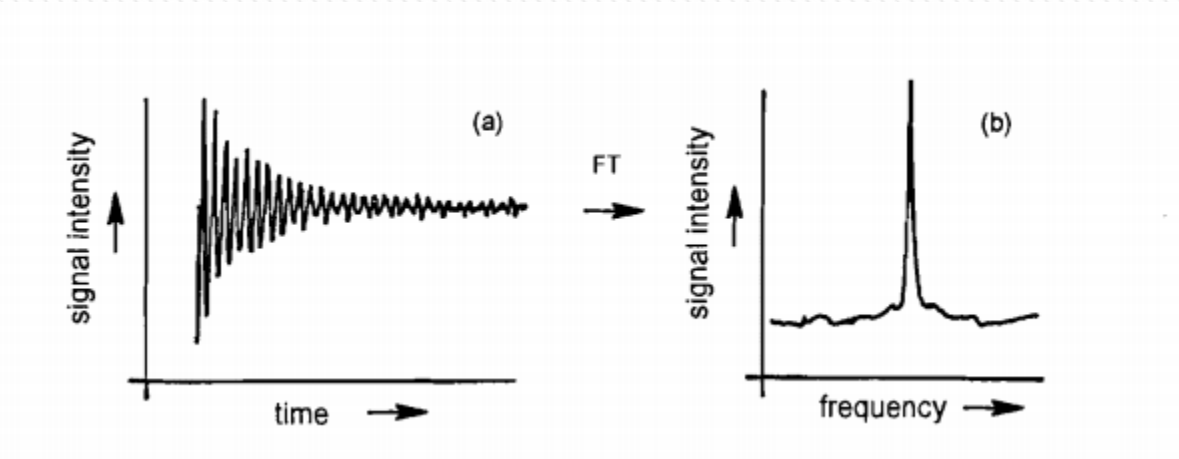
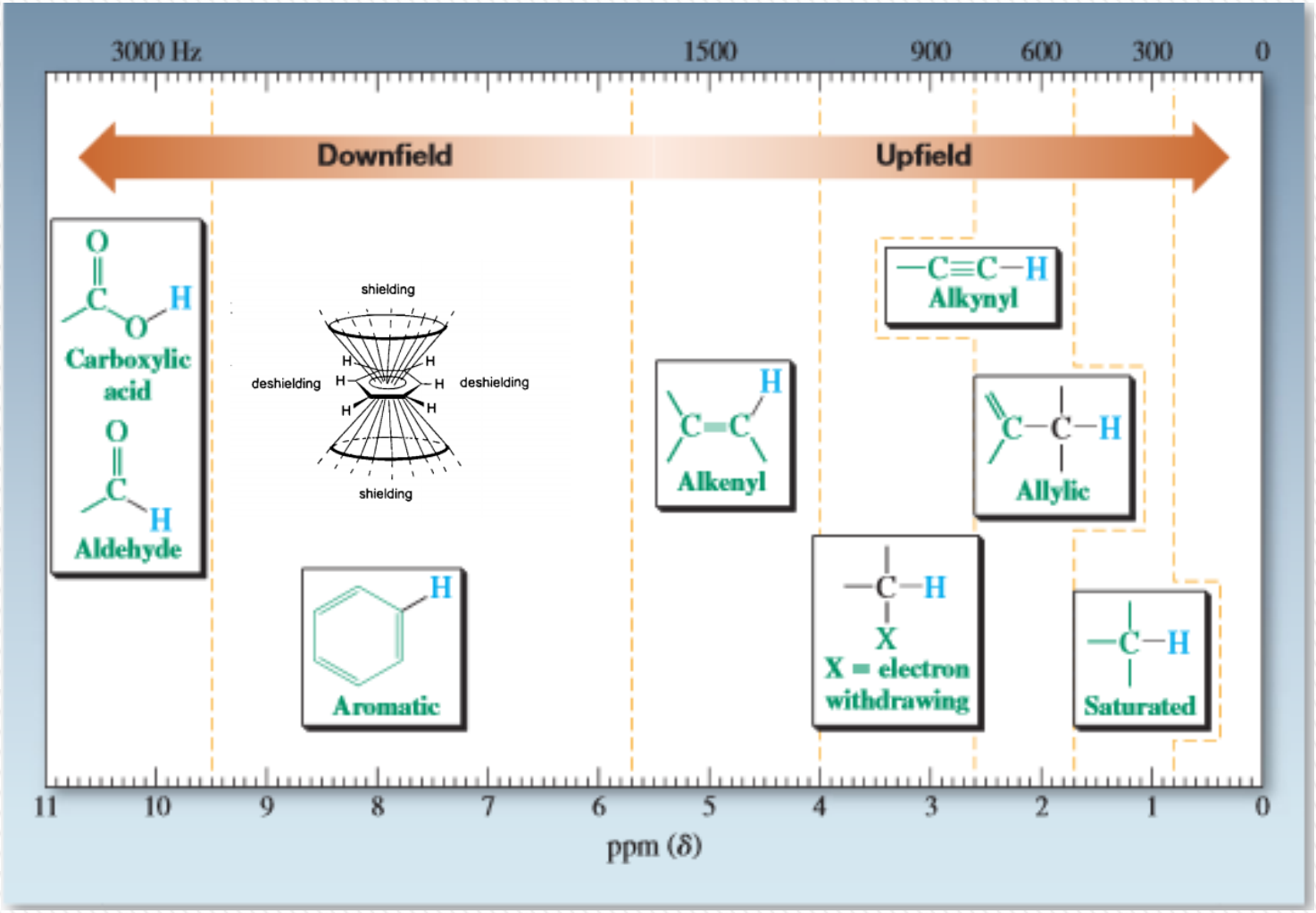
- Určeno pouze ke studijním účelům

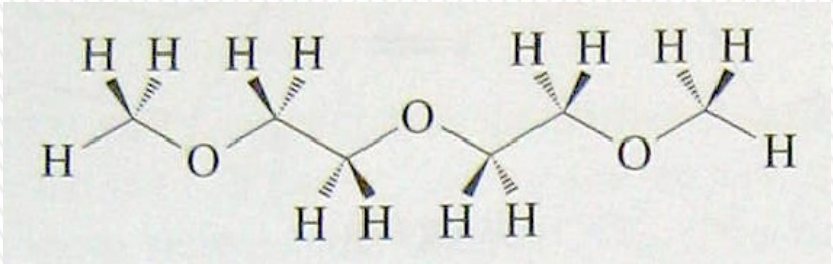
- Zdroje: Peter Vollhardt, K Peter C Vollhardt, Neil E Schore, Neil Schore: Organic Chemistry. Structure and Function. 6th Edition.
  ISBN: **142920494X**

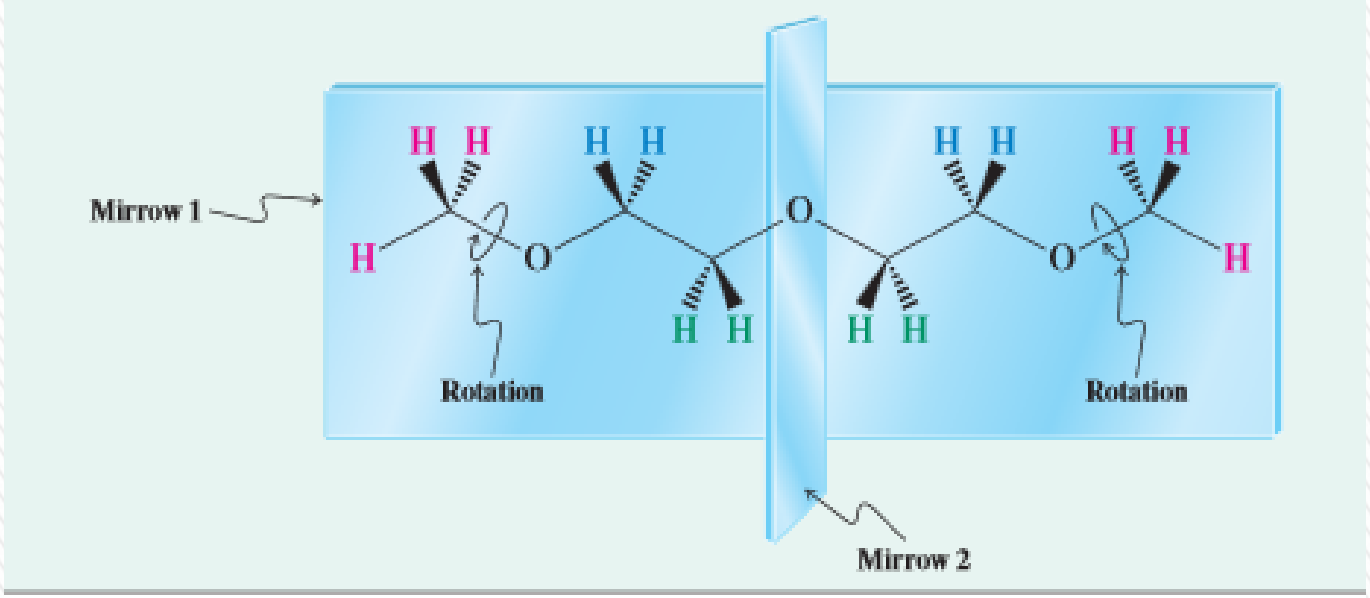
^{1}H NMR spektroskopie

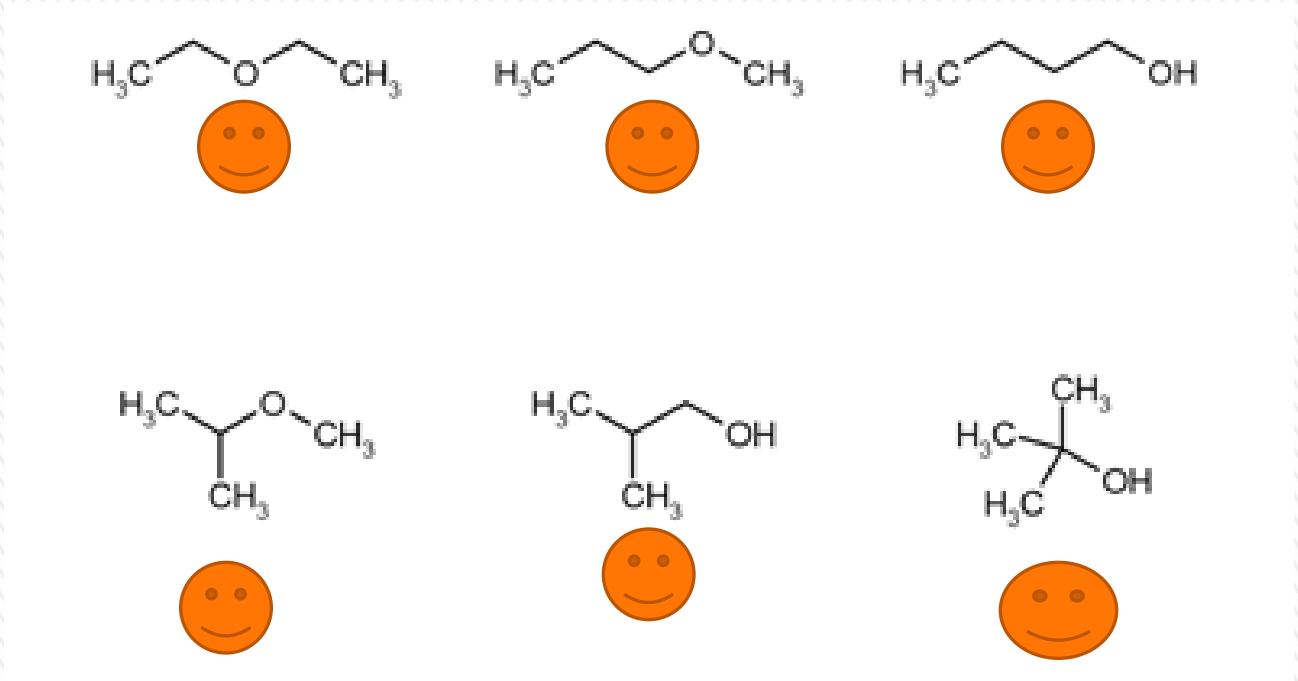


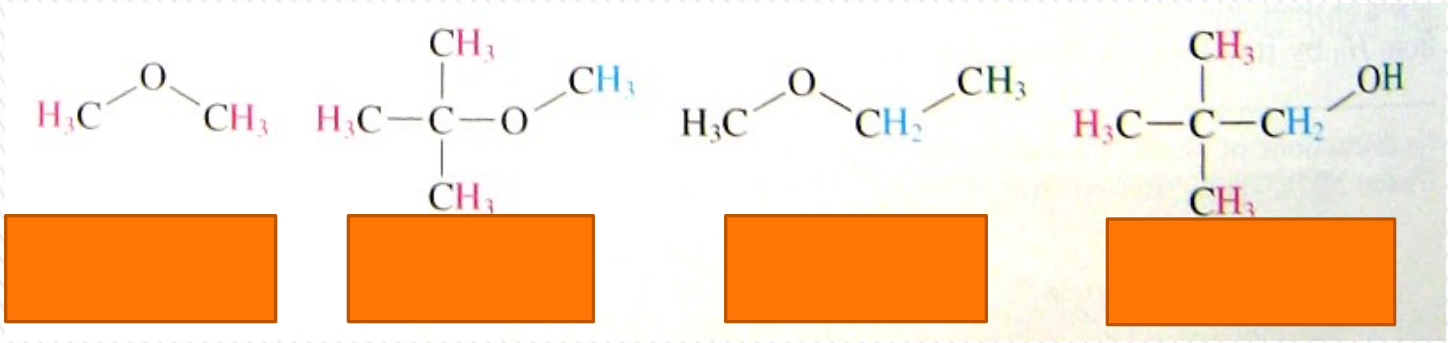

3000 Hz
1500
900
600
300
0
Downfield
Upfield
Carboxylic acid
Aldehyde
shielding
deshielding
deshielding
shielding
Aromatic
Alkenyl
Alkynyl
Allylic
X = electron withdrawing
Saturated
11
10
9
8
7
6
5
4
3
2
1
0
ppm (δ)

Kolik ^{1}H NMR signálů očekáváte u níže uvedené molekuly?





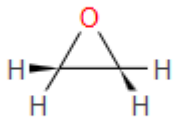

H3C O CH3
H3C O CH3
H3C OH
H3C O CH3 CH3
H3C OH CH3
CH3 H3C OH H3C

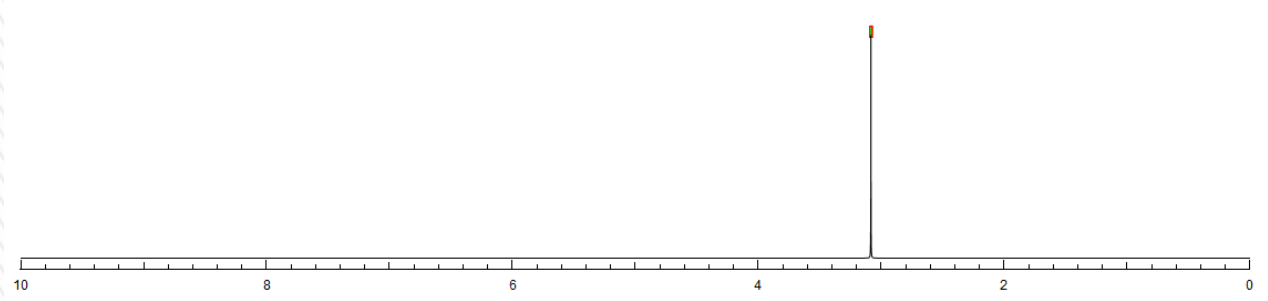

H3C O CH3
CH3 H3C C O CH3 CH3
H3C O CH2 CH3
CH3 H3C C CH2 OH CH3

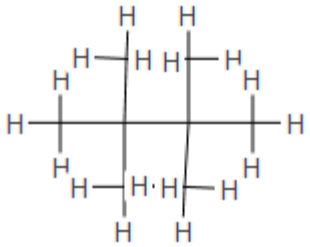
Kolik ^{1}H NMR signálů očekáváte u molekuly

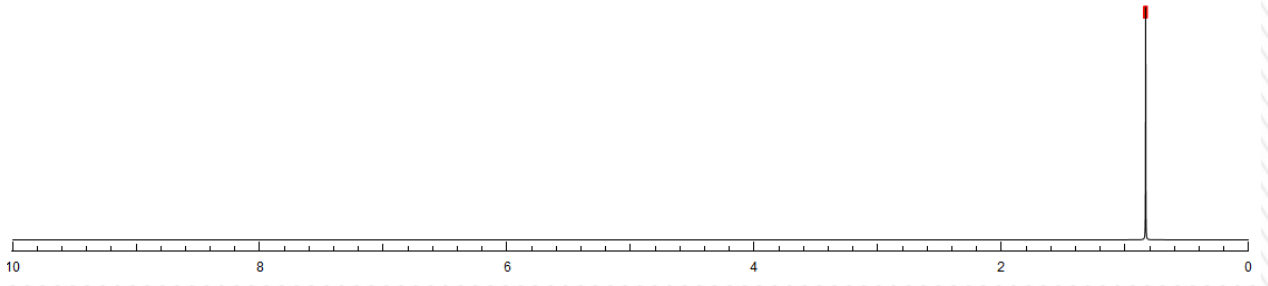
a) oxacyklopropanu

b) 2,2,3,3-tetramethylbutanu









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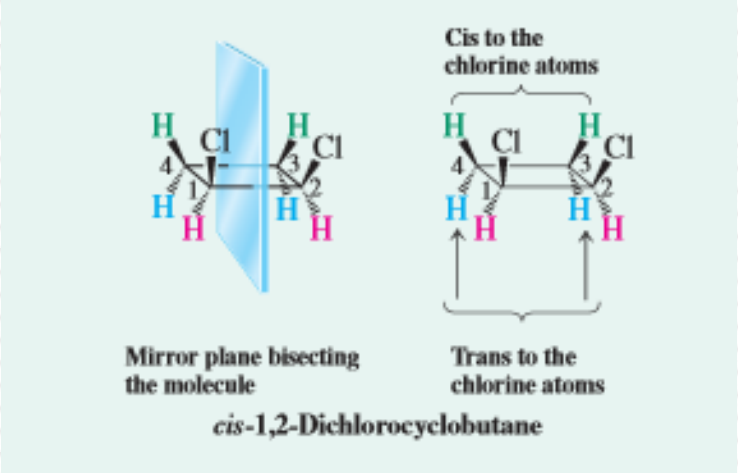
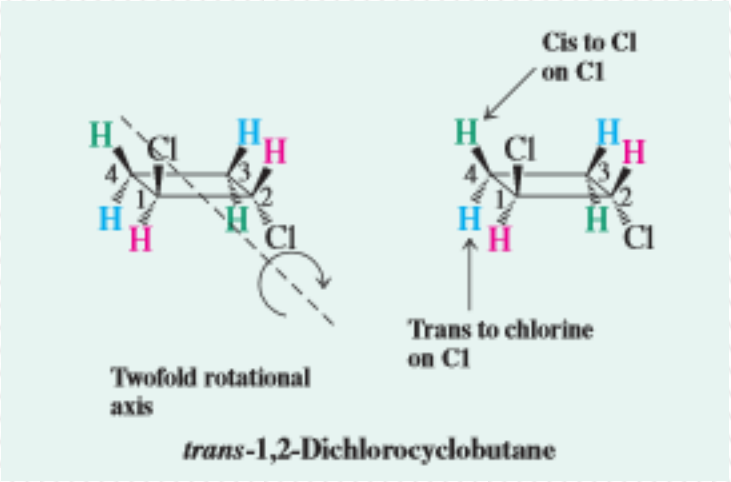
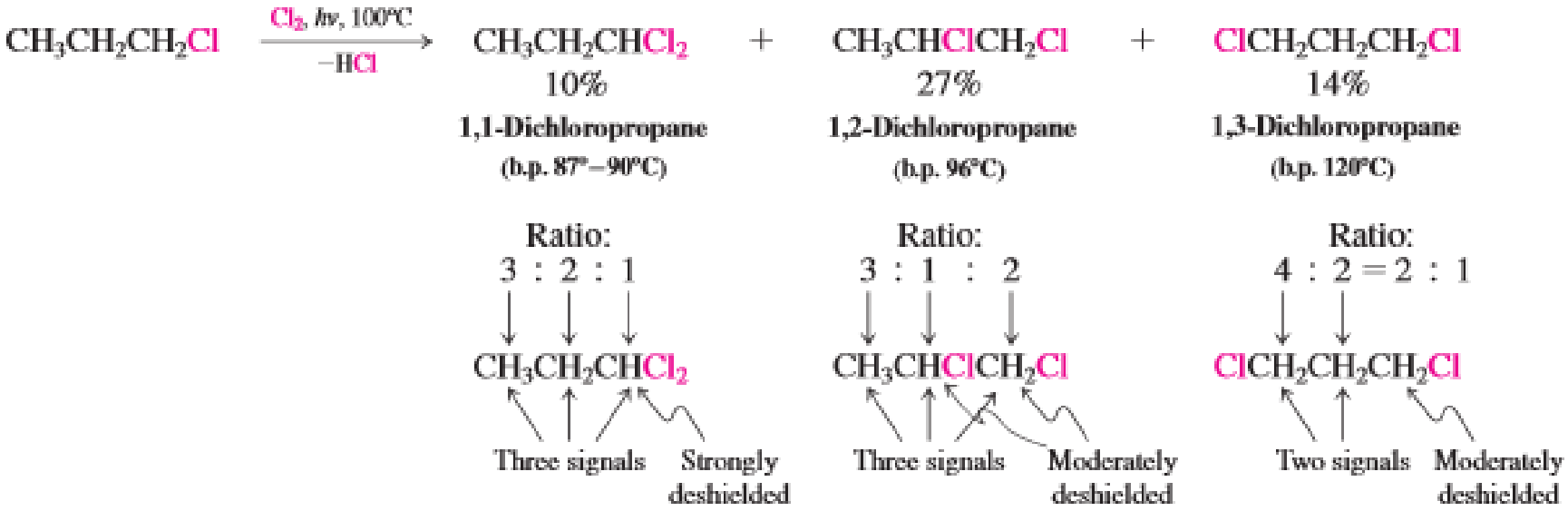
Database of NMR spectra

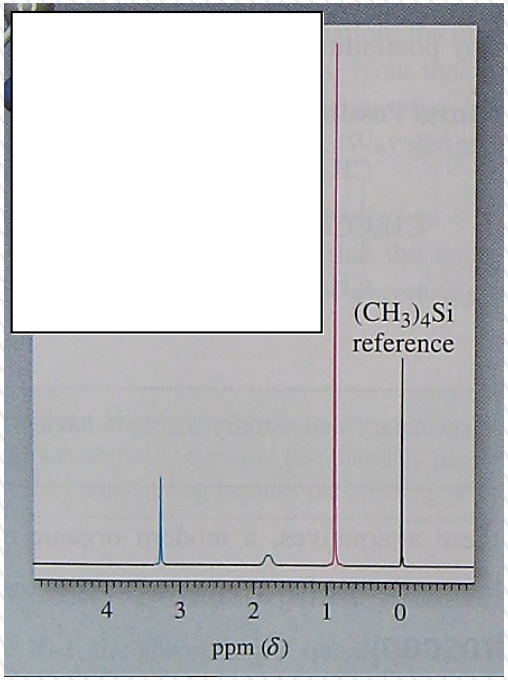
Kolik signálů očekáváte v ^{1}H NMR spektru *cis*- a *trans*-1,2-dichlorcyklobutanu?

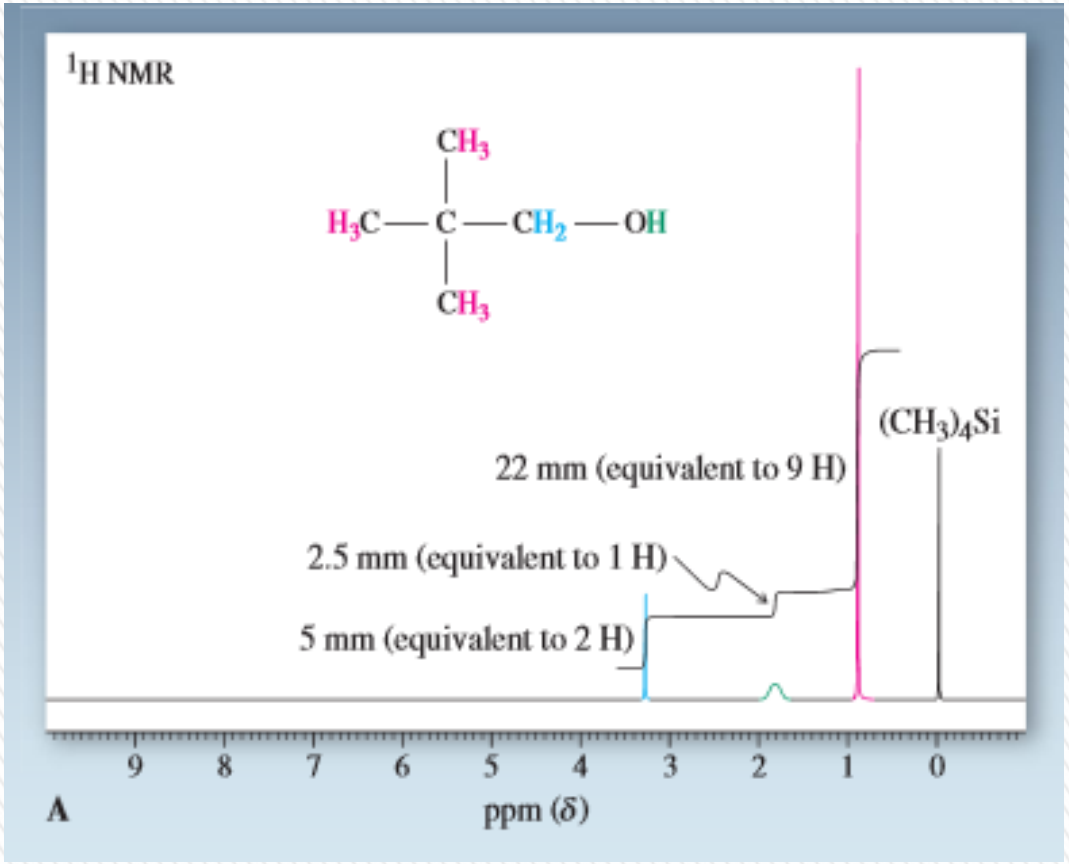


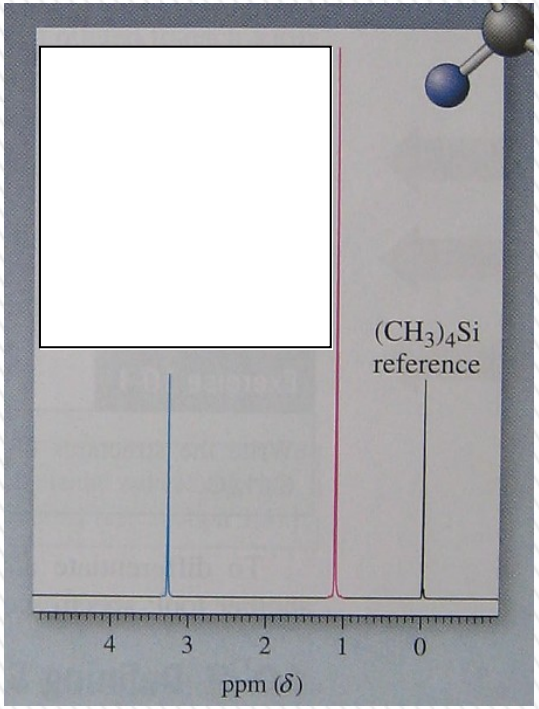


» Chemický posun a integrace plochy píků slouží k určení struktury molekul



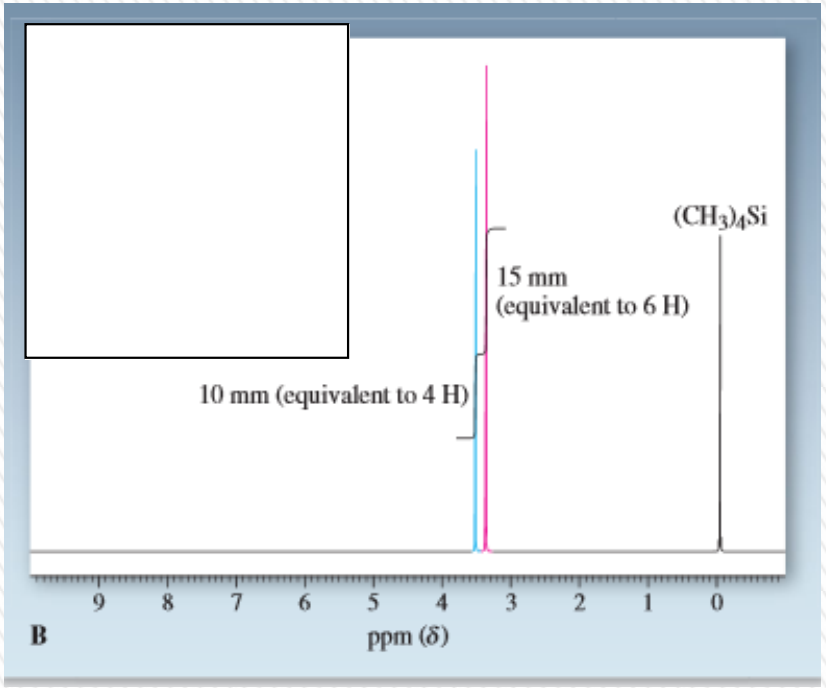


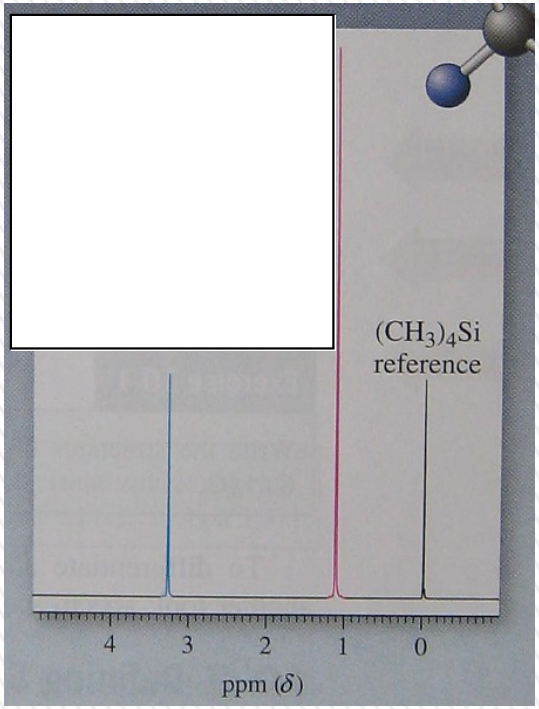


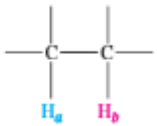
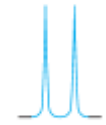
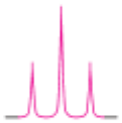
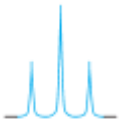
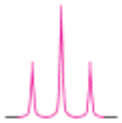
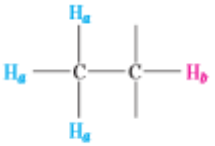
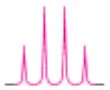
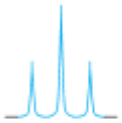
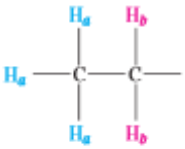
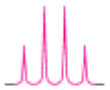
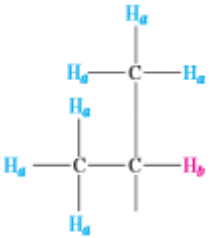
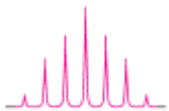


Rozhodněte, které spektrum náleží molekule (*t*-butyl)(methyl)etheru
a které molekule 2,2-dimethylpropanolu?

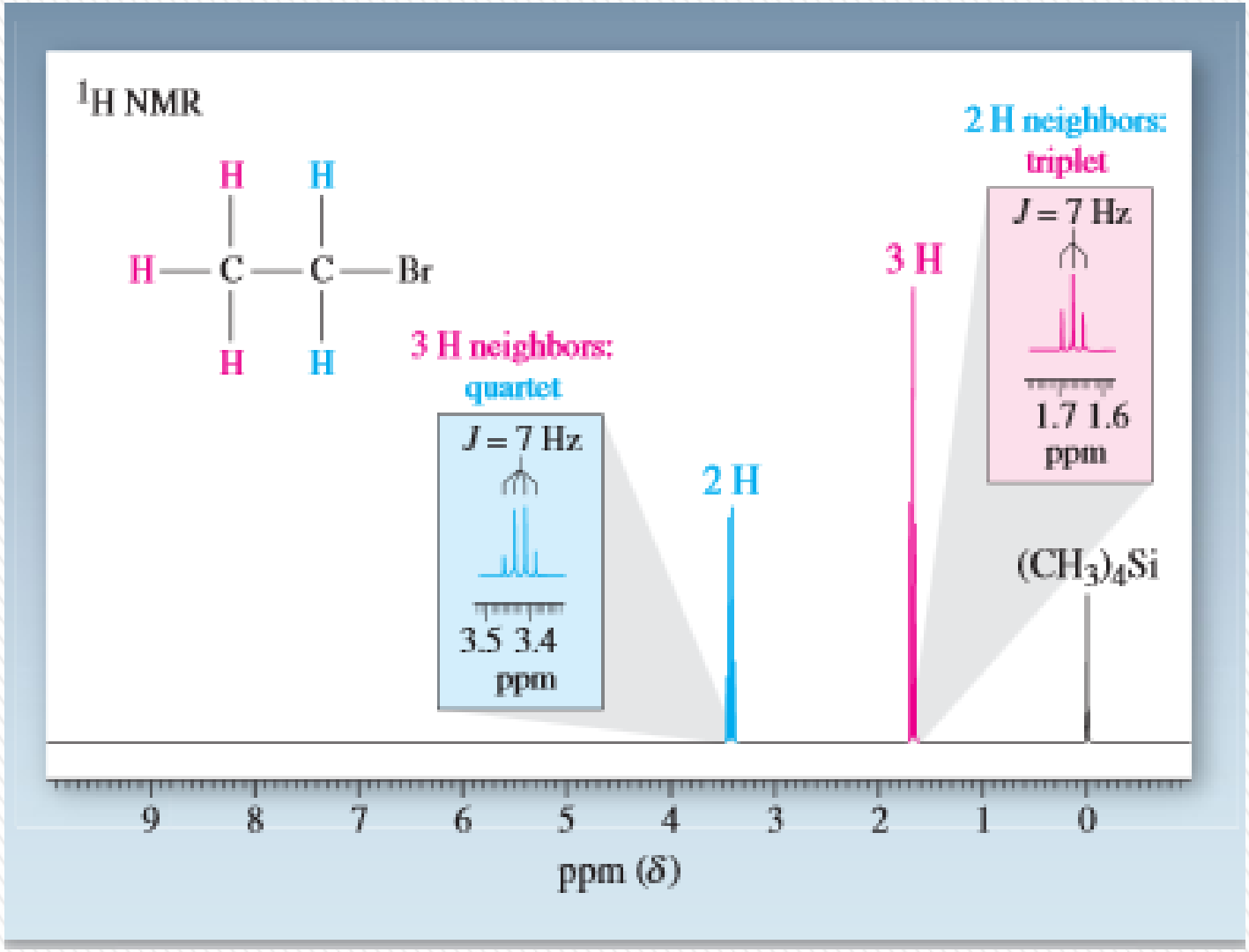
Rozhodněte, které spektrum náleží molekule (*t*-butyl)(methyl)etheru a které molekule 1,2-dimethoxyethanu.

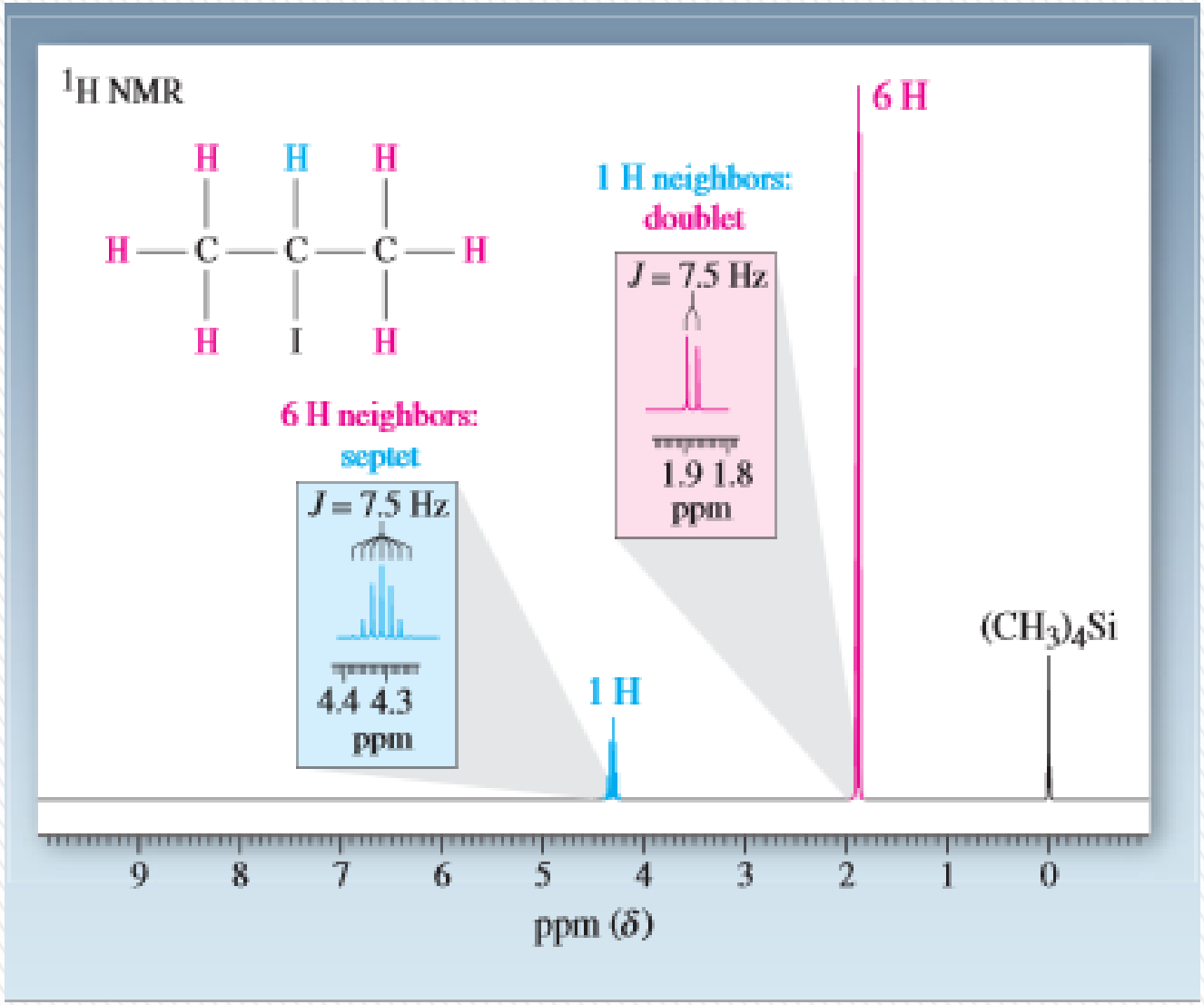


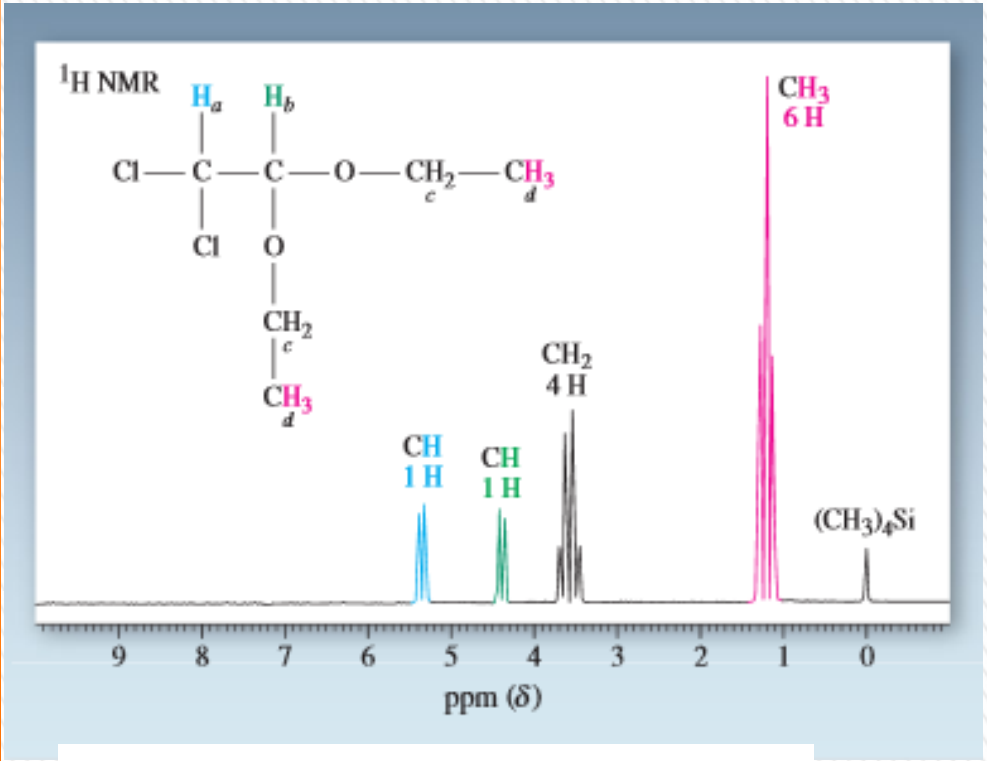


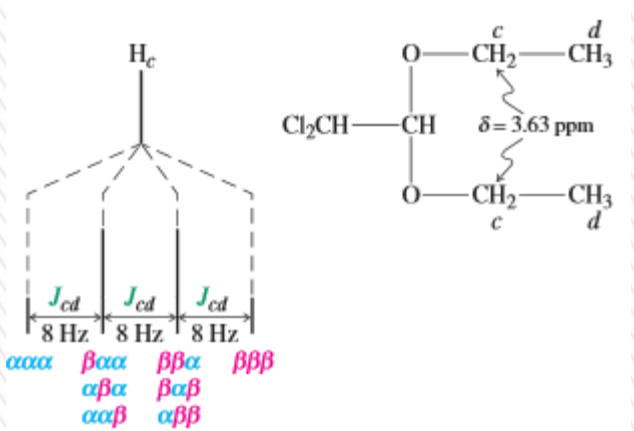
Splitting pattern for H_a	Structure	Splitting pattern for H_b
H_a has **one neighbor** H_b: 2 peaks or doublet				H_b has **one neighbor** H_a: 2 peaks or doublet
H_a has **one neighbor** H_b: 2 peaks or doublet				H_b has **two neighbors** H_a: 3 peaks or triplet
H_a has **two neighbors** H_b: 3 peaks or triplet				H_b has **two neighbors** H_a: 3 peaks or triplet
H_a has **one neighbor** H_b: 2 peaks or doublet				H_b has **three neighbors** H_a: 4 peaks or quartet
H_a has **two neighbors** H_b: 3 peaks or triplet				H_b has **three neighbors** H_a: 4 peaks or quartet
H_a has **one neighbor** H_b: 2 peaks or doublet				H_b has **six neighbors** H_a: 7 peaks or septet

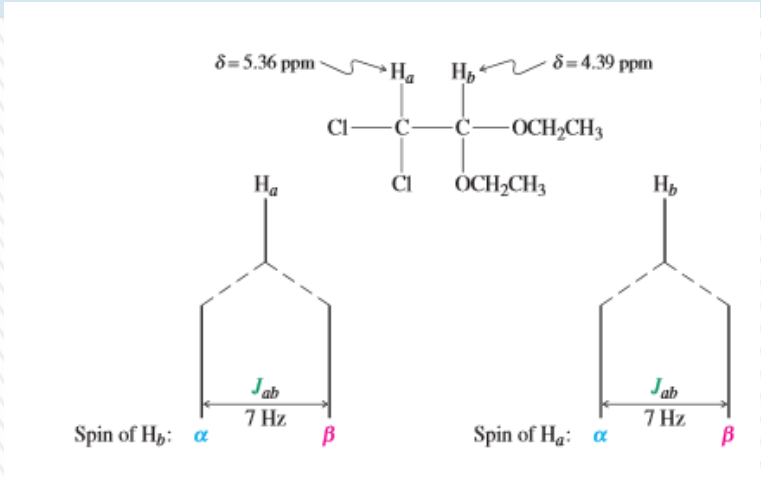
Note: H_a and H_b are not equivalent and have no other coupled nuclei in their vicinity.

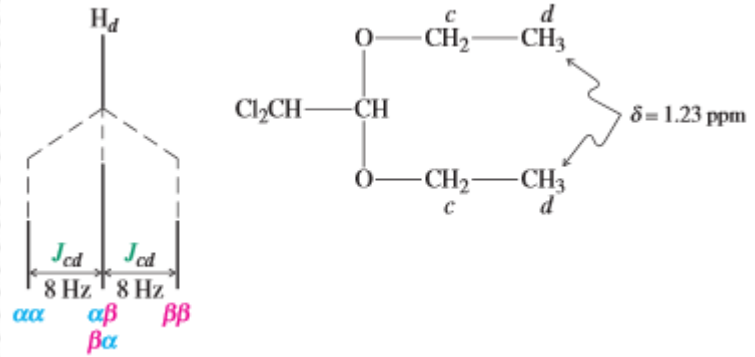

^{1}H NMR
H H
H C C Br
H H
2 H neighbors:
triplet
J = 7 Hz
1.7 1.6
ppm
3 H
3 H neighbors:
quartet
J = 7 Hz
3.5 3.4
ppm
2 H
(CH3)4Si
9 8 7 6 5 4 3 2 1 0
ppm (δ)


^{1}H NMR
6 H
1 H neighbors:
doublet
J = 7.5 Hz
1.9 1.8
ppm
6 H neighbors:
septet
J = 7.5 Hz
4.4 4.3
ppm
1 H
$(CH_3)_4Si$
9 8 7 6 5 4 3 2 1 0
ppm (δ)



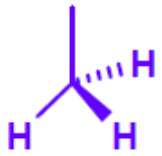


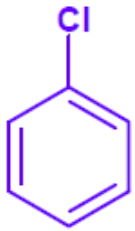


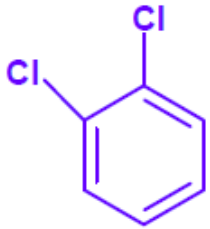


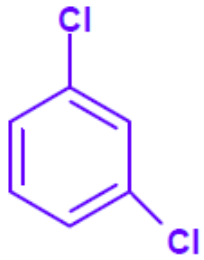
Štěpení signálů:
1,1-dichlor-2,2-diethoxyethan

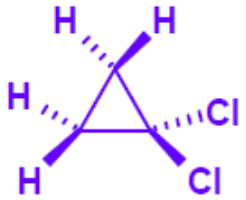
Počet signálů ve spektru:
zjištění počtu ekvivalentních jader

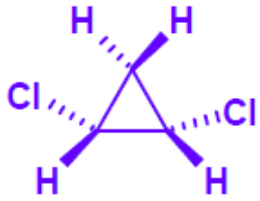


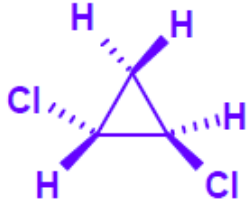




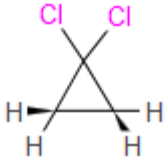


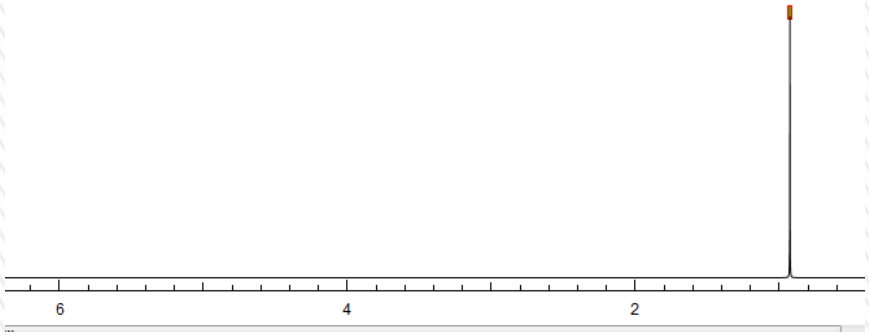


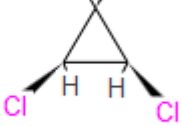


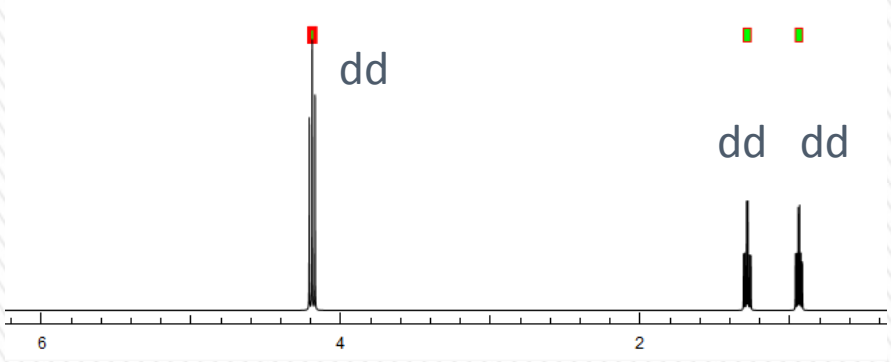


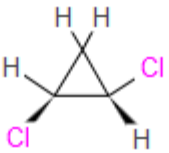
Chlorace chlorcyklopropanu poskytuje tři sloučeniny se sumárním vzorcem $C_3H_4Cl_2$. Nakreslete jejich strukturu a popište, jak byste je rozlišili pomocí jejich ^1H NMR spekter.

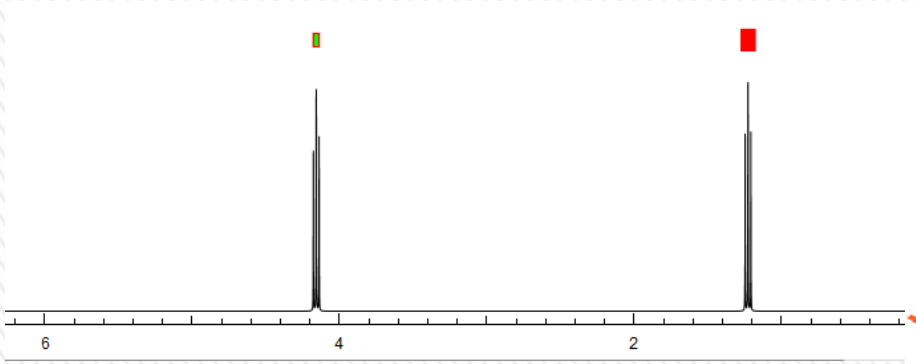






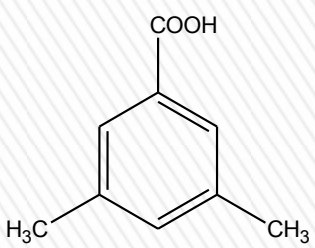


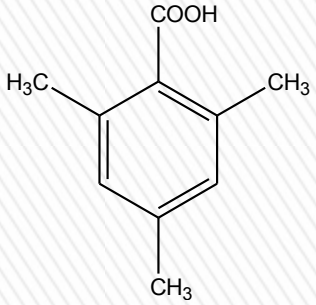


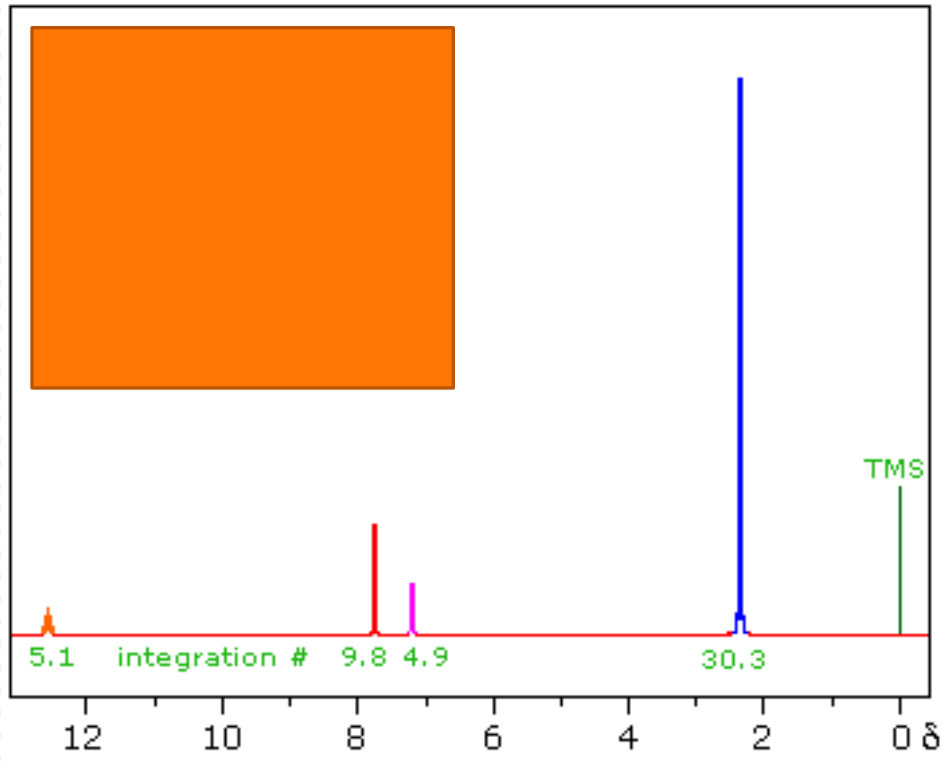


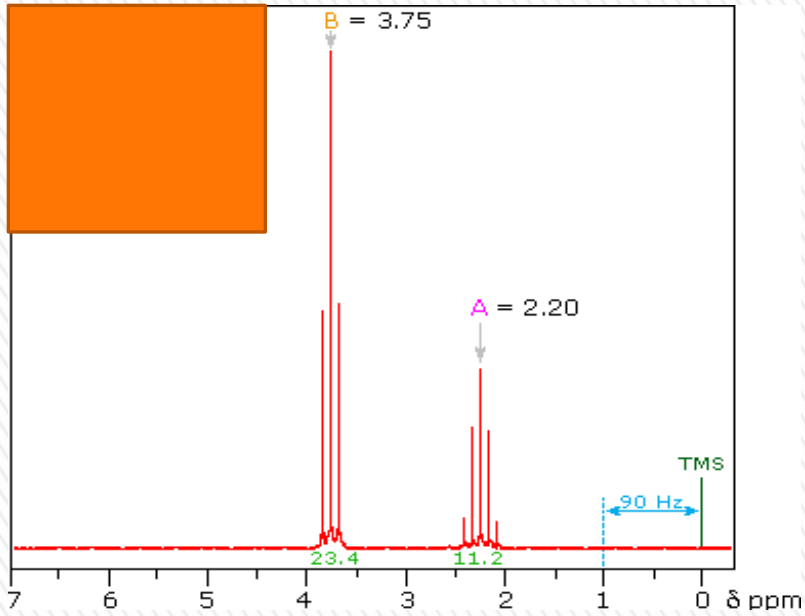
nmrdb.org
Database of NMR spectra

Rozhodněte, které z následujících sloučenin odpovídá níže uvedené ^{1}H NMR spektrum.







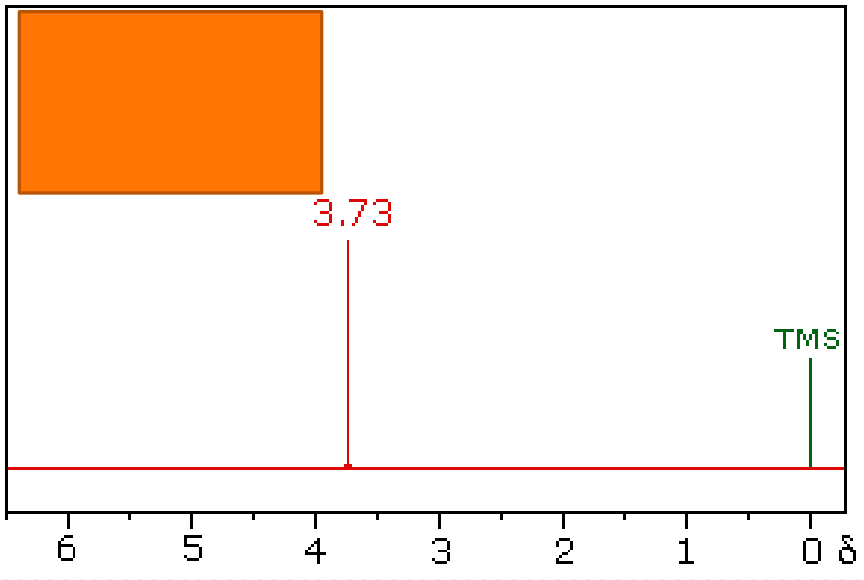


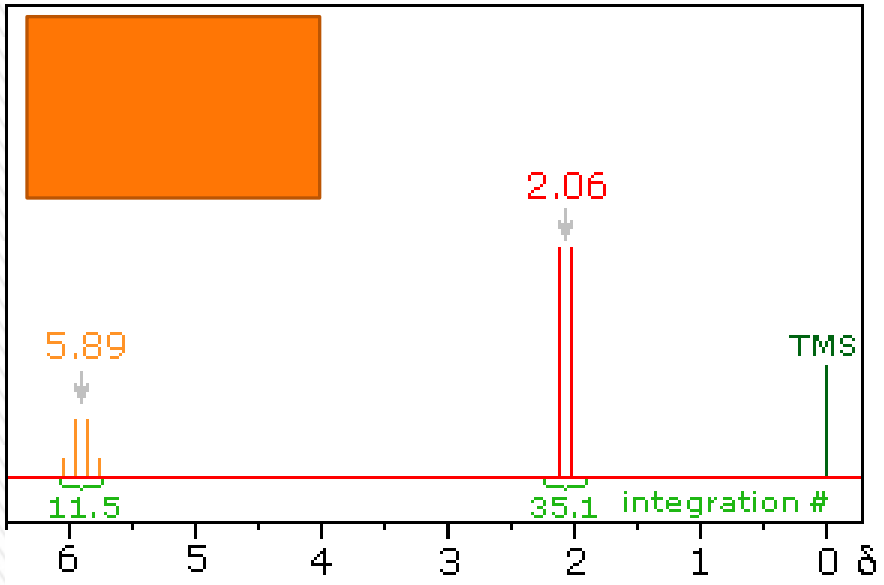
Přiřaďte následující ^{1}H NMR spektra níže uvedeným sloučeninám:

1,1-dichlorethan

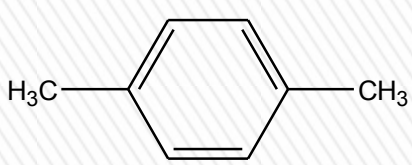
1,2-dichlorethan

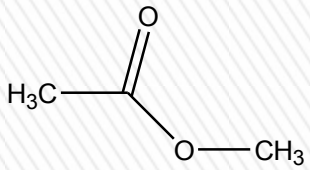
1,3-dichlorpropan

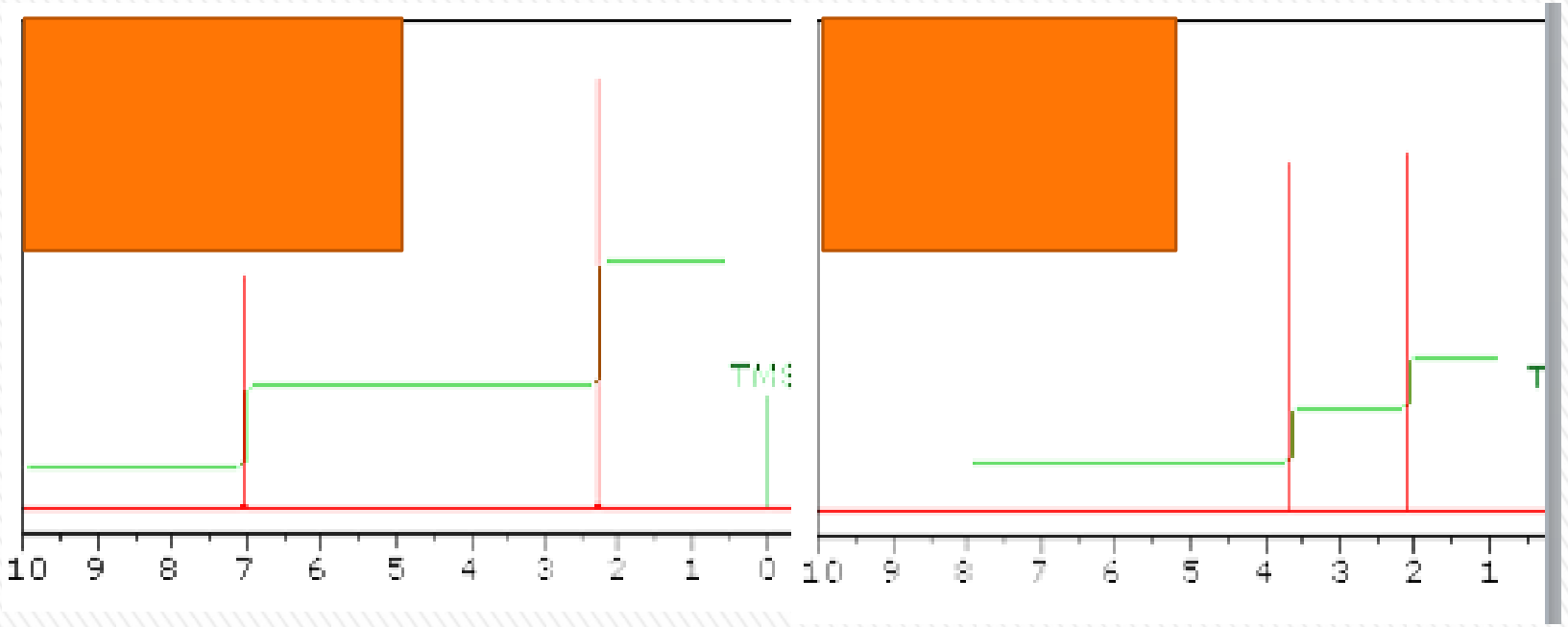




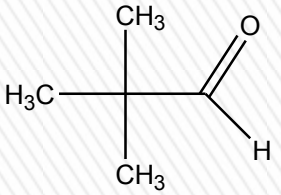
Rozhodněte, které z následujících sloučenin odpovídá níže uvedené ^{1}H NMR spektrum.

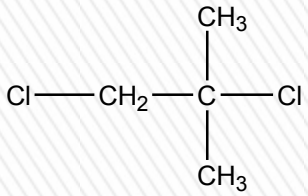


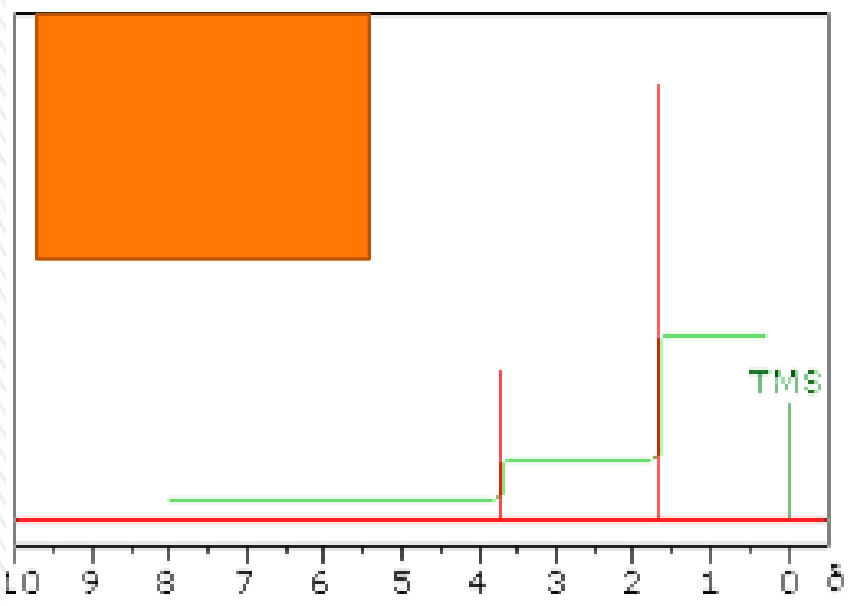


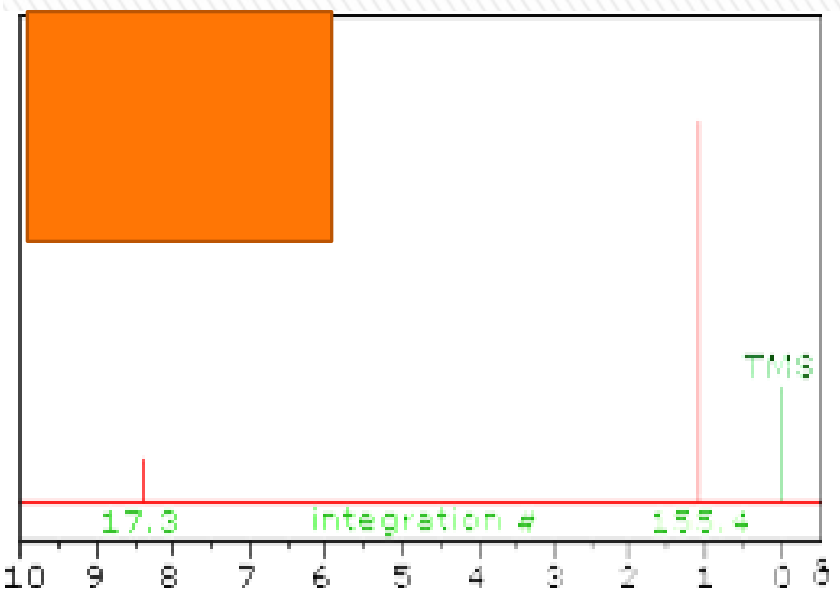


Rozhodněte, které z následujících sloučenin odpovídá níže uvedené ^{1}H NMR spektrum.



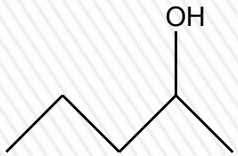


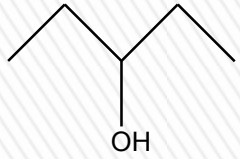


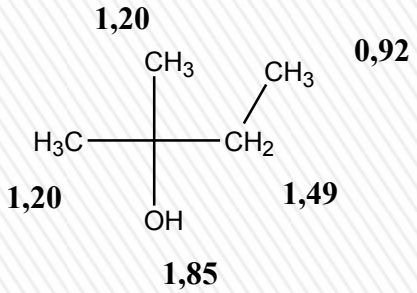


Pokuste se odhadnout, kterému z izomerních alkoholů sumárního vzorce $C_5H_{12}O$ odpovídá následující ^1H NMR spektrum.

- 0,92 (t, 3H)
- 1,20 (s, 6H)
- 1,49 (k, 2H)
- 1,85 (š. s, 1H)

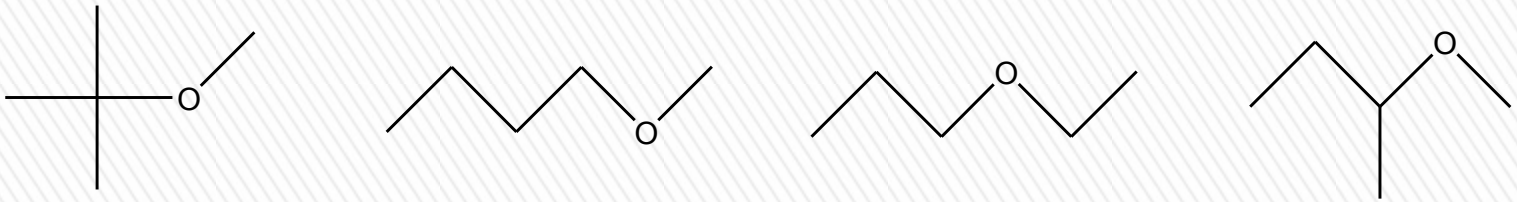






Pokuste se odhadnout, jak byste na základě ^{1}H NMR spekter rozlišili izomerní ethery sumárního vzorce $C_5H_{12}O$ a kterému z nich odpovídá následující spektrum.

- 1,19 (s, 9H)
- 3,21 (s, 3H)



^{13}C NMR spektroskopie

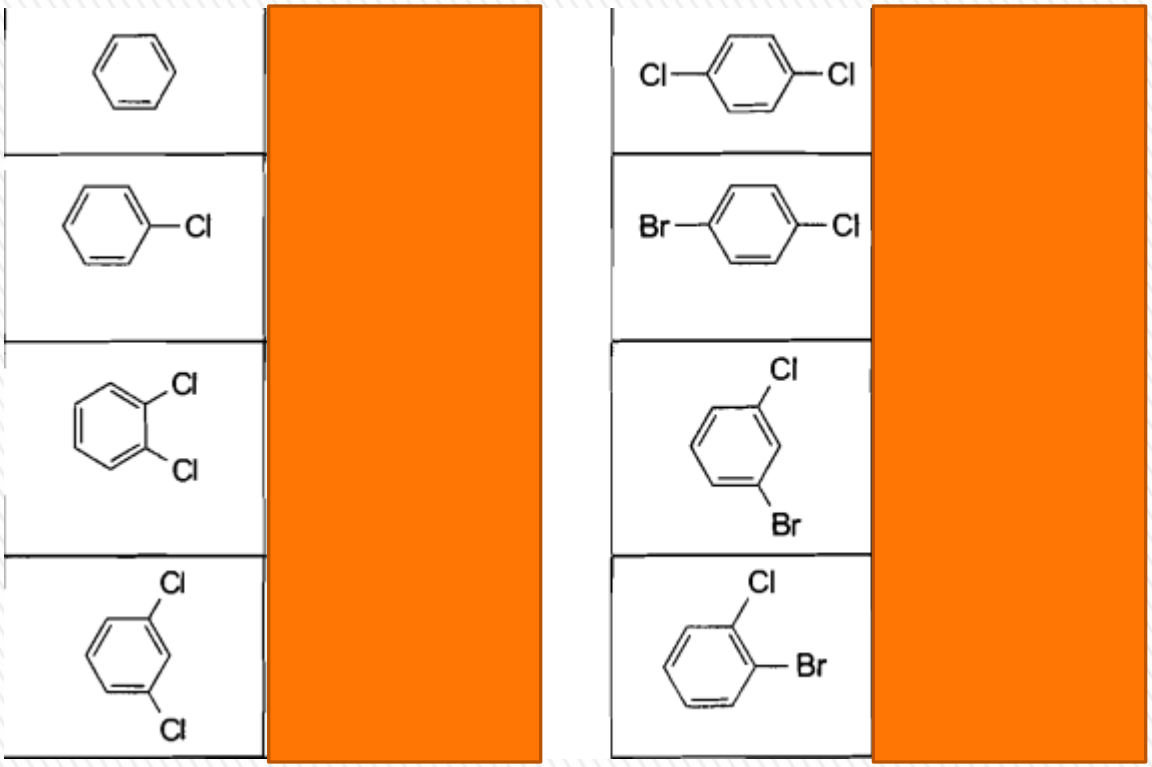
Stejná jako v ^{1}H NMR spektru, tj. odpovídá počtu ekvivalentních jader.

Ale značně závislá na způsobu měření neboť ^{13}C jádra mají velmi rozdílné ***relaxační časy*** ...

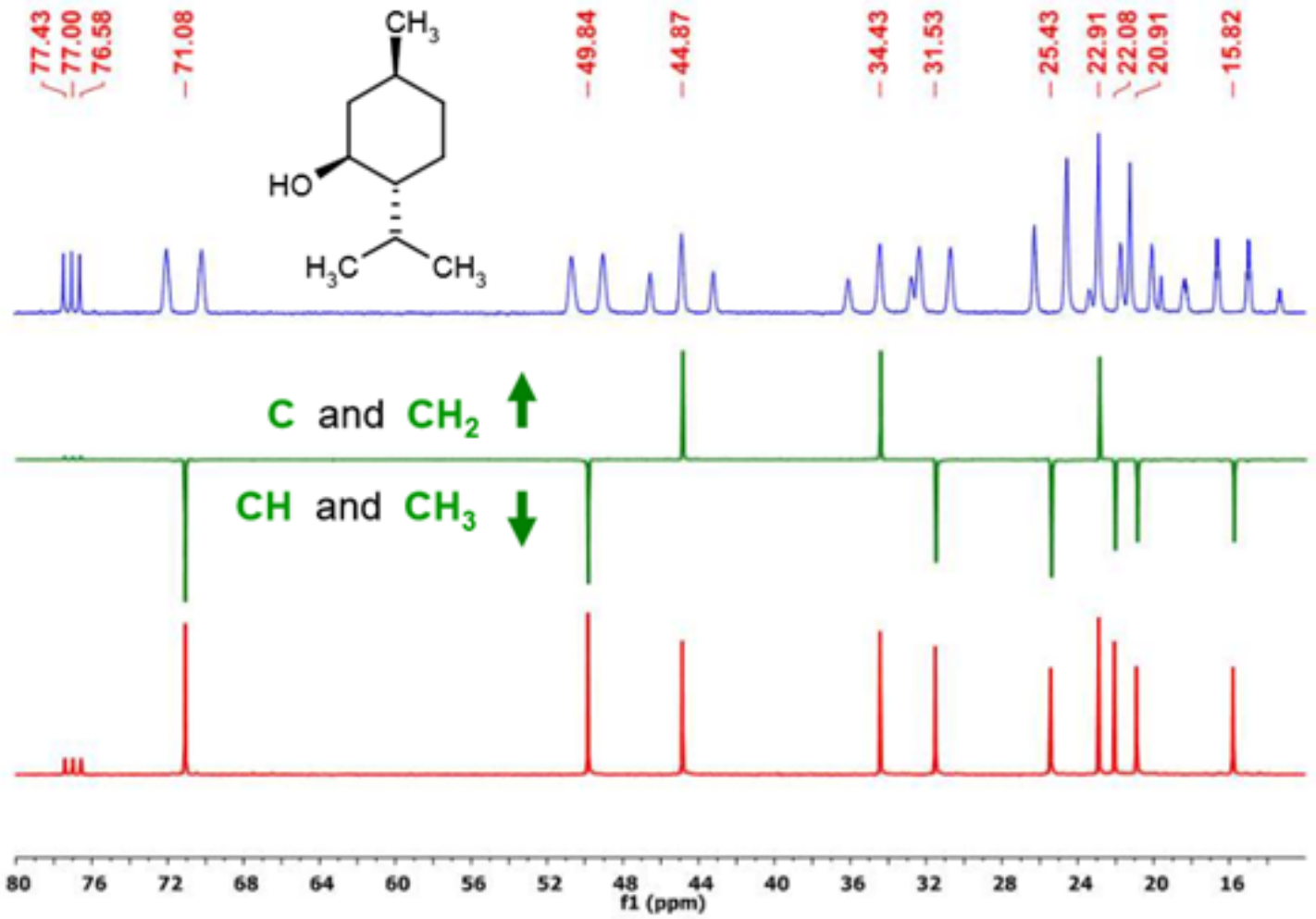
Obvykle tedy v ^{13}C neintegrujeme ... Ale!
Mají-li uhlíky blízké relaxační časy, pak je lze integrovat: např. fenyl skupina, směsi rotačních či konfiguračních izomerů, atp.

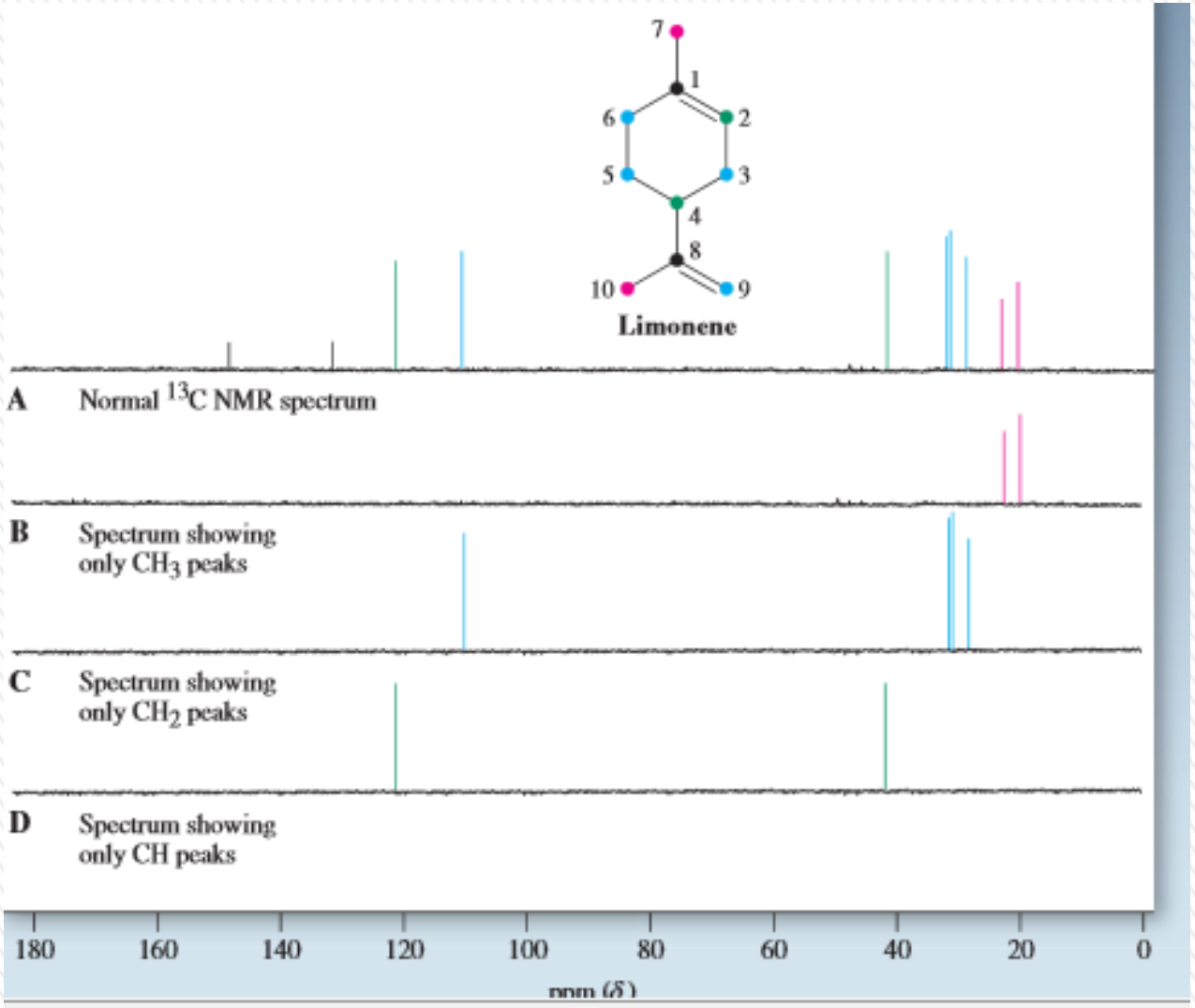
Počet vodíků, respektive množství spin-spin interakcí zrychluje relaxaci ^{13}C.

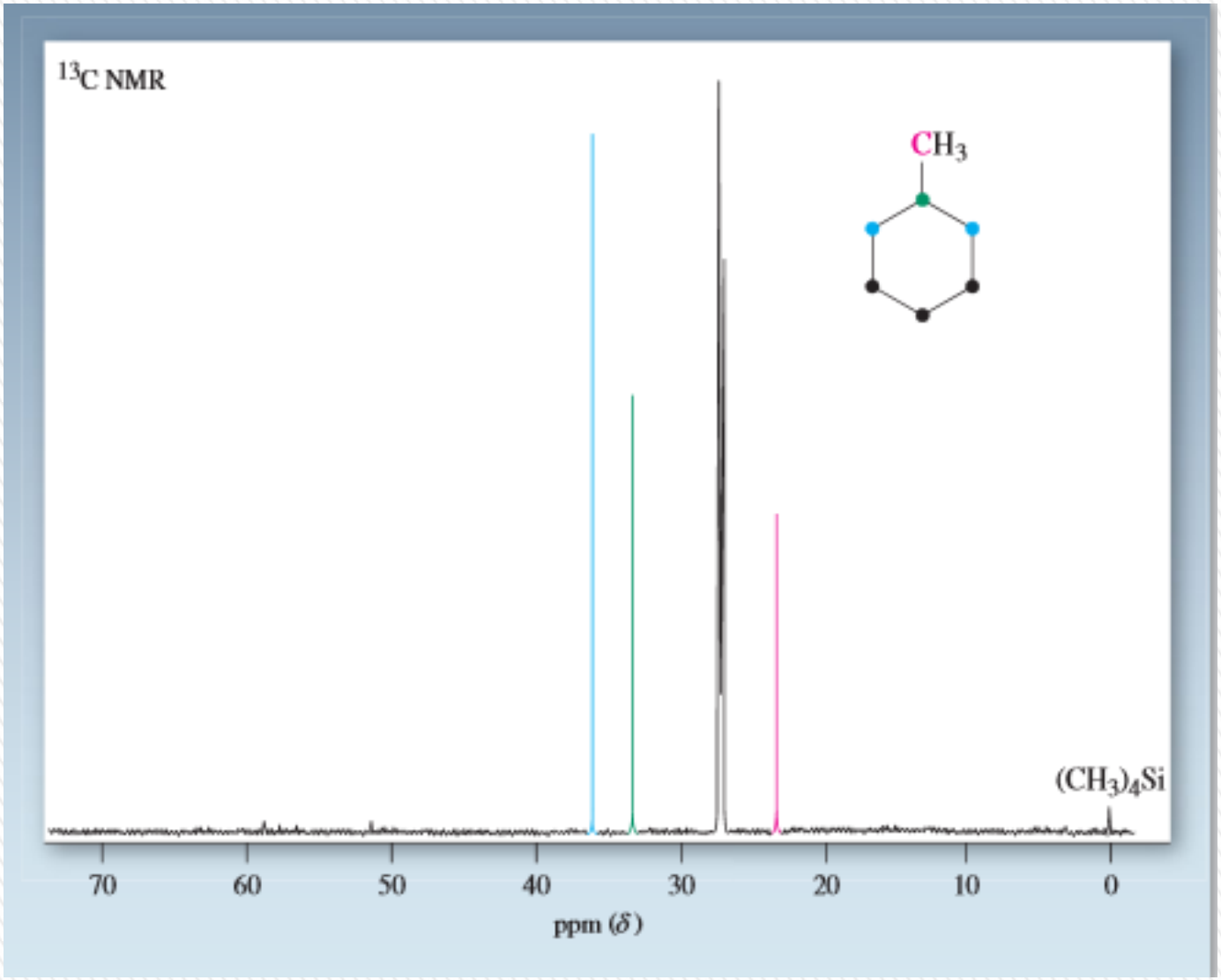
^{13}C NMR počet signálů

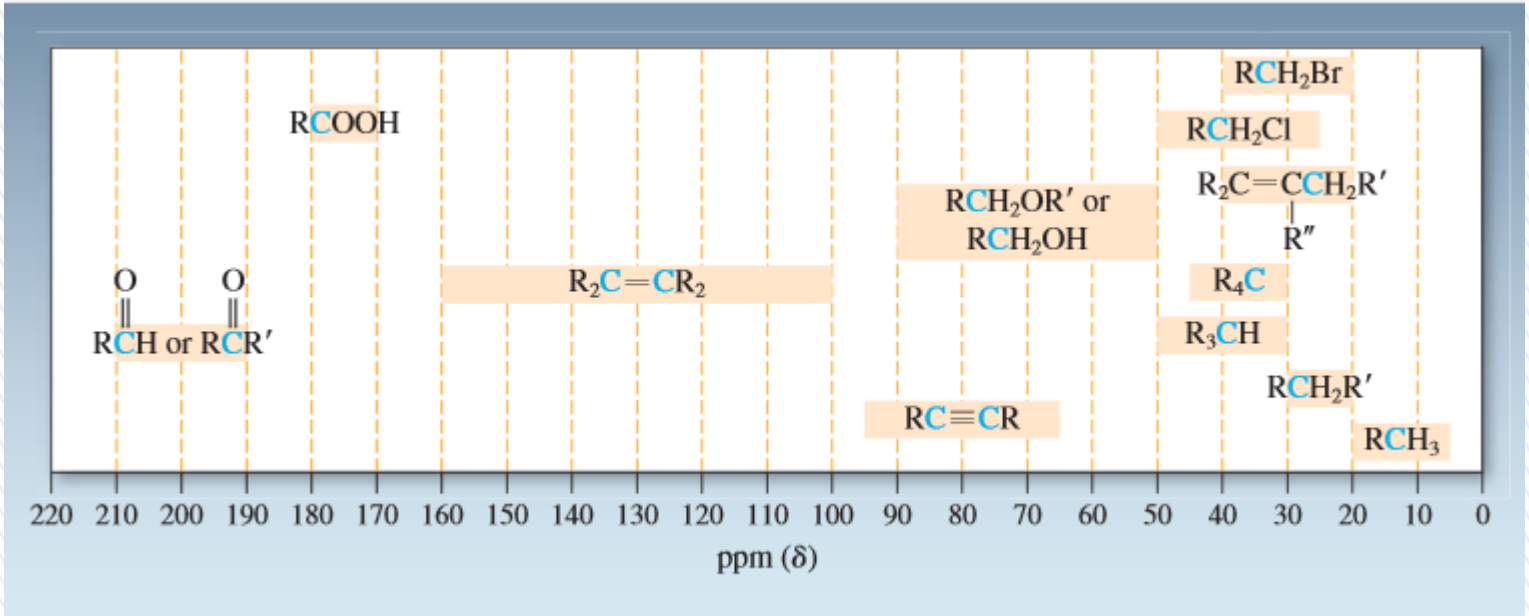


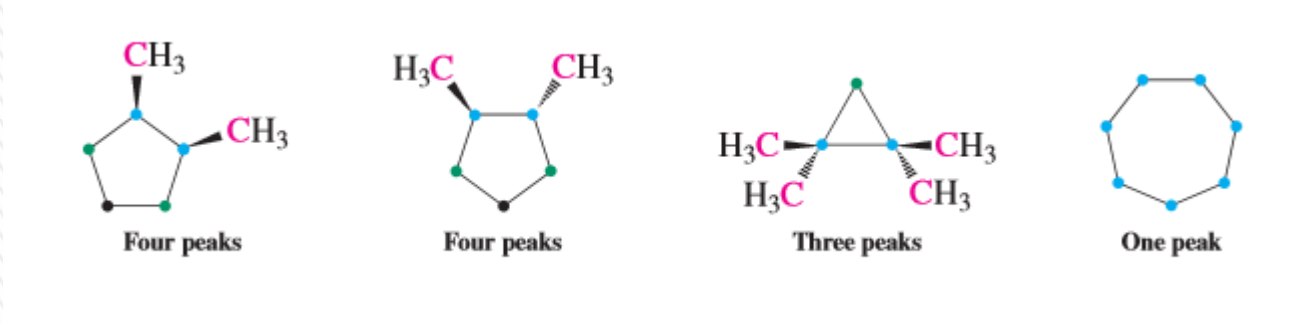
^{13}C NMR dekapling **OFF** or **ON**, and **APT**



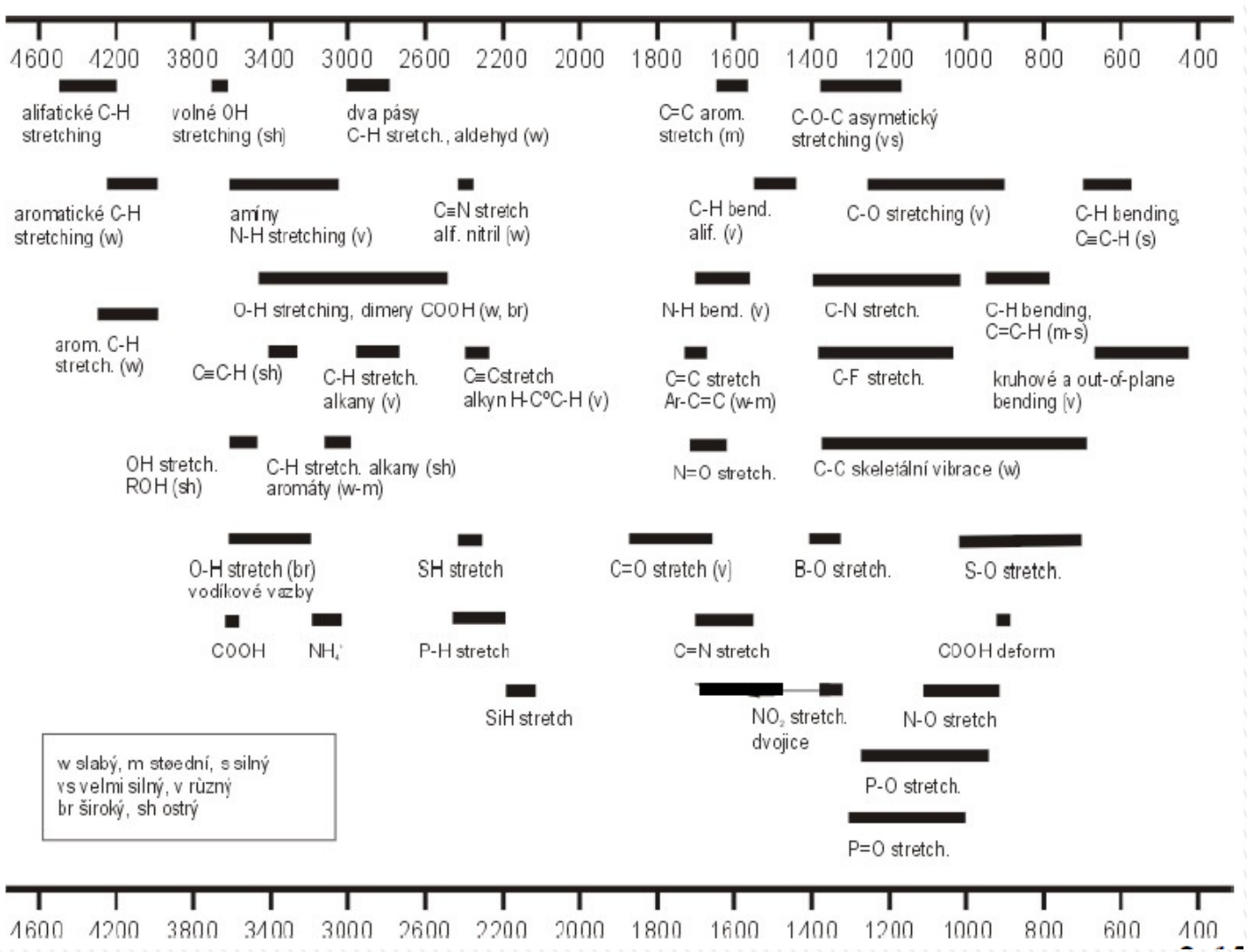

7
1
6
2
5
3
4
8
10
9
Limonene
A Normal ^{13}C NMR spectrum
B Spectrum showing only CH_3 peaks
C Spectrum showing only CH_2 peaks
D Spectrum showing only CH peaks
180
160
140
120
100
80
60
40
20
0
ppm (δ)

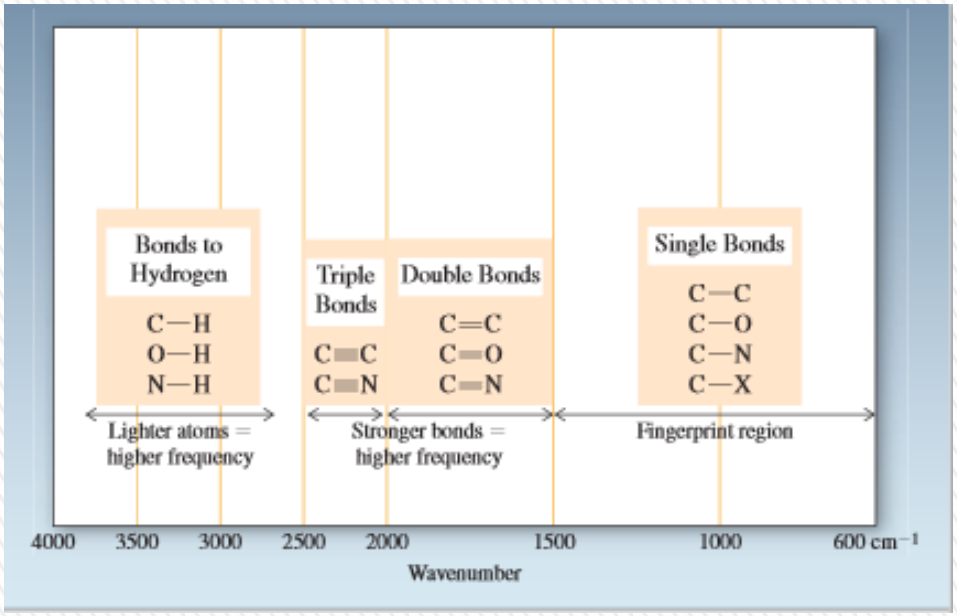

^{13}C NMR
CH3
(CH3)4Si
70
60
50
40
30
20
10
0
ppm (δ)

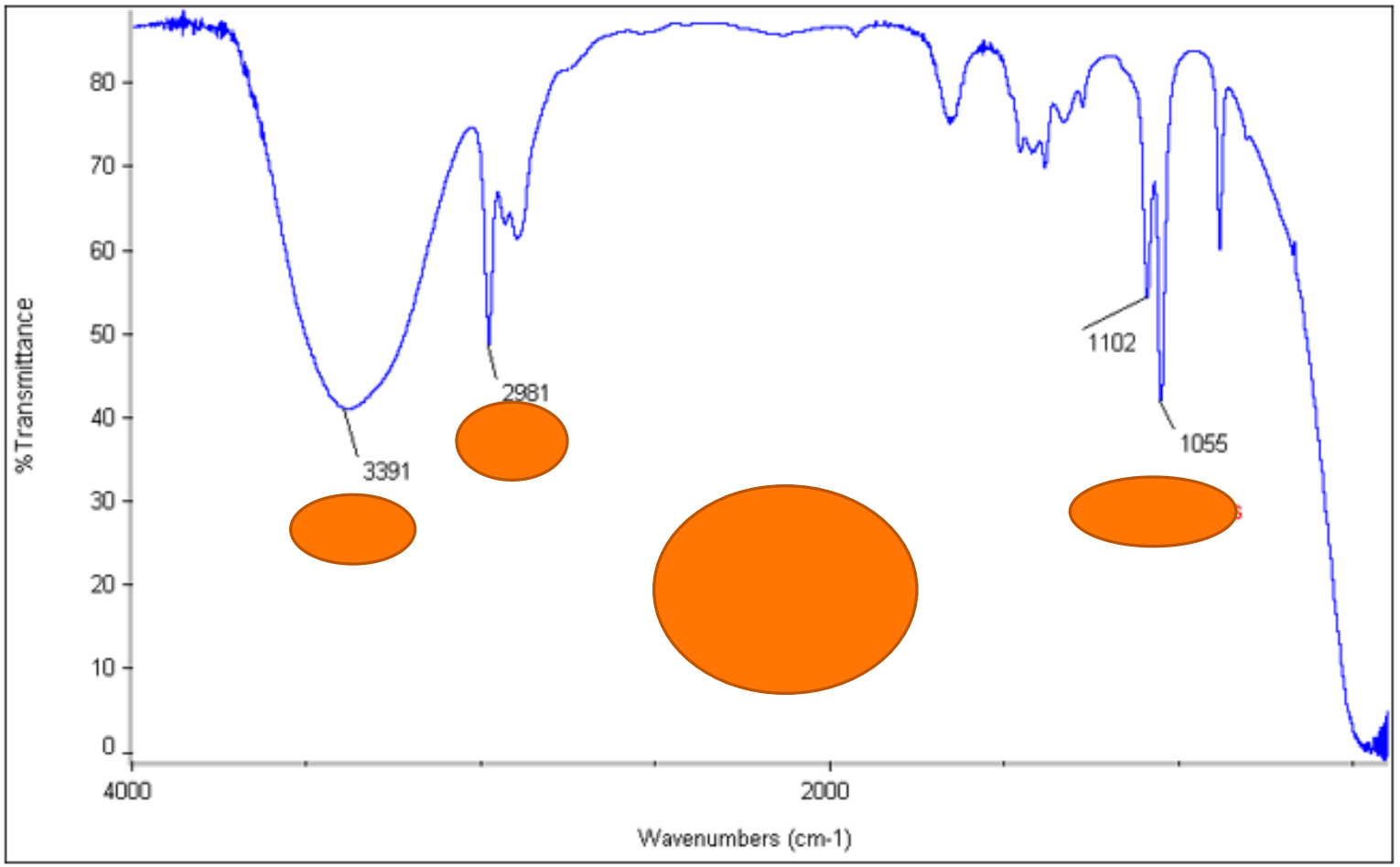

RCH2Br
RCH2Cl
R2C=CCH2R′
R″
RCH2OR′ or
RCH2OH
R4C
R3CH
RCH2R′
RCH3
RCOOH
O
O
RCH or RCR′
R2C=CR2
RC≡CR
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm (δ)

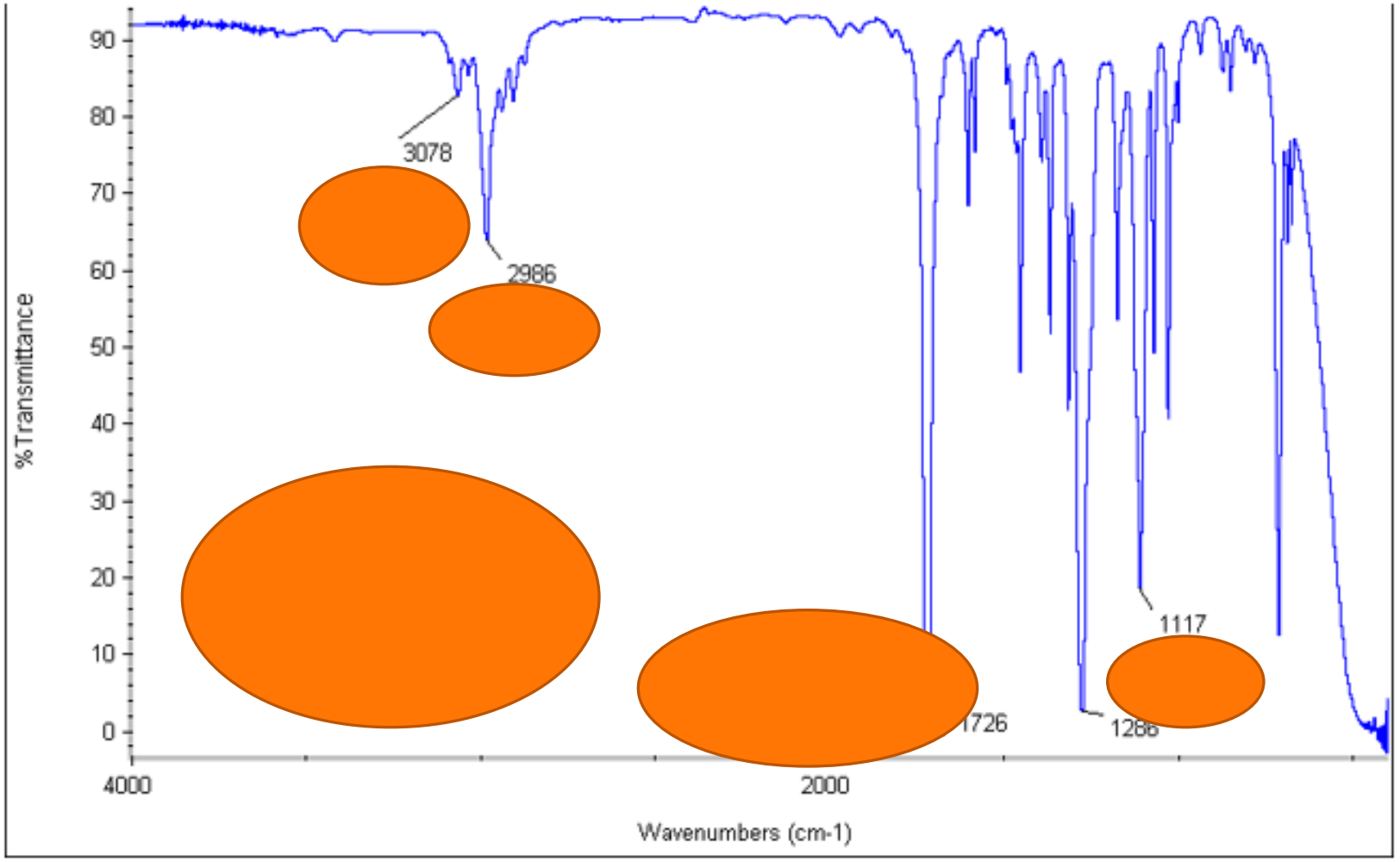

CH3
CH3
Four peaks
H3C
CH3
Four peaks
H3C
CH3
H3C
CH3
Three peaks
One peak

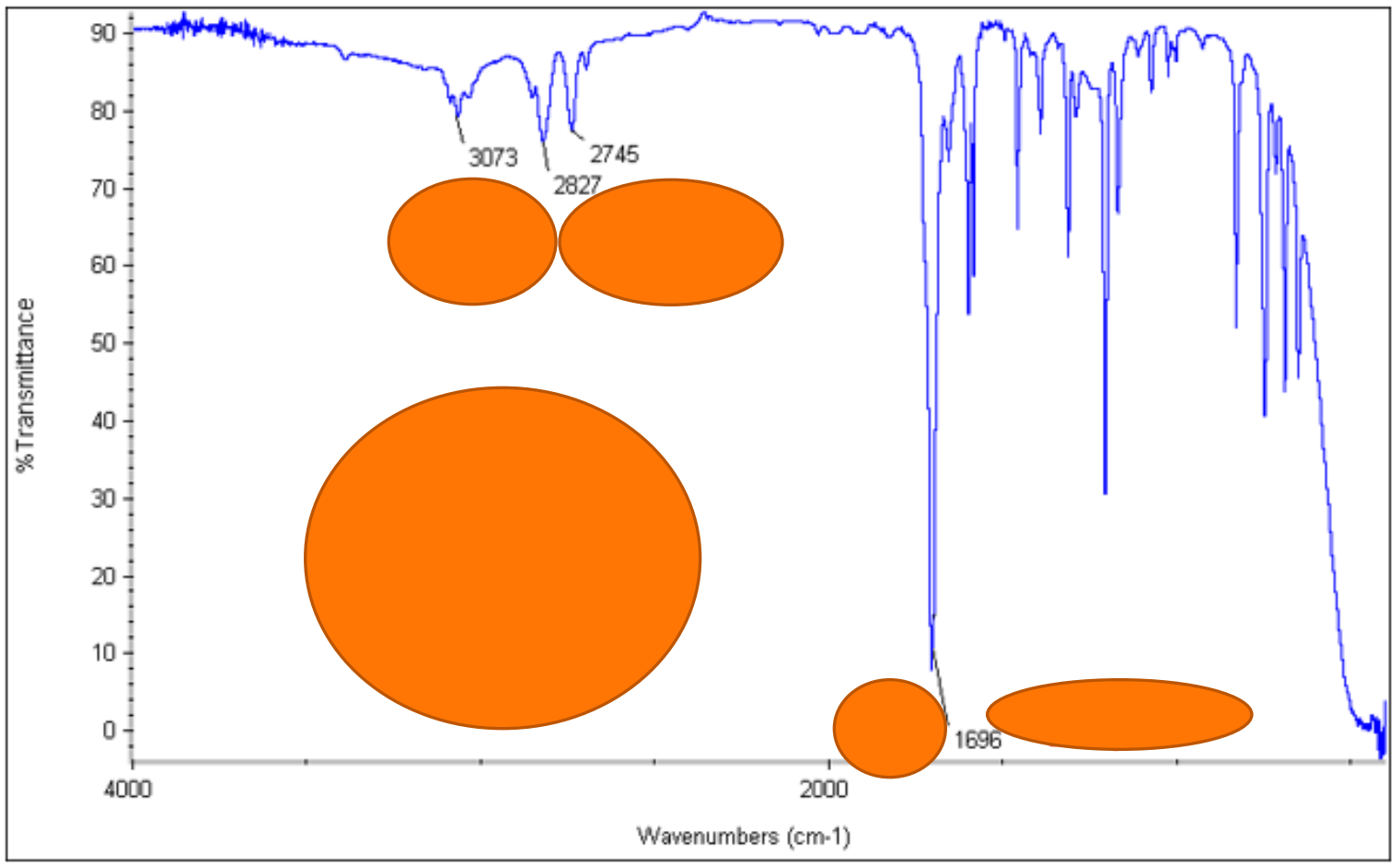
» Charakteristické vibrace cm^{-1}

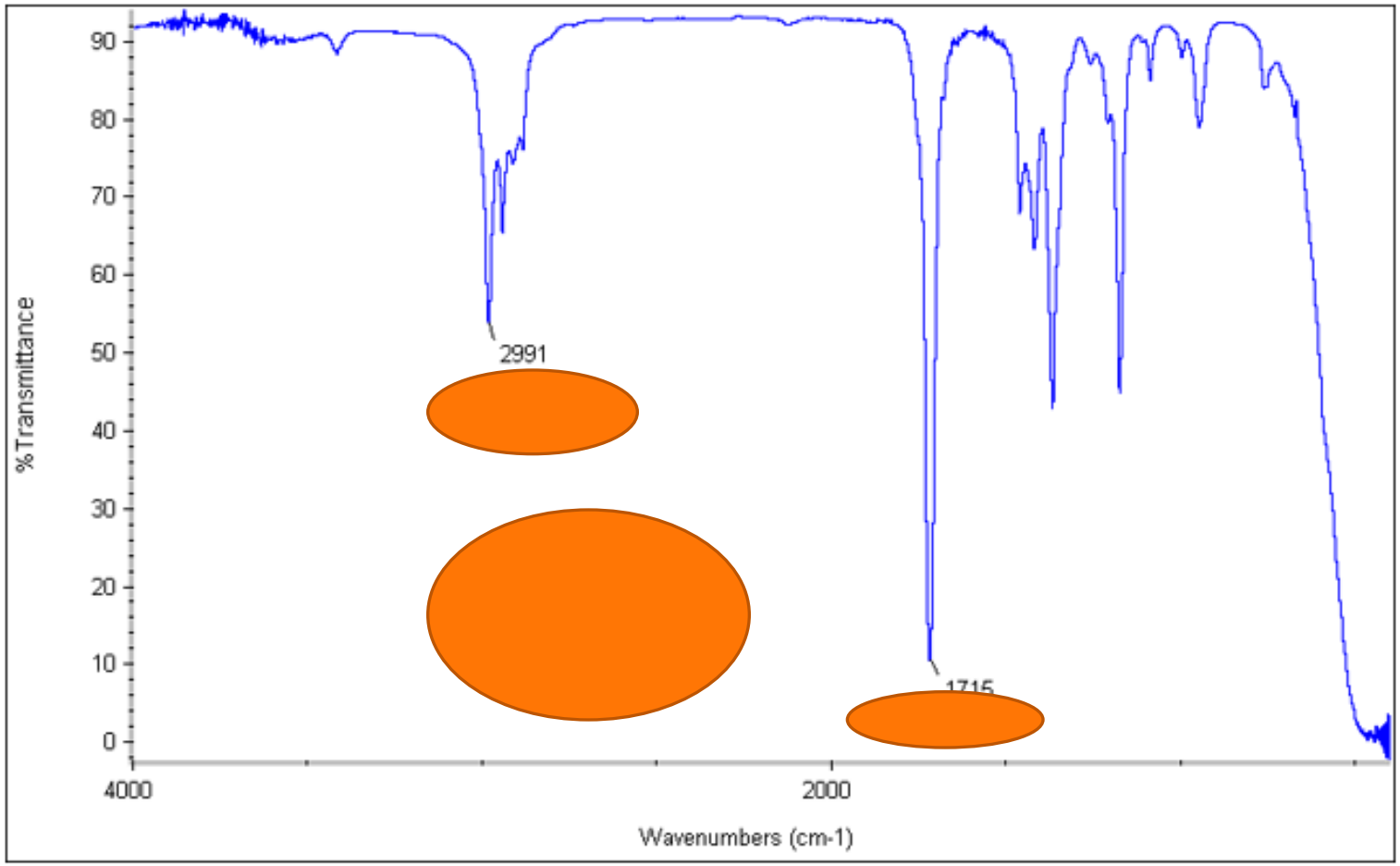


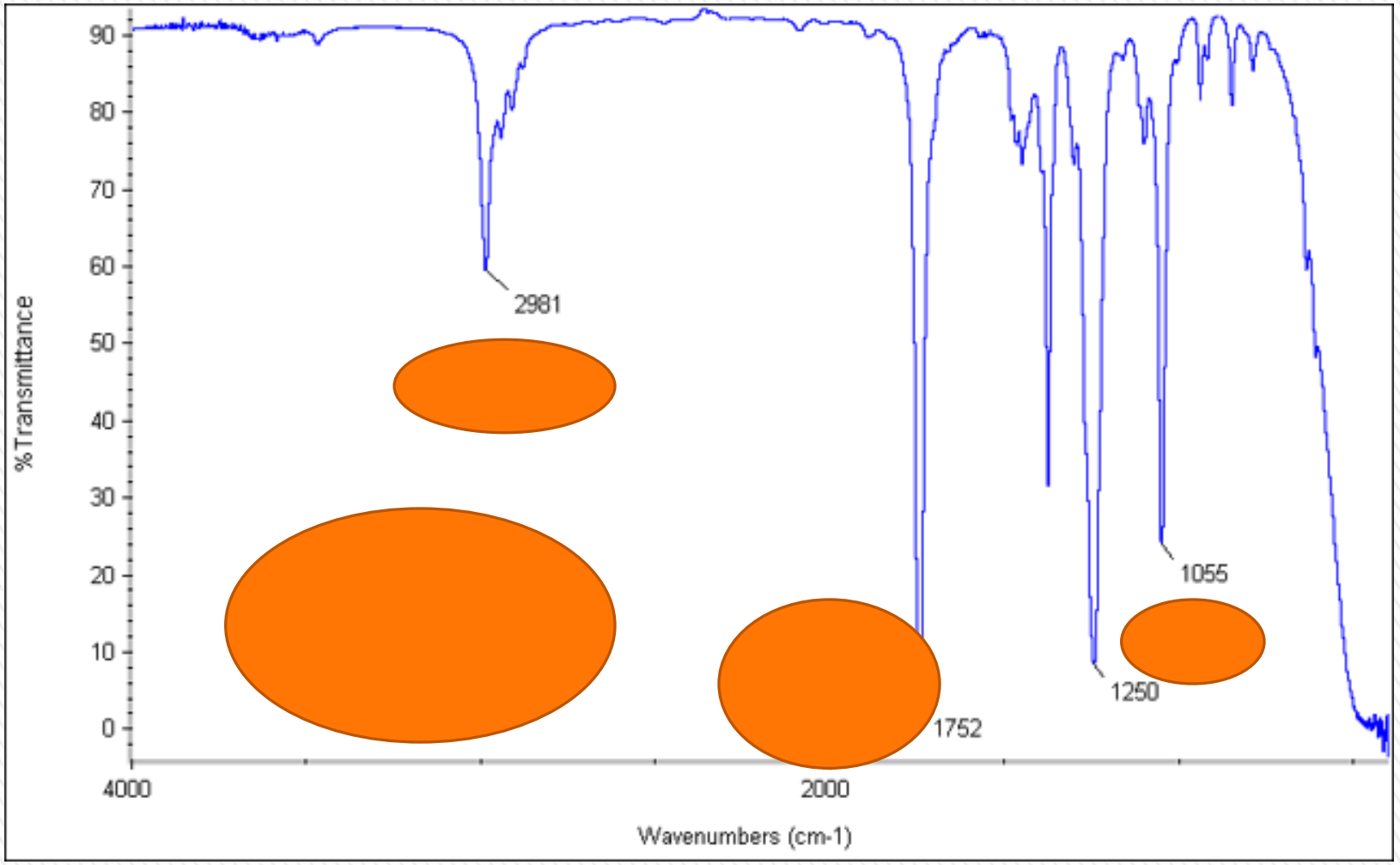

Bonds to Hydrogen
C—H
O—H
N—H
Triple Bonds
C≡C
C≡N
Double Bonds
C=C
C=O
C=N
Single Bonds
C—C
C—O
C—N
C—X
Lighter atoms = higher frequency
Stronger bonds = higher frequency
Fingerprint region
4000
3500
3000
2500
2000
1500
1000
600 cm⁻¹
Wavenumber


% Transmittance
80
70
60
50
40
30
20
10
0
4000
2000
Wavenumbers (cm-1)
3391
2981
1102
1055


%Transmittance
90
80
70
60
50
40
30
20
10
0
3078
2986
1726
1286
1117
4000
2000
Wavenumbers (cm-1)


%Transmittance
90
80
70
60
50
40
30
20
10
0
3073
2827
2745
1696
4000
2000
Wavenumbers (cm-1)


90
80
70
60
50
40
30
20
10
0
% Transmittance
2991
1715
4000
2000
Wavenumbers (cm-1)


90
80
70
60
50
40
30
20
10
0
%Transmittance
2981
1055
1250
1752
4000
2000
Wavenumbers (cm-1)