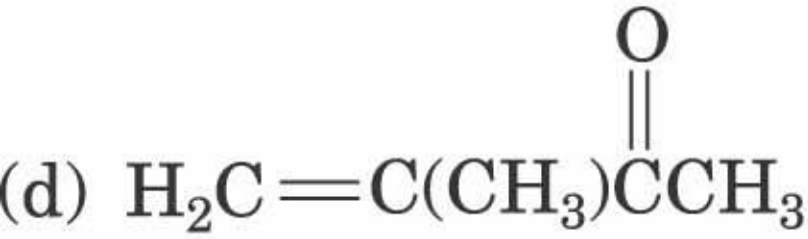
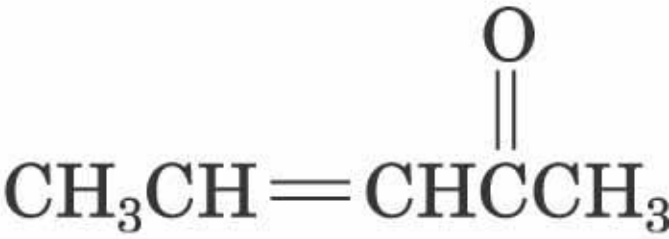


Differentiate using ^{1}H NMR

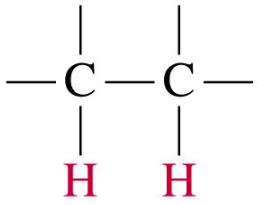
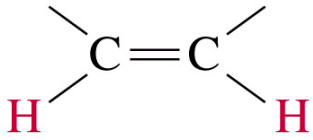
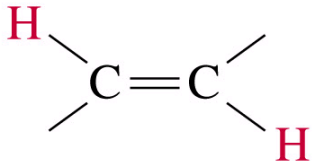
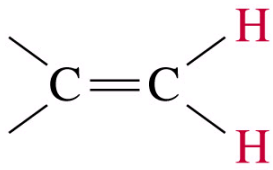
(a) $CH_3CH=CHCH_2CH_3$ and 

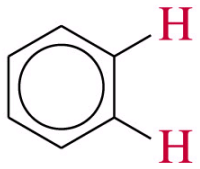
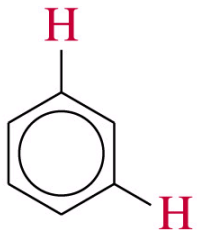
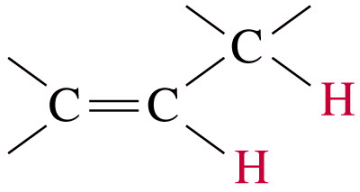
(b) $CH_3CH_2OCH_2CH_3$ and $CH_3OCH_2CH_2CH_3$

(c)  and 

(d)  and 

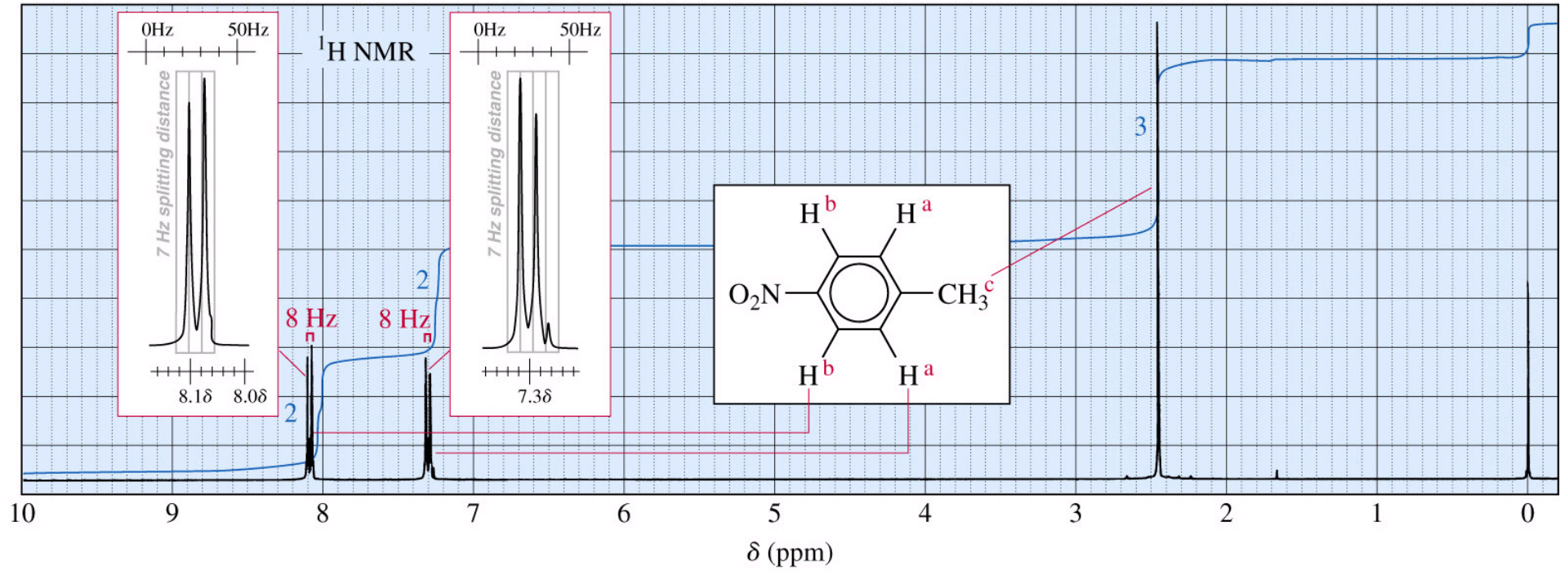
Coupling Constants (J values)

		Approx. *J*
	(free rotation)	7 Hz[a]
	(cis)	10 Hz
	(trans)	15 Hz
	(geminal)	2 Hz

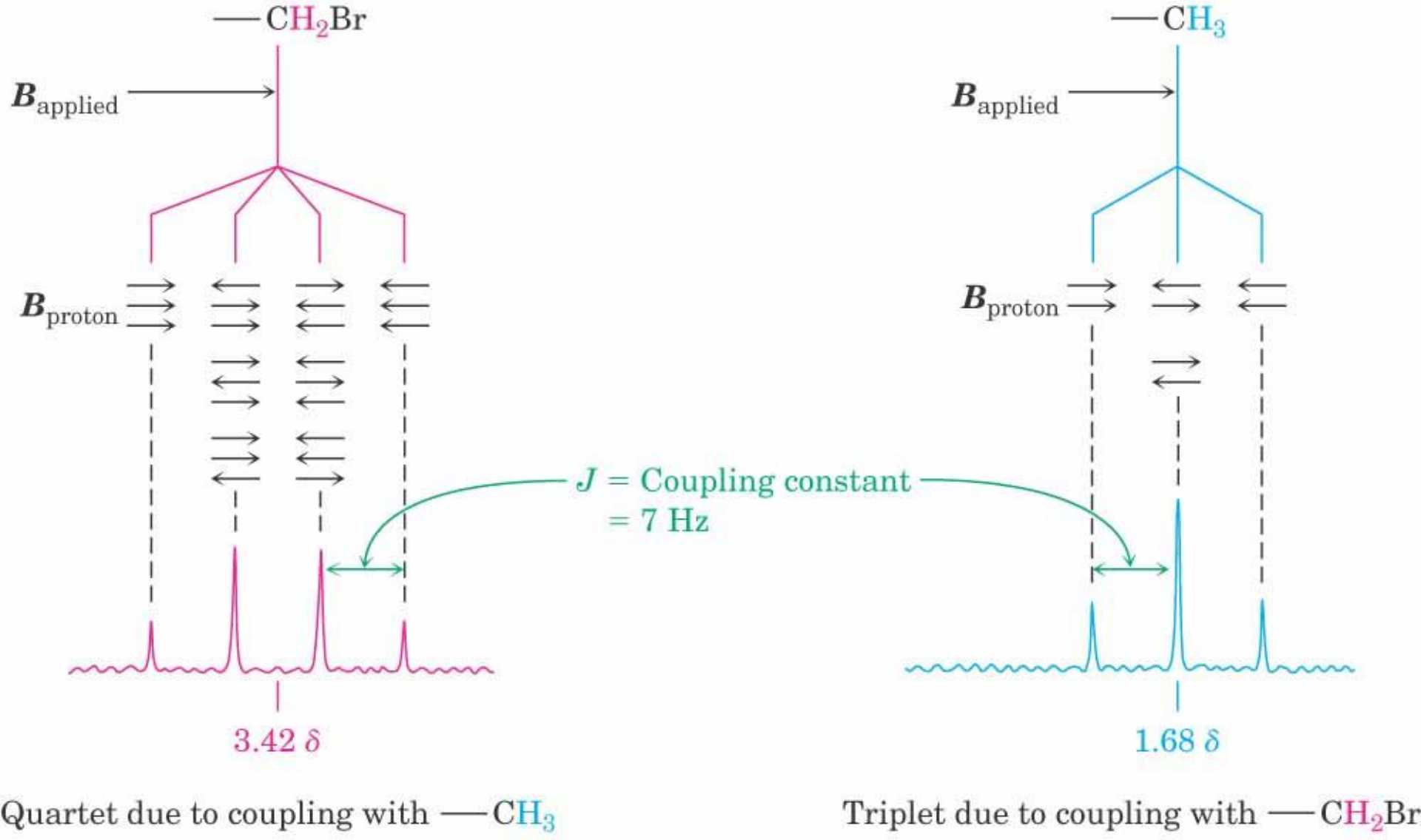
		Approx. *J*
 (ortho)		8 Hz
 (meta)		2 Hz
 (allylic)		6 Hz

[a]The value of 7 Hz in an alkyl group is averaged for rapid rotation about the carbon–carbon bond. If rotation is hindered by a ring or bulky groups, other splitting constants may be observed.

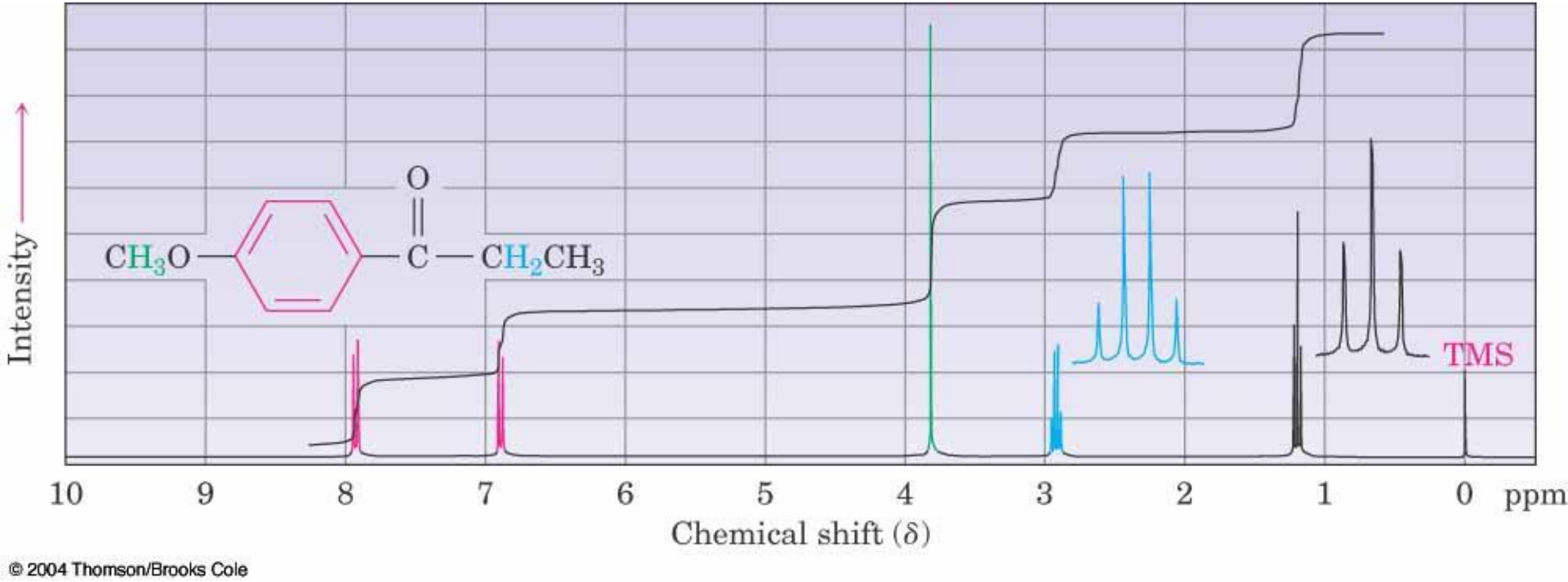
Para Nitrotoluene



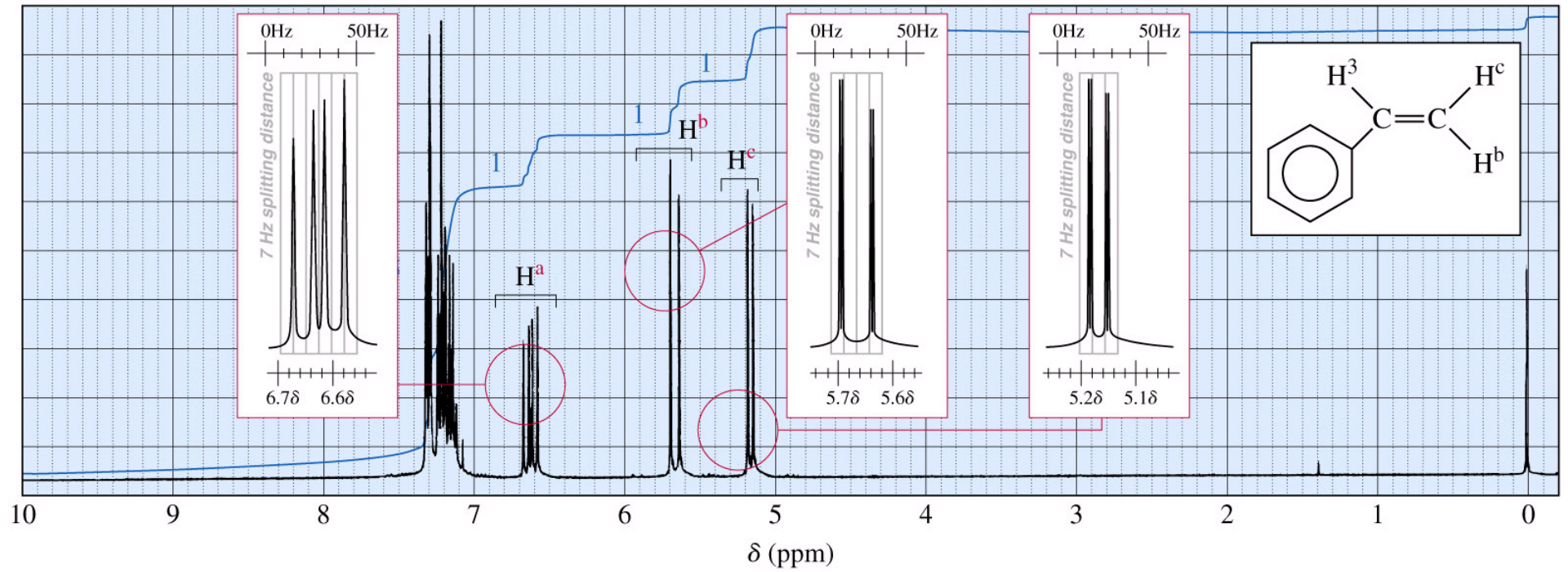
Bromoethane



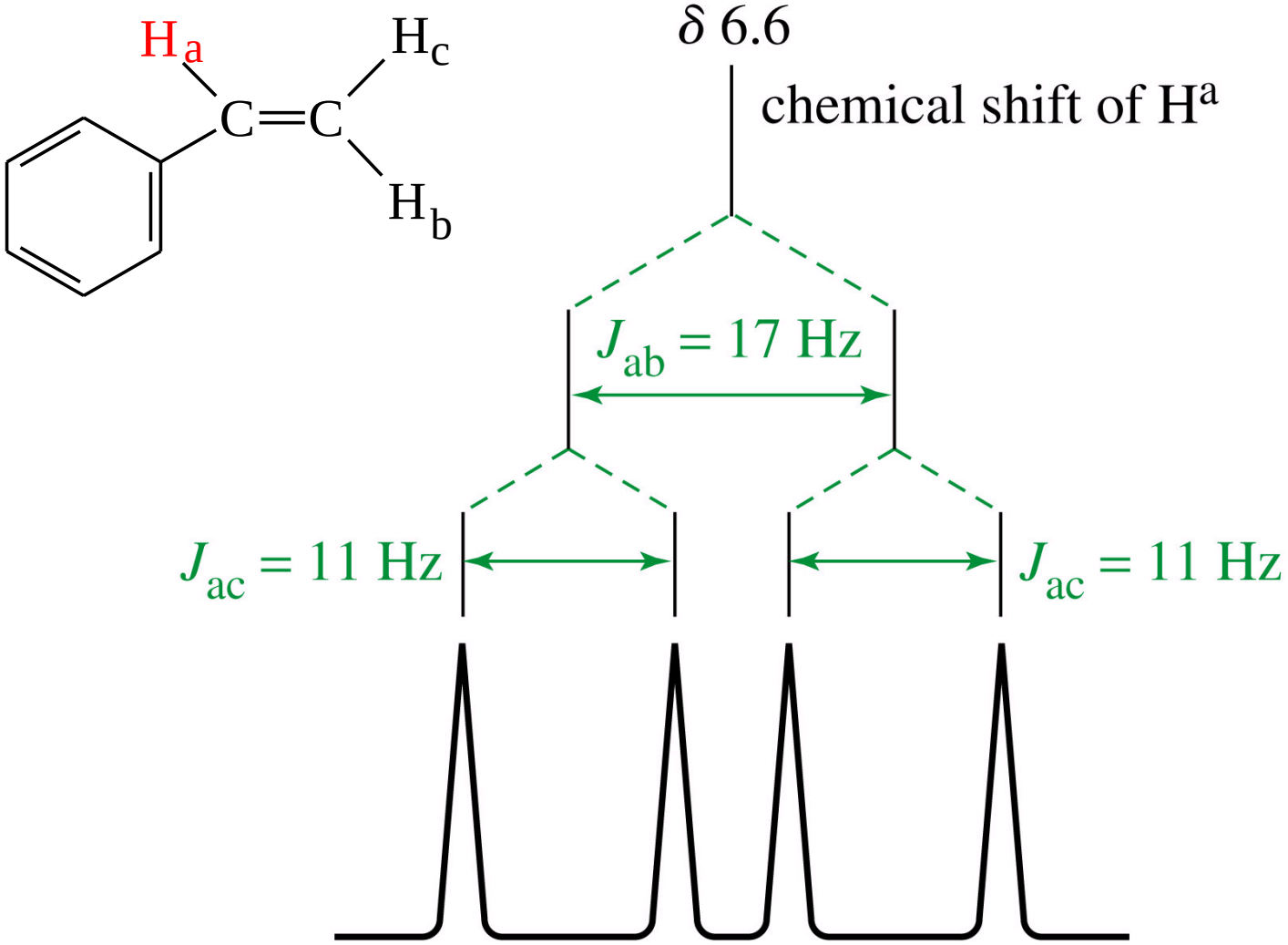
para-Methoxypropiophenone



Styrene

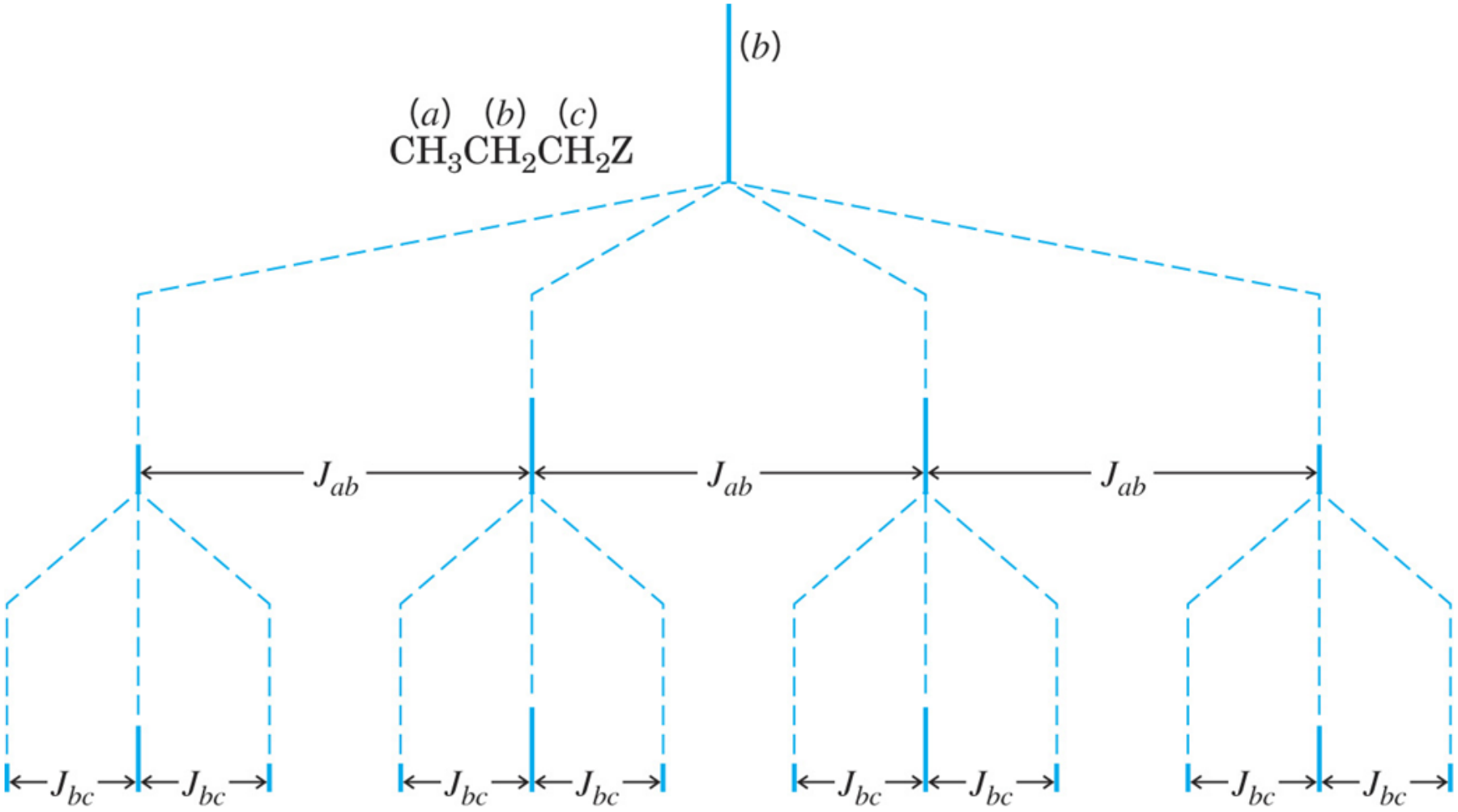

0Hz
50Hz
7 Hz splitting distance
6.7δ
6.6δ
5.7δ
5.6δ
5.2δ
5.1δ
H^a
H^b
H^c
H^e
H^3
1
1
1
10
9
8
7
6
5
4
3
2
1
0
δ (ppm)

H_a splitting in Styrene "Tree" Diagram

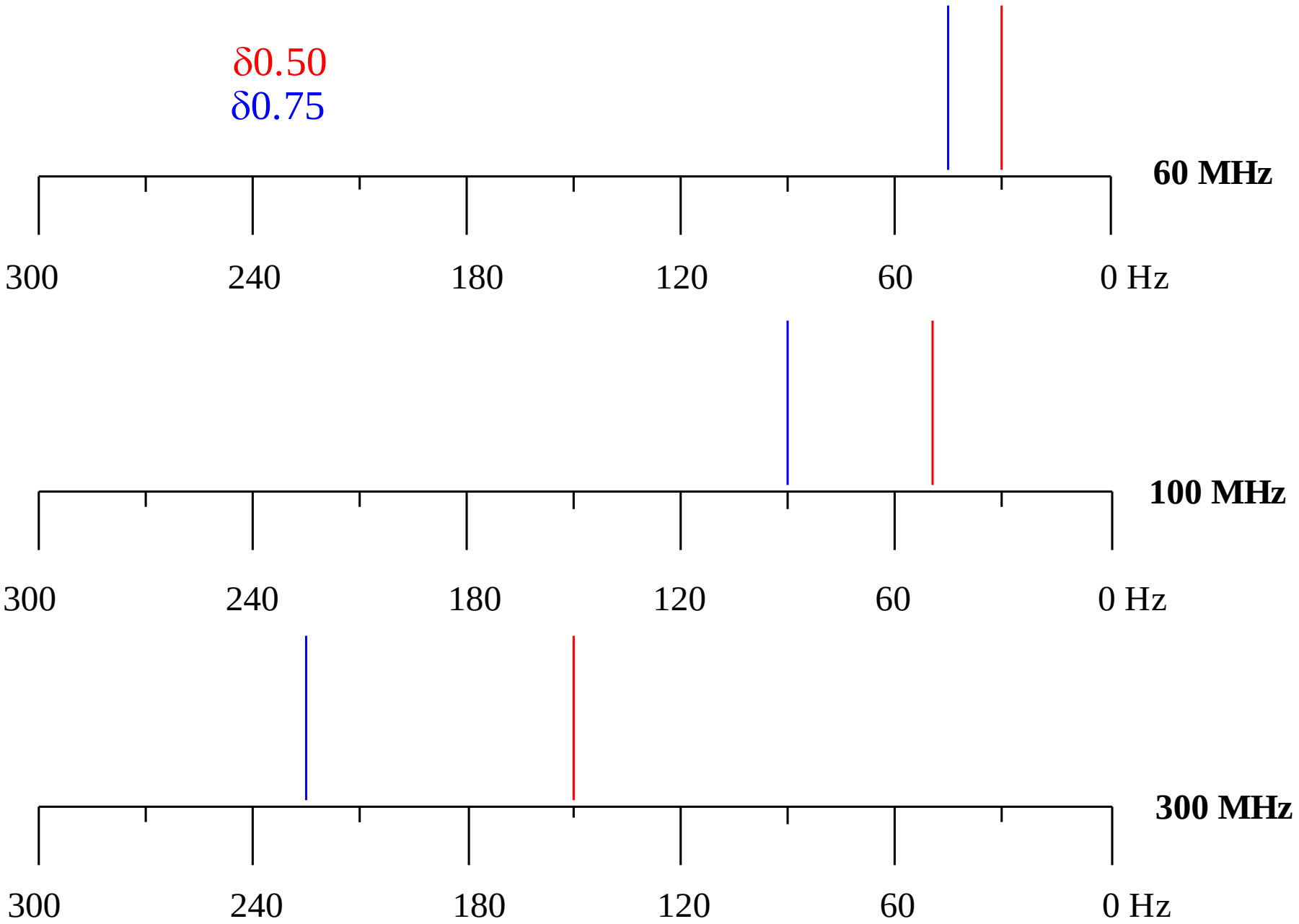


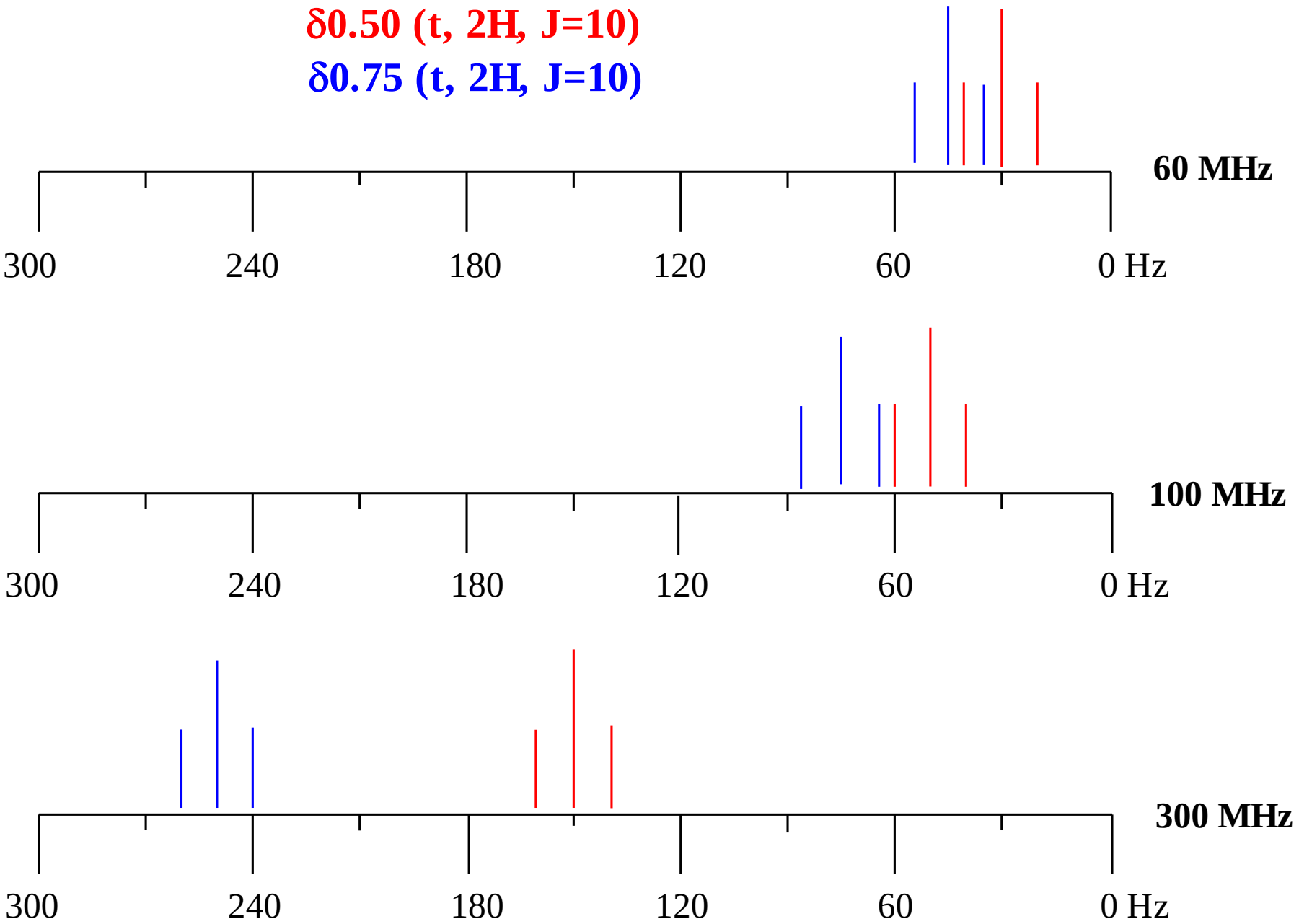
In the system below, Hb is split by two different sets of hydrogens : Ha and Hc

- **Theortically Hb could be split into a triplet of quartets (12 peaks) but this complexity is rarely seen in aliphatic systems**



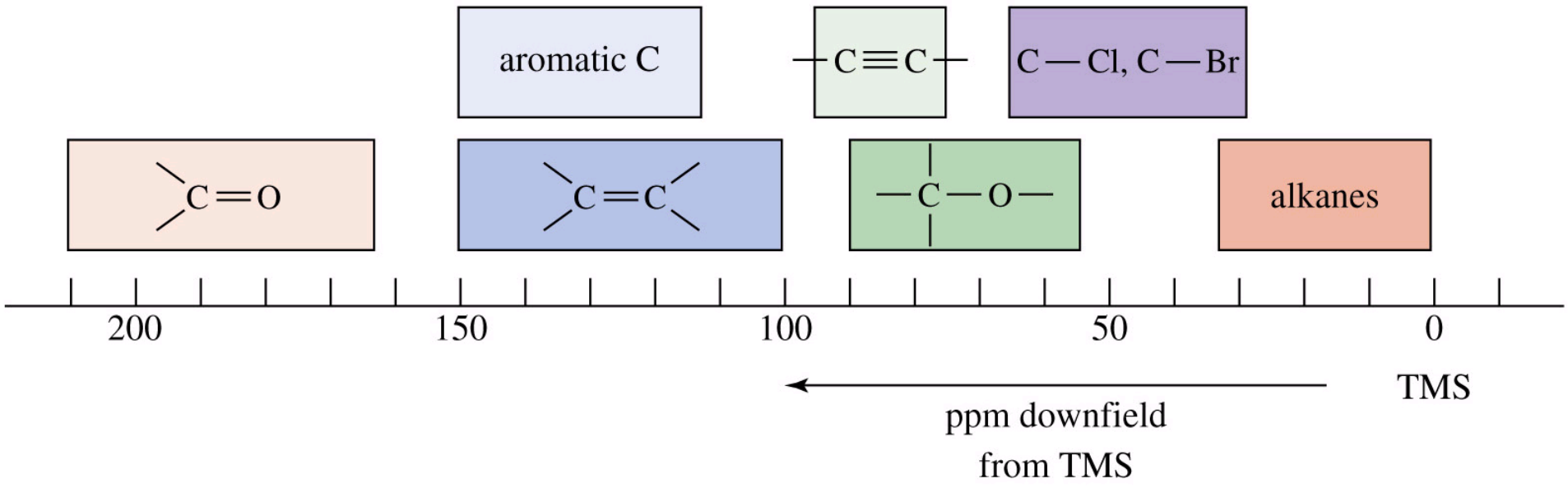
Why go to a higher field strength?




δ0.50 (t, 2H, J=10)
δ0.75 (t, 2H, J=10)
60 MHz
300
240
180
120
60
0 Hz
100 MHz
300
240
180
120
60
0 Hz
300 MHz
300
240
180
120
60
0 Hz

C-13 NMR Spectroscopy

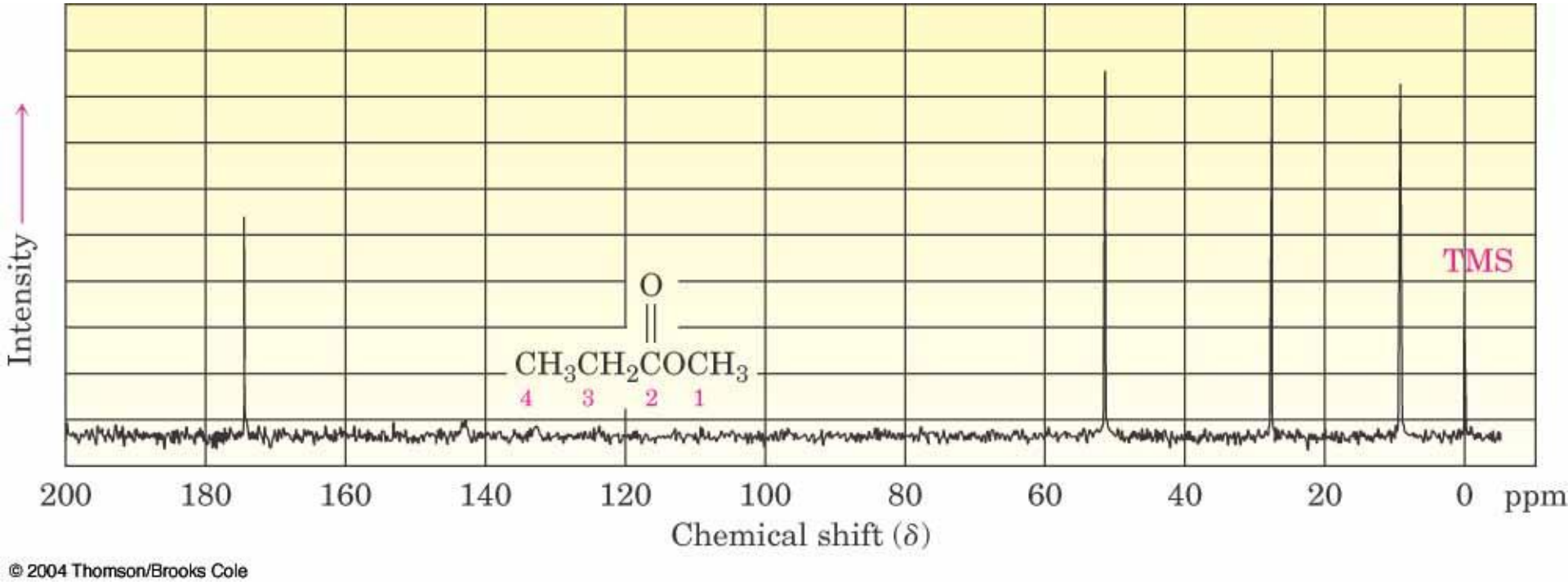
C-13 chemical shifts



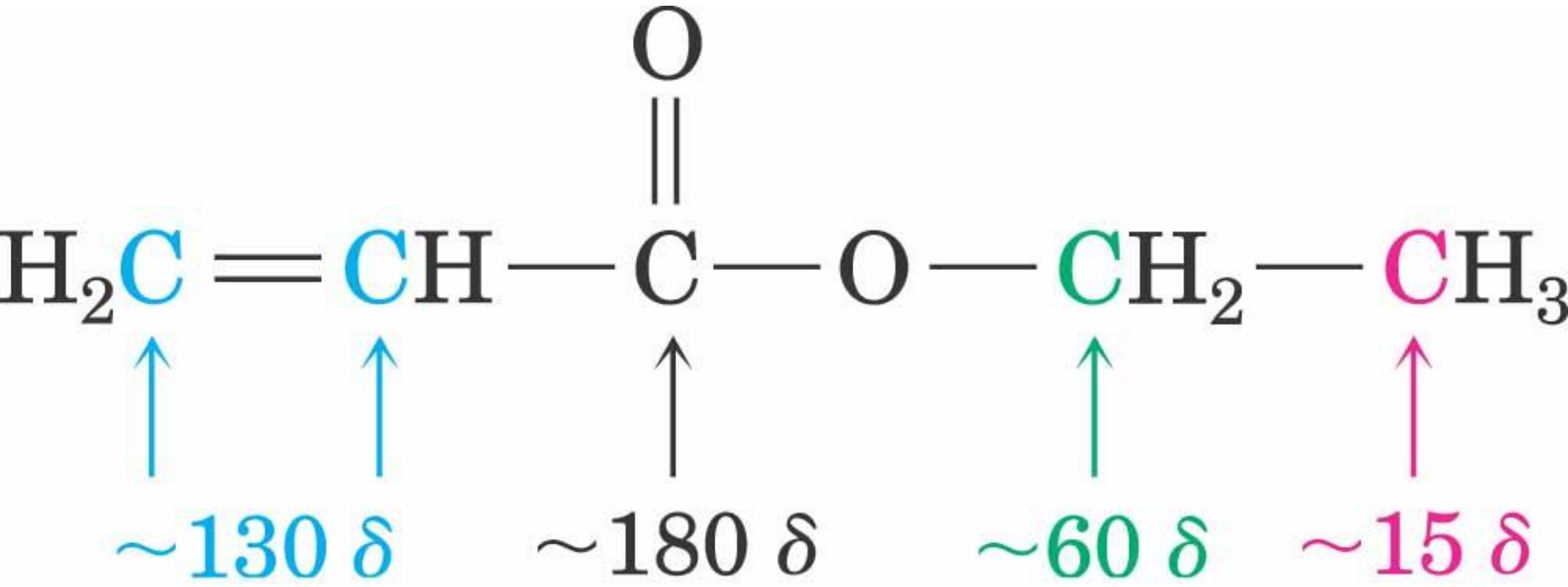
One signal for each chemically unique carbon

Methyl Propanoate

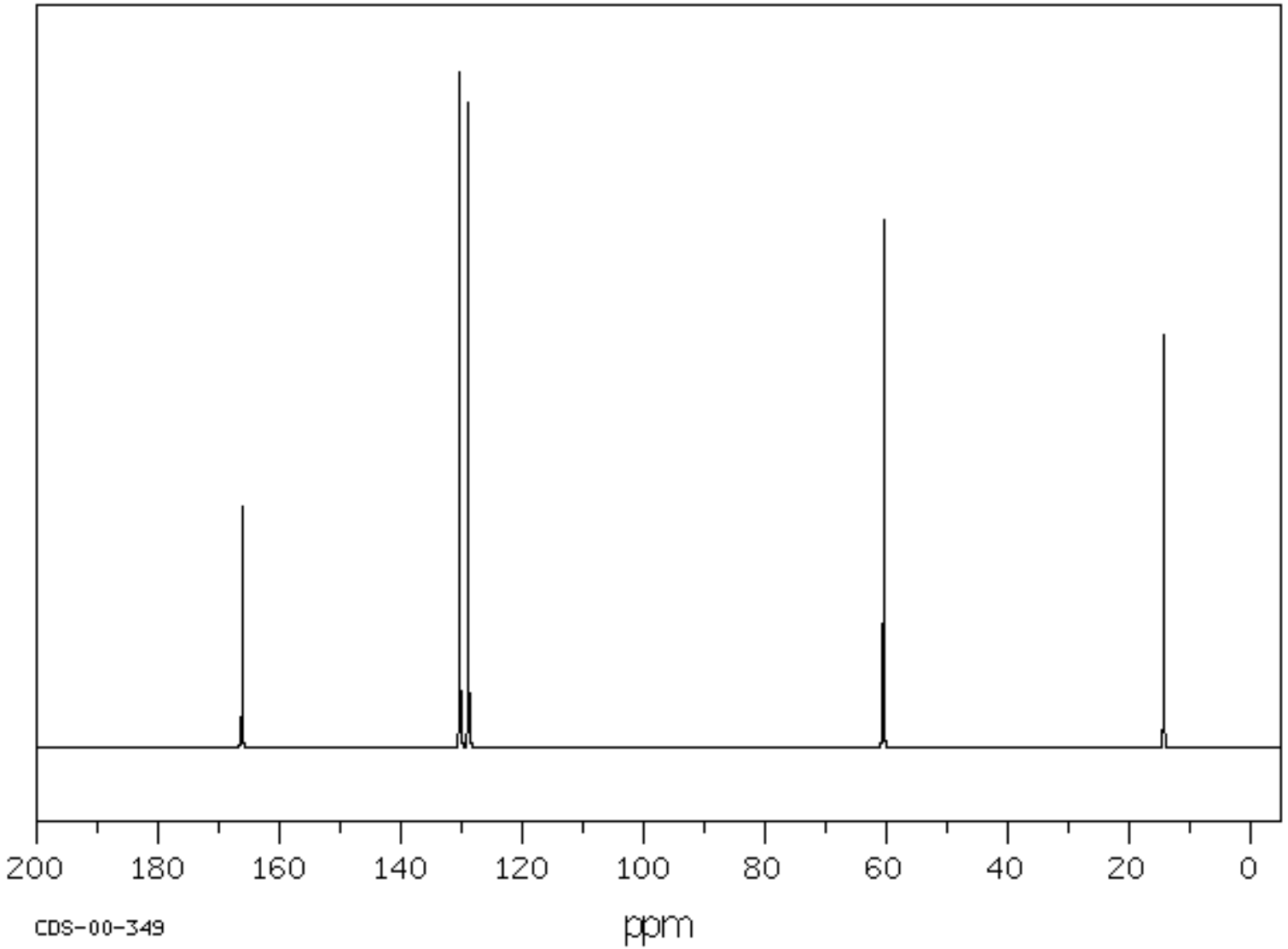
C-13 proton decoupled



Ethyl Acrylate; C-13 prediction

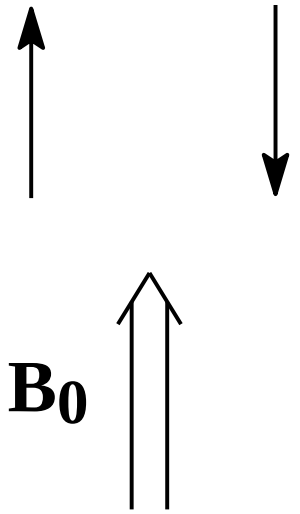


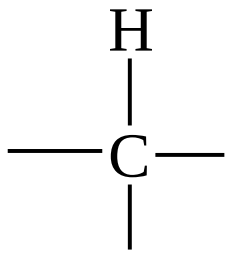
Ethyl Acrylate; C-13 NMR



Coupling in C-13 NMR

the doublet in C-13 NMR





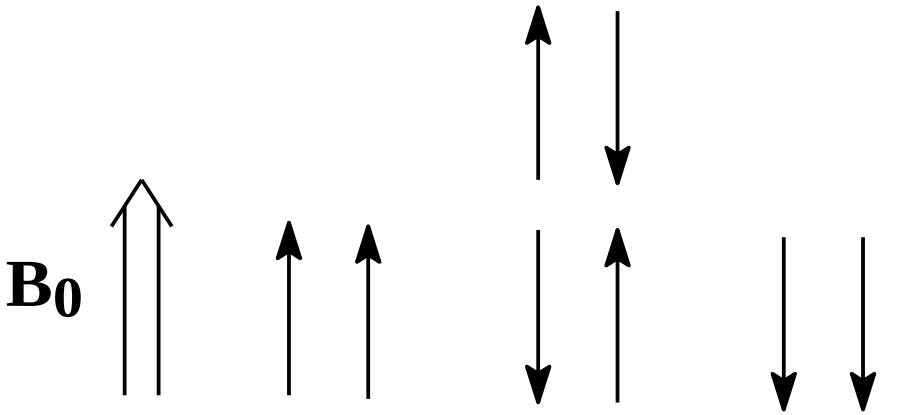
methine group

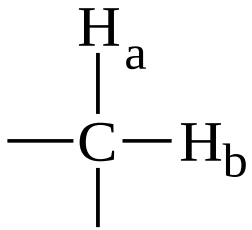
C is coupled to H

H is parallel or anti-parallel to B_0

∴ C splits into a 1:1 doublet peak

the triplet in C-13 NMR





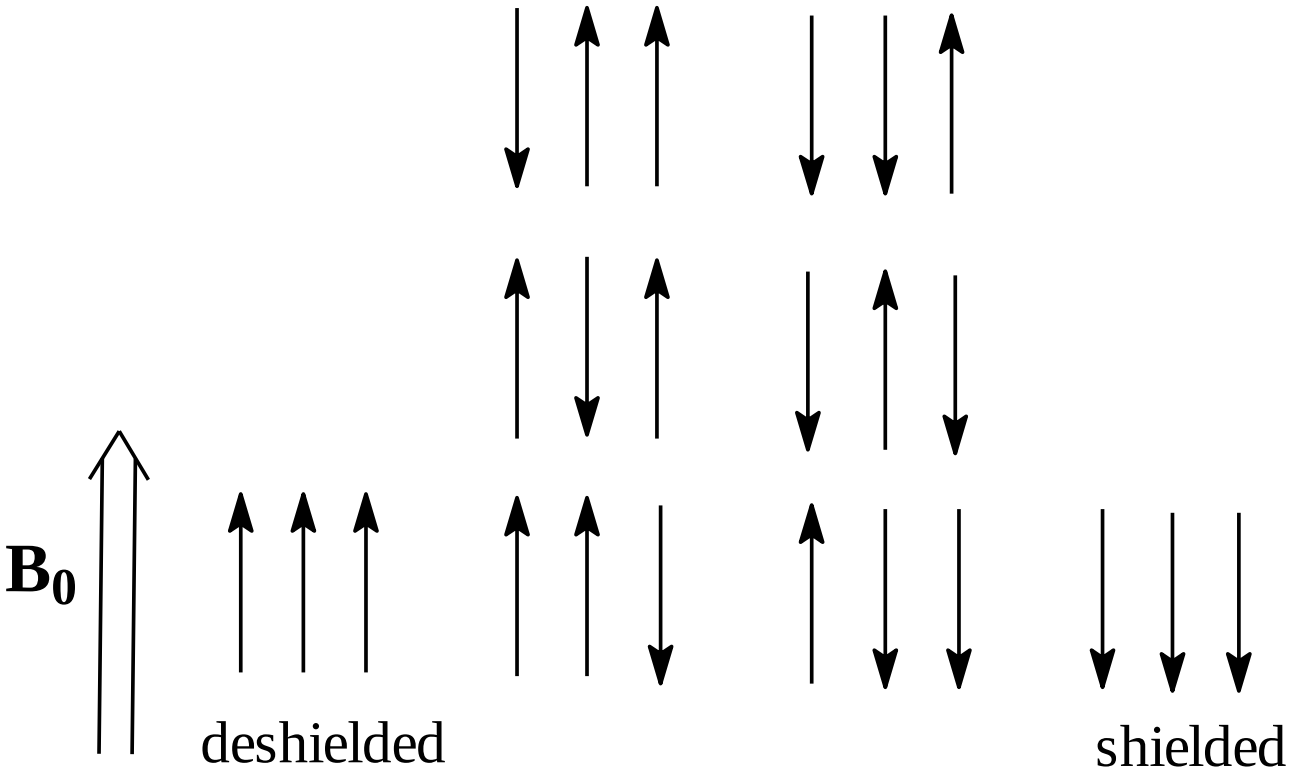
methylene group

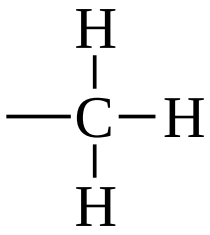
C is coupled to H_a and H_b

H_a & H_b can both be parallel, anti-paralle
or one parallel and one anti-parallel

∴ **C splits into a 1:2:1 triplet peak**

the quartet in C-13 NMR





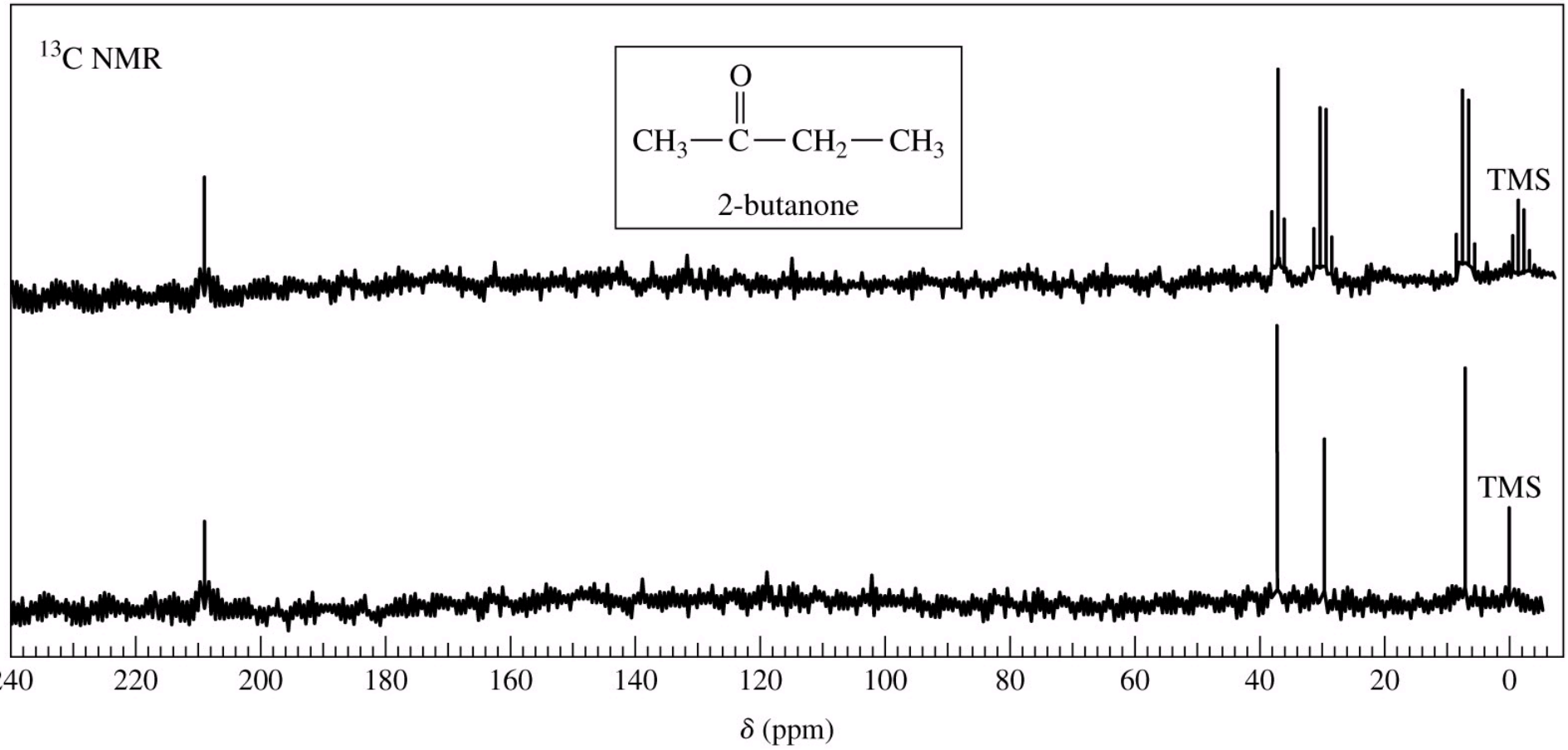
methyl group

carbon splits into n+1

quartet 1:3:3:1

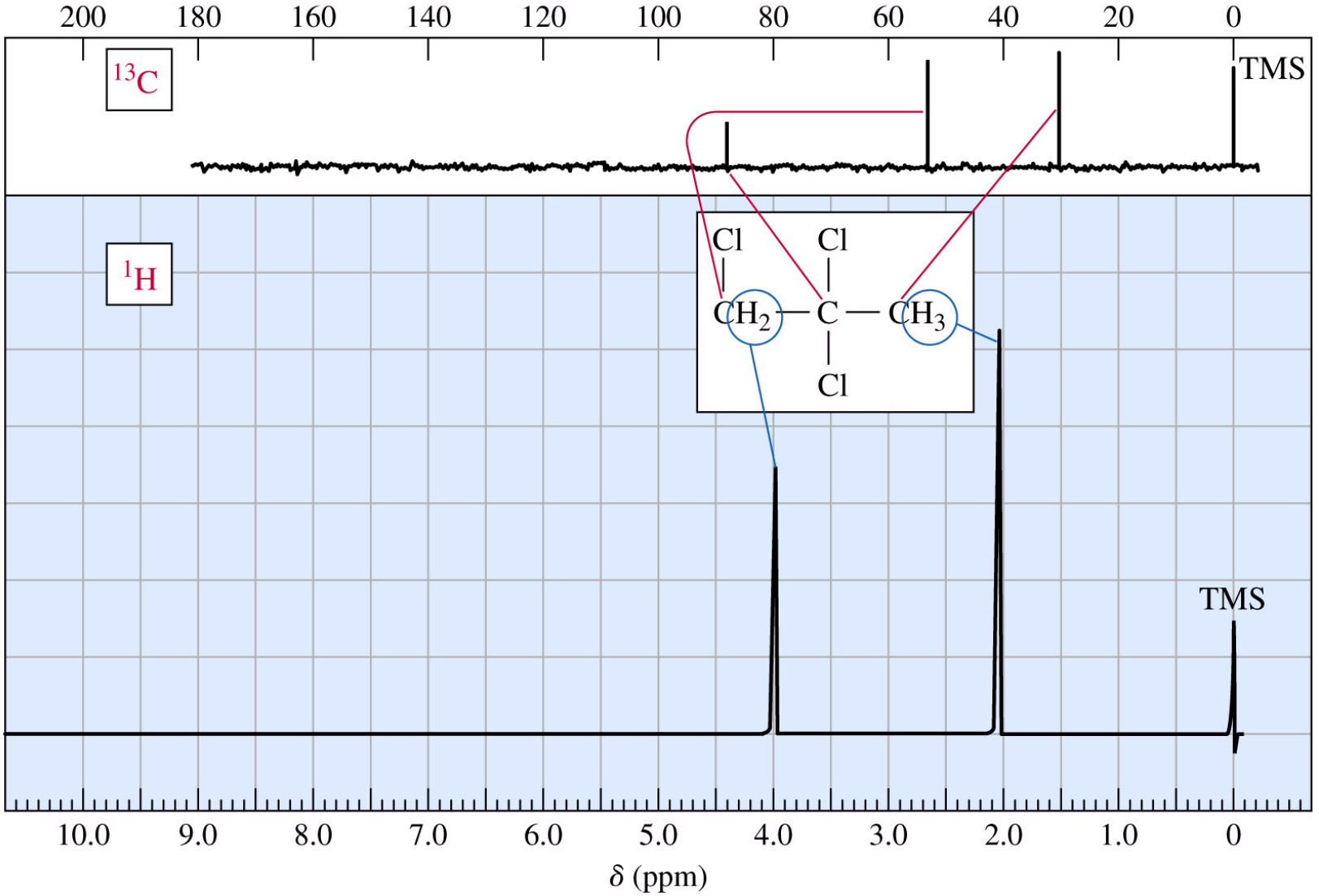
n = # attached H's

Butanone - Coupled and Decoupled

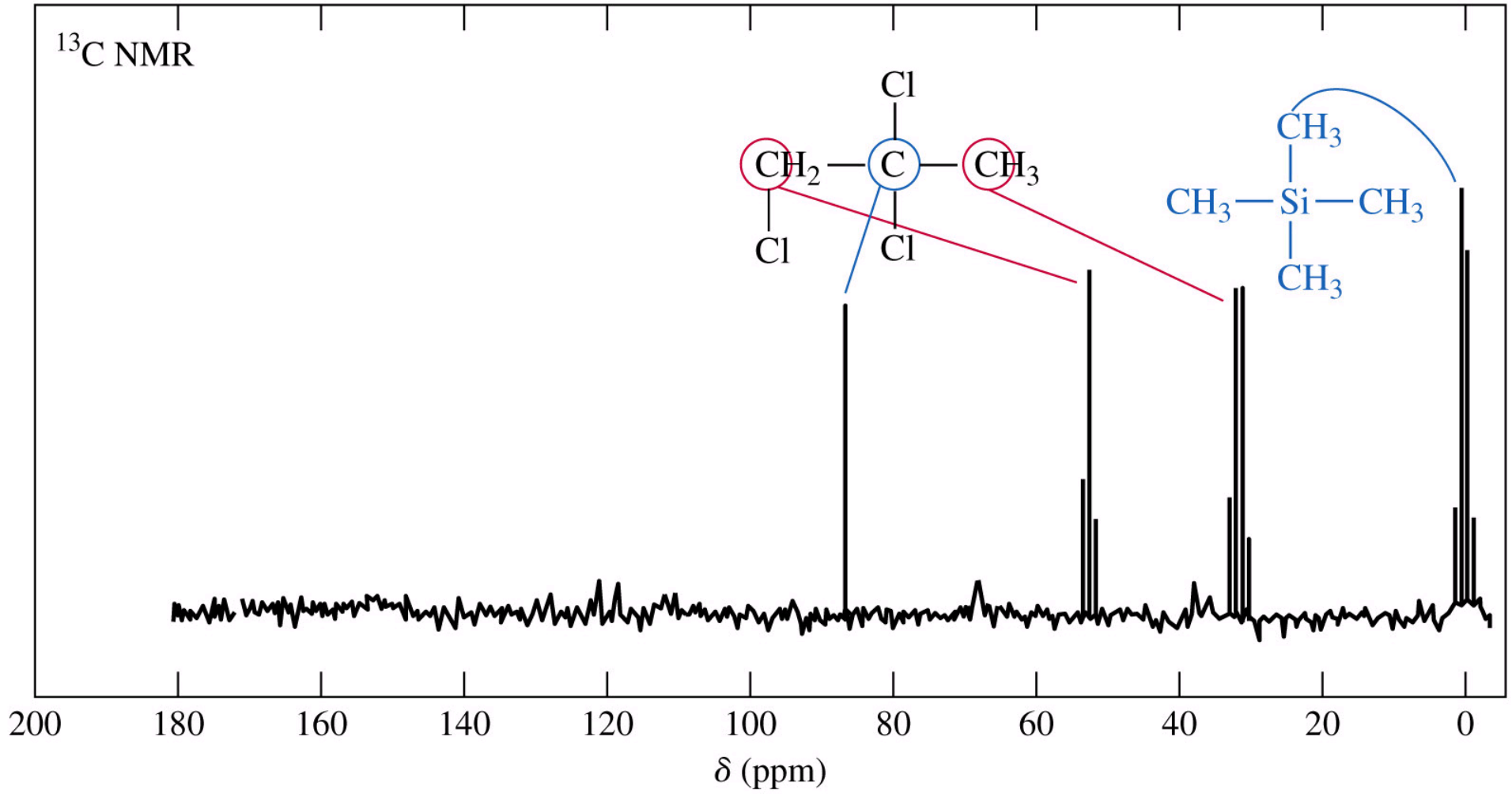


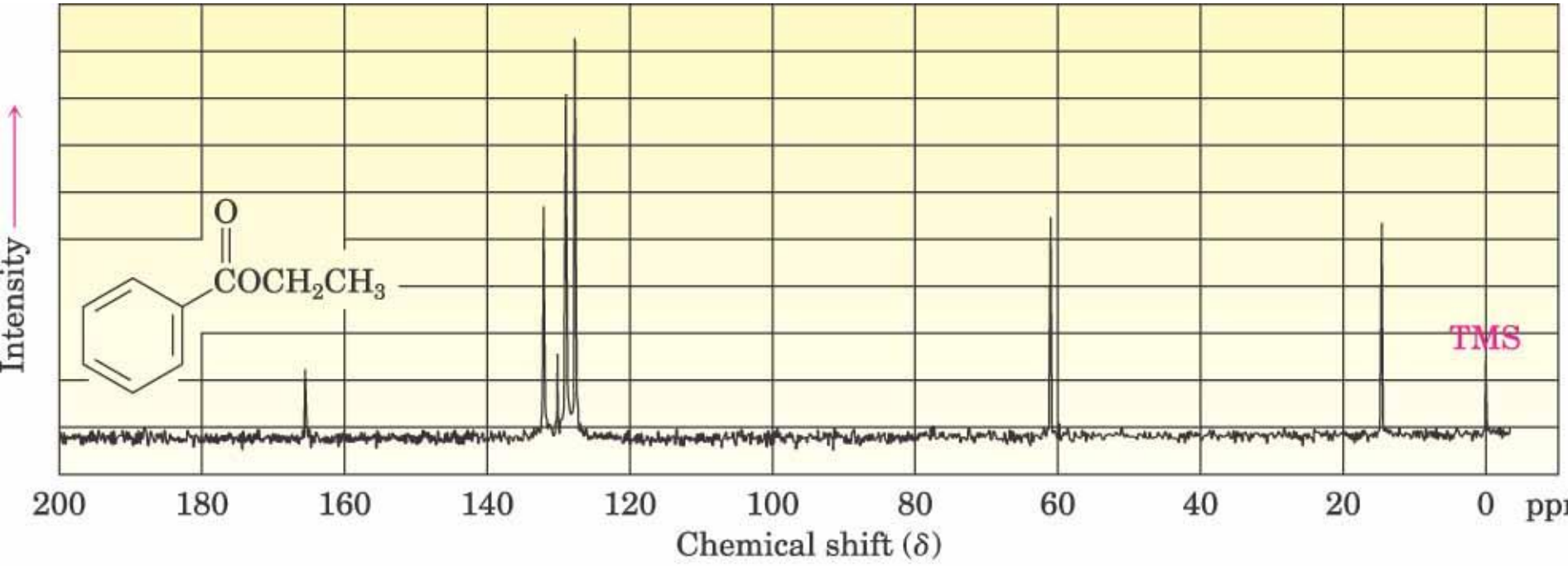
1,2,2-Trichloropropane

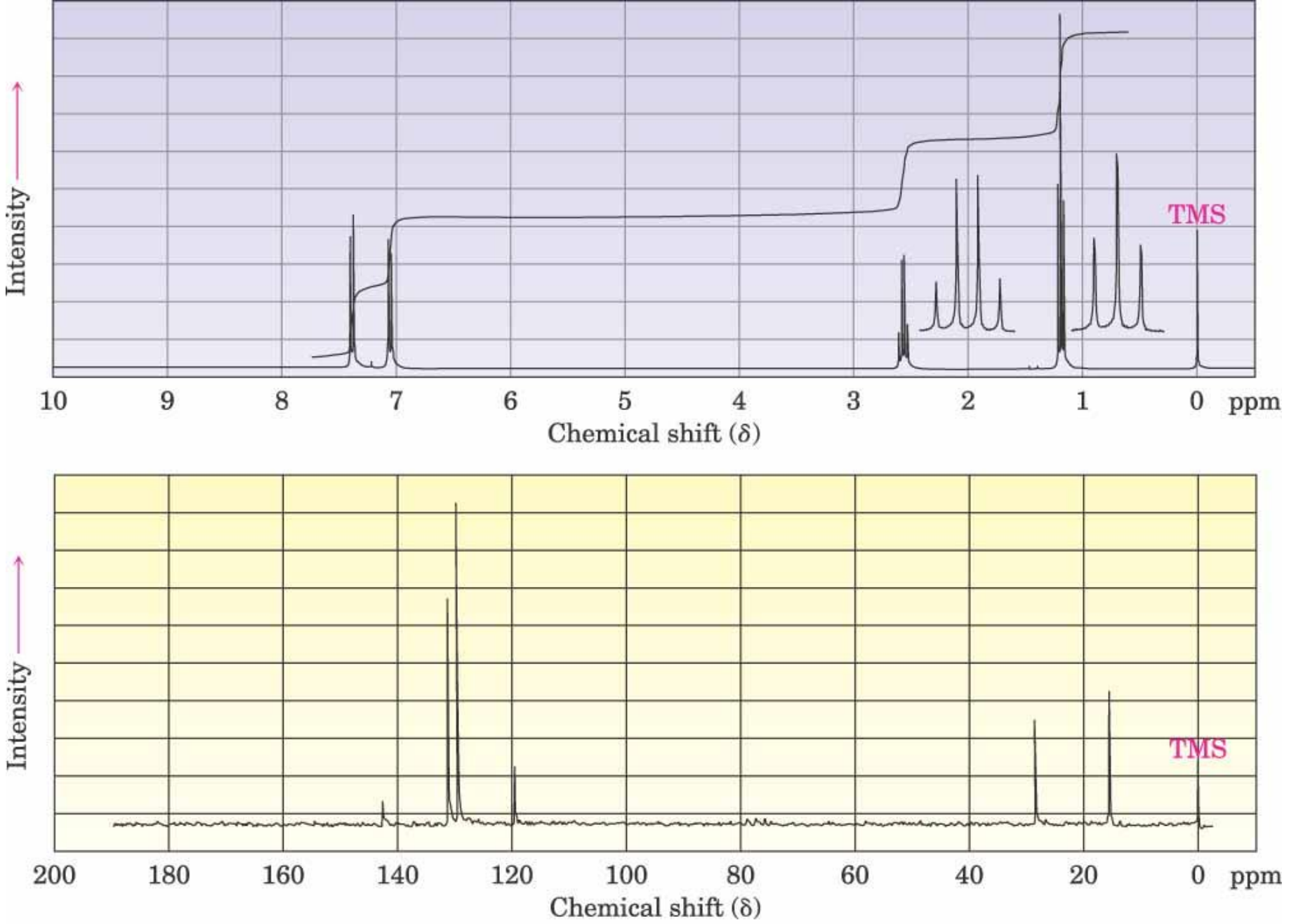
^{1}H and ^{13}C NMR Spectra

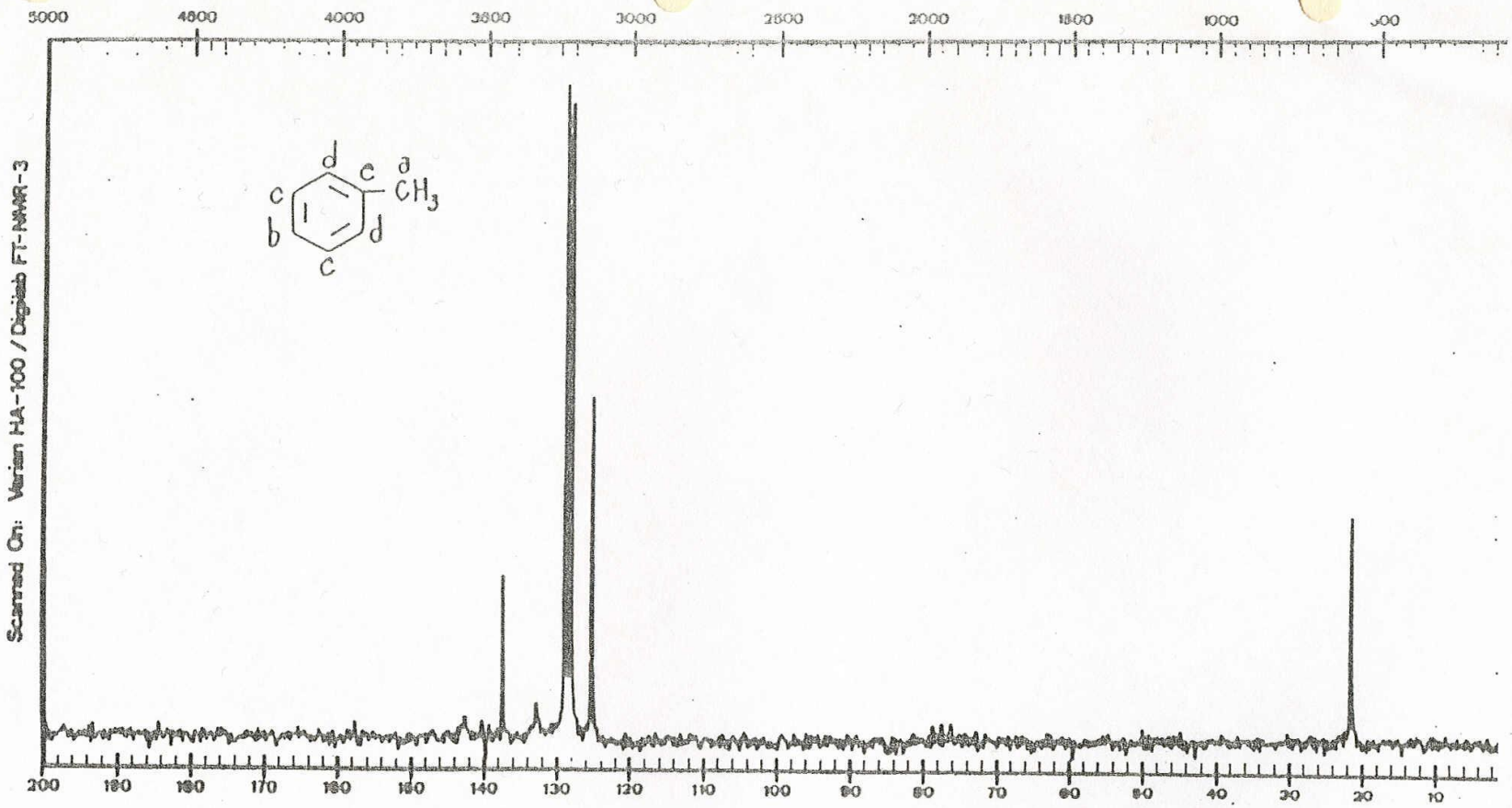


Coupled C-13 NMR Spectrum





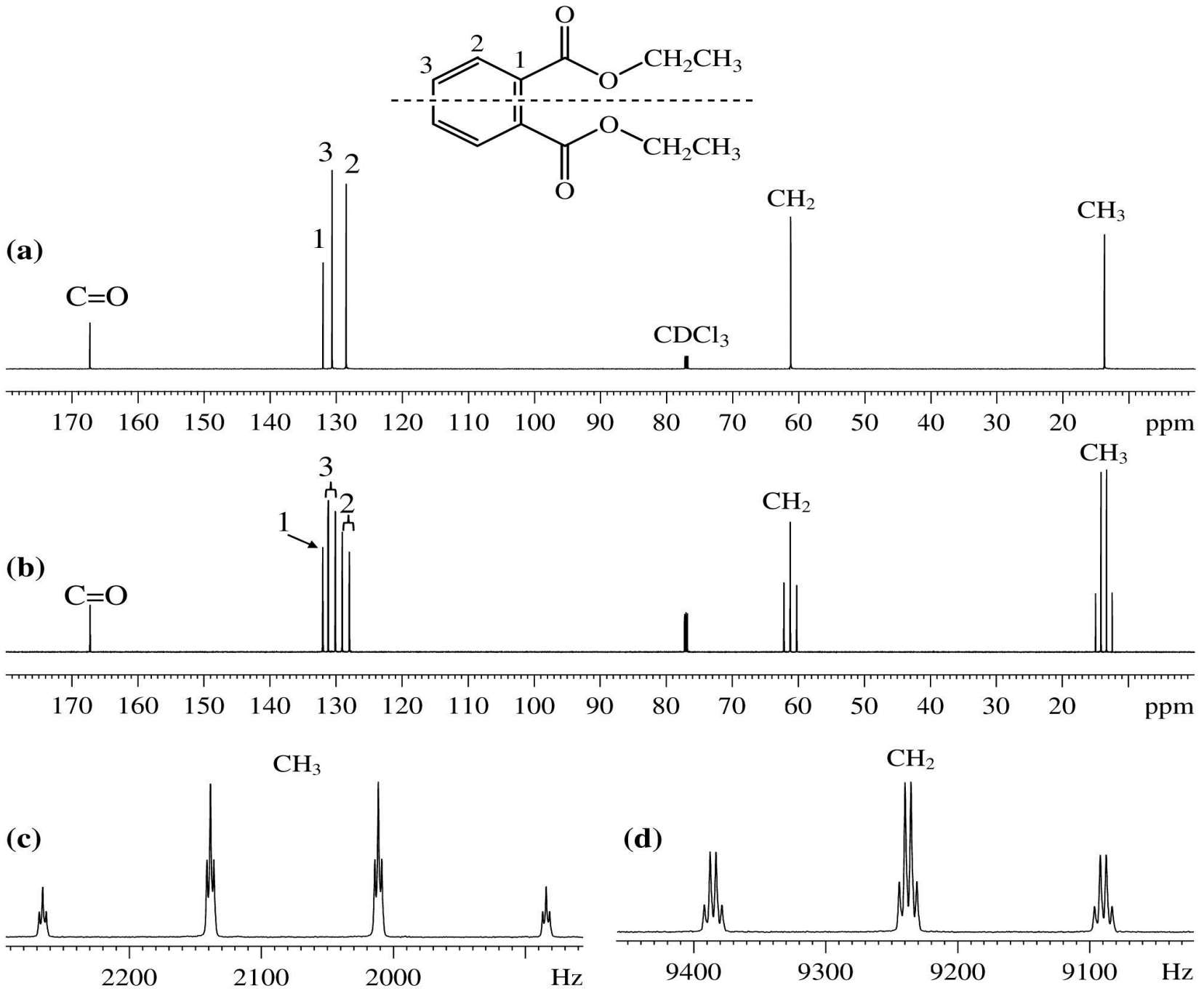


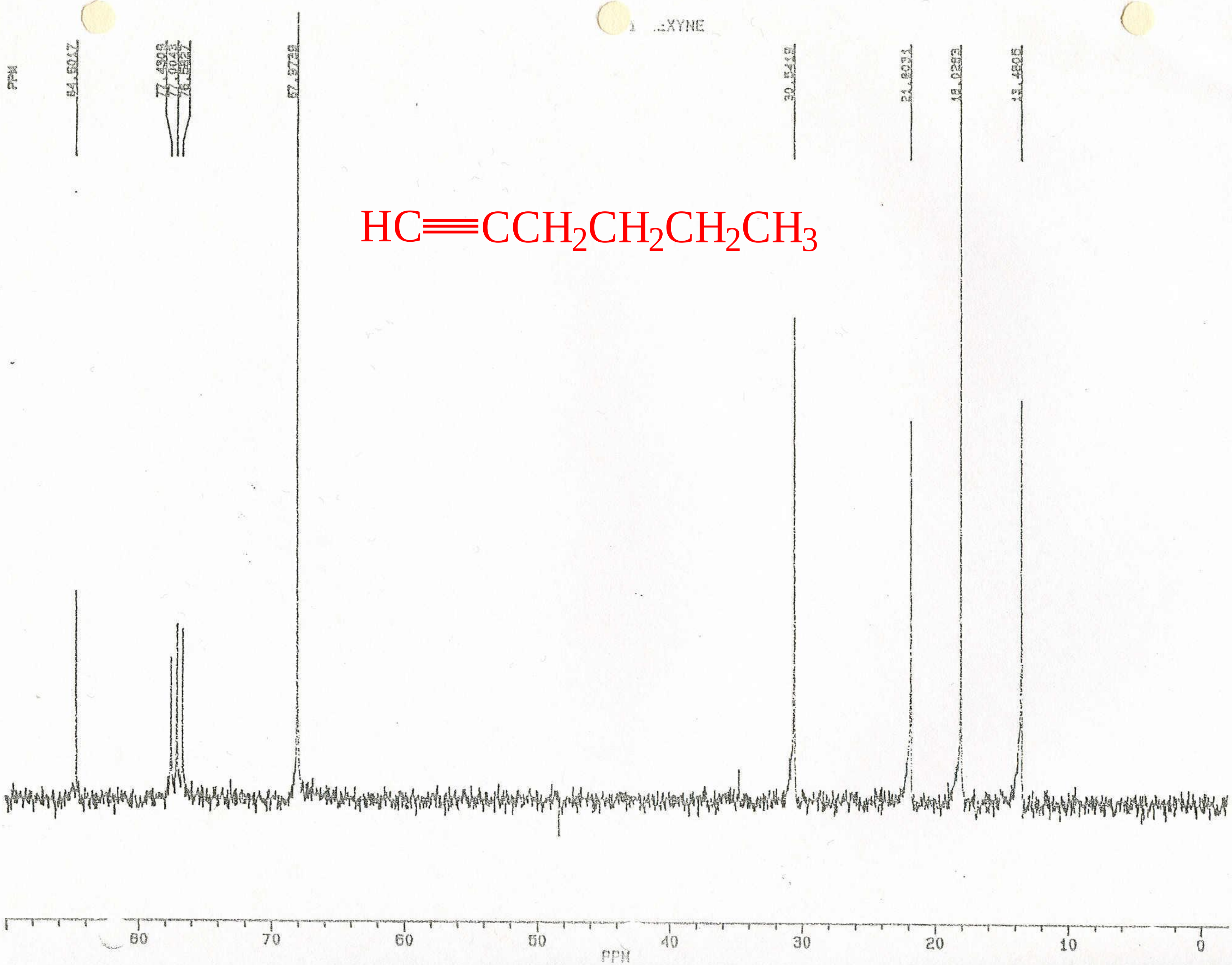


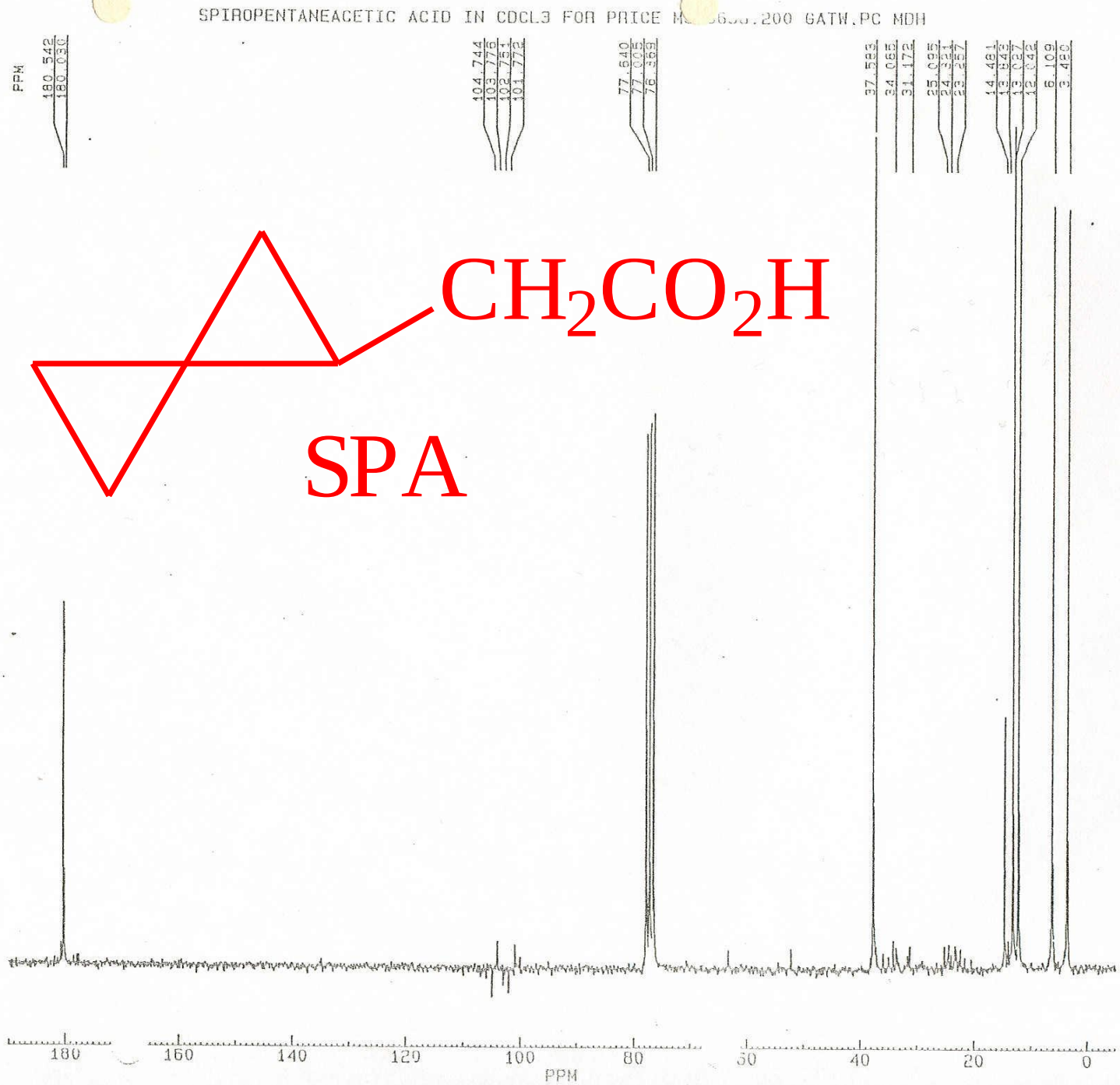
COMPOUND	TOLUENE
SOURCE OF SAMPLE	U.S. Testing Company Hoboken, New Jersey
CHEMICAL FORMULA	C_7H_8
MOLECULAR WT.	92.14
SOLUTION CONC.	50% v/v
SOLVENT	$CDCl_3$
REFERENCE	TMS

ASSIGNMENT

A	21.4	N	
B	125.6	O	
C	129.2	P	
D	130.0	Q	
E	137.7	R	
F		S	
G		T	
H		U	
I		V	
		W	


O
2
3
1
CH2CH3
O
O
CH2CH3
O
3
2
1
CH2
CH3
(a)
C=O
CDCl3
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm
CH3
3
2
1
CH2
(b)
C=O
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm
CH3
(c)
2200 2100 2000 Hz
CH2
(d)
9400 9300 9200 9100 Hz

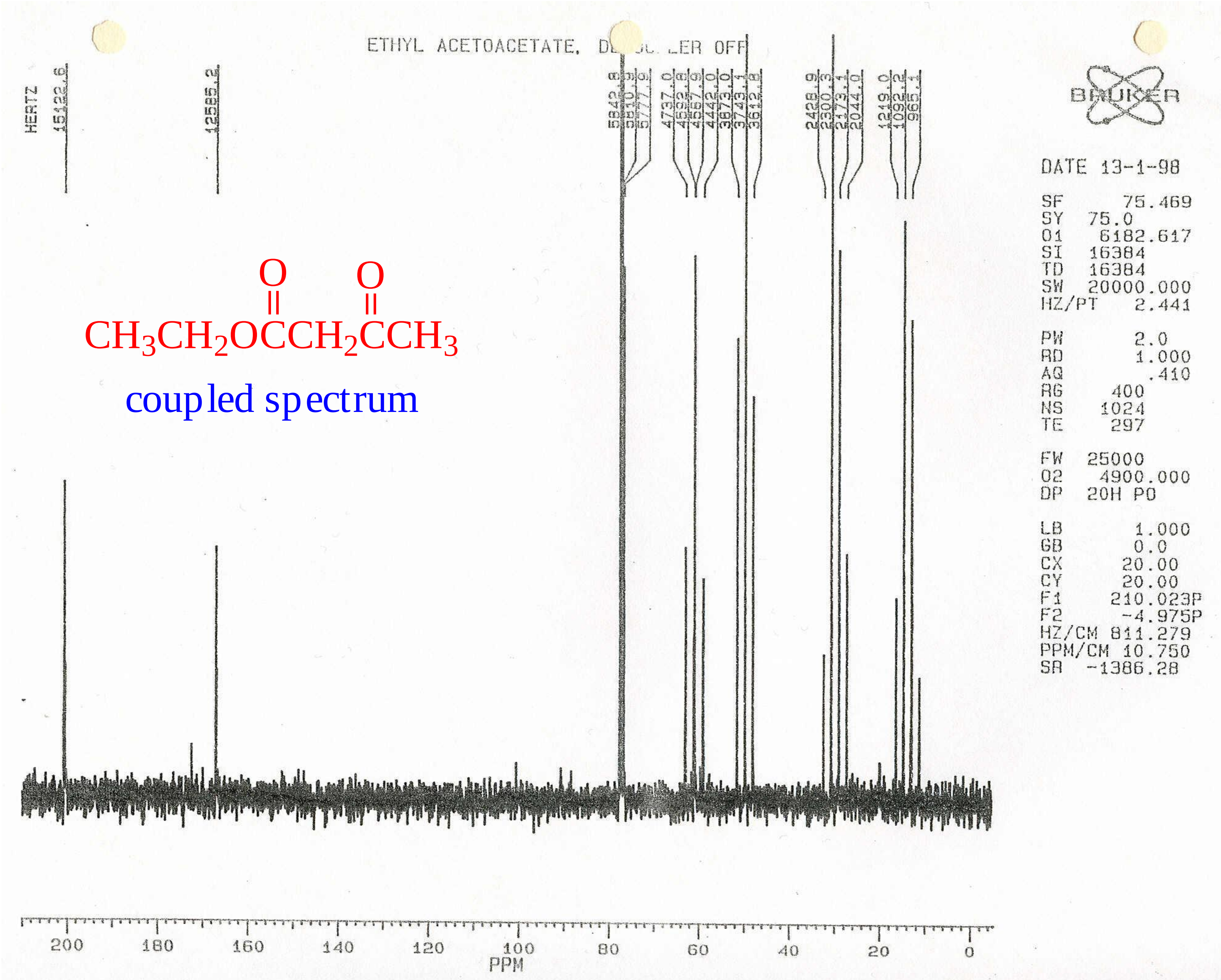

PPM
84.5047
77.4309
77.0043
30.5415
18.0283
HC≡CCH$_2$CH$_2$CH$_2$CH$_3$
80
70
60
50
40
30
20
10
0
PPM



BRUKER

MSL3638.200
AU:
SAVDAT.AU
PPG:
6ATW.PC
DATE 13-11-91

SF	50.323
O1	5351.572
SI	32768
TD	32768
SW	11111.111
HZ/PT	.678
RG	20
NE	1
NS	2009
TE	297
DW	45.0
FW	13400
O2	3040.000
DP	25H D0
D0	2.000S
D1	4.200U
D2	1.000U
D3	50.000U
D4	1.000U
D5	1.000U
D6	1.000U
LB	3.000
GB	0.0
NC	4
CX	20.00
CY	15.00
HZ/CM	490.723
SR	317.71


ETHYL ACETOACETATE,
LER OFF
HERTZ
15122.6
12585.2
5842.8
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5777.9
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4567.9
4442.0
3873.0
3743.1
3612.8
2428.9
2300.3
2173.1
2044.0
1219.0
1092.2
965.1
BRUKER
DATE 13-1-98
SF 75.469
SY 75.0
O1 6182.617
SI 16384
TD 16384
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HZ/PT 2.441
PW 2.0
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RG 400
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FW 25000
O2 4900.000
DP 20H PO
LB 1.000
GB 0.0
CX 20.00
CY 20.00
F1 210.023P
F2 -4.975P
HZ/CM 811.279
PPM/CM 10.750
SR -1386.28
200
180
160
140
120
100
80
60
40
20
0
PPM
$CH_3CH_2OC(=O)CH_2C(=O)CH_3$
coupled spectrum

Broadband decoupled	DEPT-90	DEPT-135
C, CH, CH_2, CH_3	CH	CH_3, CH are positive CH_2 is negative

C	Subtract DEPT-135 from broadband decoupled
CH	DEPT-90
CH_2	Negative DEPT-135
CH_3	Subtract DEPT-90 from positive DEPT-135