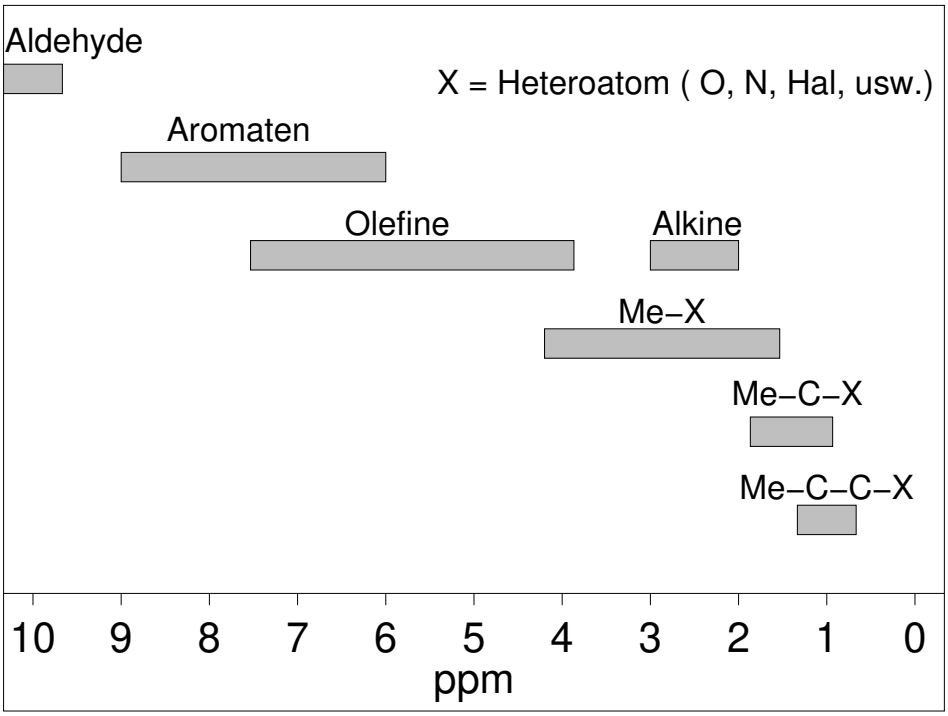
Übungen zur Spektroskopie 2

C. Ober und Dr. D. S. Stephenson
Department Chemie, Universität München

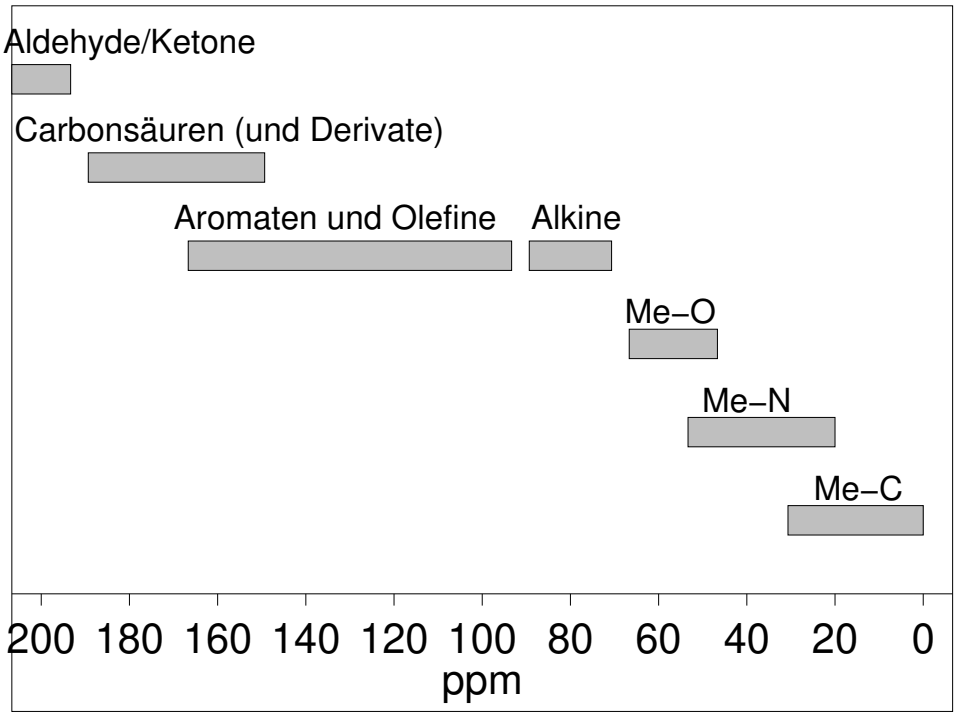
Sie finden diese Übungen und alte Klausuren (mit Lösung) auf unserer Homepage:

https://www.cup.uni-muenchen.de/oc/nmr/uebungen/
https://www.cup.uni-muenchen.de/oc/nmr/alte-klausuren/

- Die ^{1}H chemischen Verschiebungen liegen meistens zwischen 0 ppm und 10 ppm.



- Die ^{13}C chemischen Verschiebungen liegen meistens zwischen 0 ppm und 200 ppm.

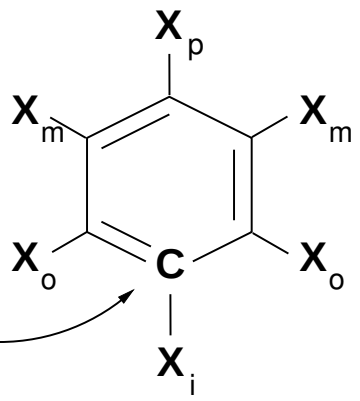


8. ^{13}C - „Inkremente“

- Benzole

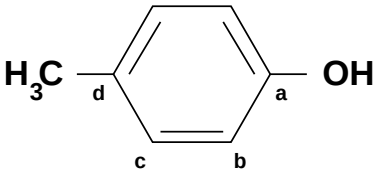
$$\delta_C = 128.5 + \sum_k S_k \, n_k$$

(k = i, o, m, p)



X	S_{ipso}	S_{ortho}	S_{meta}	S_{para}
CH_3	9.2	0.7	-0.1	-3.1
CH_2CH_3	15.6	-0.5	0.0	-2.7
$CH(CH_3)_2$	20.1	-2.0	0.0	-2.5
$C(CH_3)_3$	22.1	-3.4	-0.4	-3.1
CH_2Cl	9.3	0.3	0.2	0
CH_2Br	9.5	0.7	0.3	0.2
CH_2OH	12.4	-1.2	0.2	-1.1
$CH{=}CH_2$	8.9	-2.3	-0.1	-0.8
C_6H_5	13.1	-1.1	0.4	-1.1
$C{\equiv}CH$	-6.2	3.6	-0.4	-0.3
CHO	8.4	1.2	0.5	5.7
$COCH_3$	8.9	0.1	-0.1	4.4
COOH	2.1	1.6	-0.1	5.2
$COOCH_2CH_3$	2.1	1.0	-0.5	3.9
$CONR_2$	5.0	-1.2	0.1	3.4
OH	26.9	-12.8	1.4	-7.4
OCH_3	31.4	-14.4	1.0	-7.7
$OCOCH_3$	22.4	-7.1	0.4	-3.2
CN	-15.7	3.6	0.7	4.3
NH_2	18.2	-13.4	0.8	-10.0
NO_2	19.9	-4.9	0.9	6.1
F	34.8	-13.0	1.6	-4.4
Cl	6.3	0.4	1.4	-1.9
Br	-5.8	3.2	1.6	-1.6
I	-34.1	8.9	1.6	-1.1

– Beispiel: p-Kresol



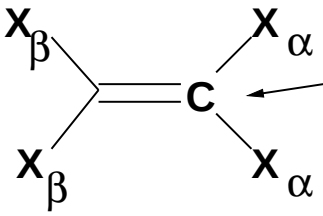
δ_a = 128.5 + 26.9 – 3.1 = 152.3 (gem.: 152.6)

δ_b = 128.5 – 12.8 – 0.1 = 115.6 (gem.: 115.3)

δ_c = 128.5 + 1.4 + 0.7 = 130.6 (gem.: 130.2)

δ_d = 128.5 – 7.4 + 9.2 = 130.3 (gem.: 130.5)

- Olefine

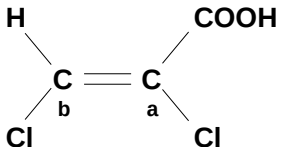


$$\delta = 123.5 + \sum_k S_k n_k$$

$$(k = \alpha, \beta)$$

X	S_α	S_β
CH_3	10.6	-7.9
CH_2CH_3	15.5	-9.7
$CH_2CH_2CH_3$	14.0	-8.2
$CH(CH_3)_2$	20.4	-11.5
$C(CH_3)_3$	25.3	-13.3
CH_2Cl	10.2	-6.0
CH_2Br	10.9	-4.5
CH_2I	14.2	-4.0
CH_2OH	14.2	-8.4
$CH{=}CH_2$	13.6	-7.0
$C{\equiv}CH$	-7.5	8.9
C_6H_5	12.5	-11.0
CHO	13.1	12.7
$COCH_3$	15.0	5.8
COOH	4.2	8.9
$COOCH_2CH_3$	6.3	7.0
OCH_3	29.4	-38.9
OCH_2CH_3	28.5	-39.8
$OCOCH_3$	18.4	-26.7
CN	-15.1	14.2
NO_2	22.3	-0.9
F	24.9	-34.3
Cl	2.6	-6.1
Br	-7.9	-1.4
I	-38.1	7.0

– Beispiel: Dichloracrylsäure



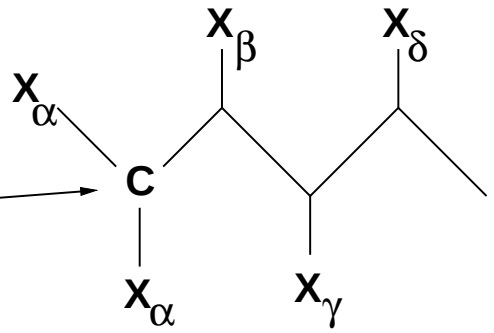
$\delta_a =$ 123.5 + 4.2 + 2.6 –6.1 = 124.2 (gem.: 129.3)

$\delta_b =$ 123.5 + 8.9 –6.1 + 2.6 = 128.9 (gem.: 132.6)

- Aliphaten

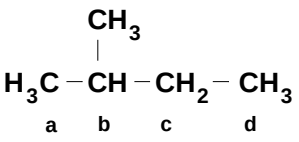
$$\delta = -2.3 + \sum_k S_k n_k$$

$$(k = \alpha, \beta, \gamma, \delta)$$



X	S_α	S_β	S_γ	S_δ
CH_3	9.1	9.4	-2.5	0.3
$CH{=}CH_2$	22.3	6.9	-2.2	0.2
CH=CH(cis)	14.2	7.3	-1.5	0
CH=CH($trans$)	19.7	7.2	-1.6	0
C≡CH	4.5	5.5	-3.5	0
C_6H_5	22.3	8.6	-2.3	0.2
CHO	31.9	0.7	-2.3	0
$COCH_3$	30.9	2.3	-0.9	2.7
COOH	20.8	2.7	-2.3	1.0
$COOCH_3$	20.4	2.3	-1.9	1.2
$CONR_2$	22.0	2.6	-3.2	-0.4
CN	3.6	2.0	-3.1	-0.5
NH_2	28.6	11.5	-4.9	0.3
NO_2	64.5	3.1	-4.7	-1.0
OH($prim$)	48.3	10.2	-5.8	0.3
OH(sek)	44.5	9.7	-3.3	0.2
OH($tert$)	39.7	7.3	-1.8	0.3
OR	58.0	8.1	-4.7	1.4
$OCOCH_3$	51.1	7.1	-4.8	1.1
SH	11.1	11.8	-2.9	0.7
SCH_3	21.1	6.4	-3.0	0.5
F	70.1	7.8	-6.8	0
Cl	31.2	10.5	-4.6	0.1
Br	20.0	10.6	-3.1	0.1
I	-6.0	11.3	-1.0	0.2

– Beispiel: Isopentan



$\delta_a = -2.3 + 1 * 9.1 + 2 * 9.4 - 1 * 2.5 = 23.1$ (gem.: 21.9)

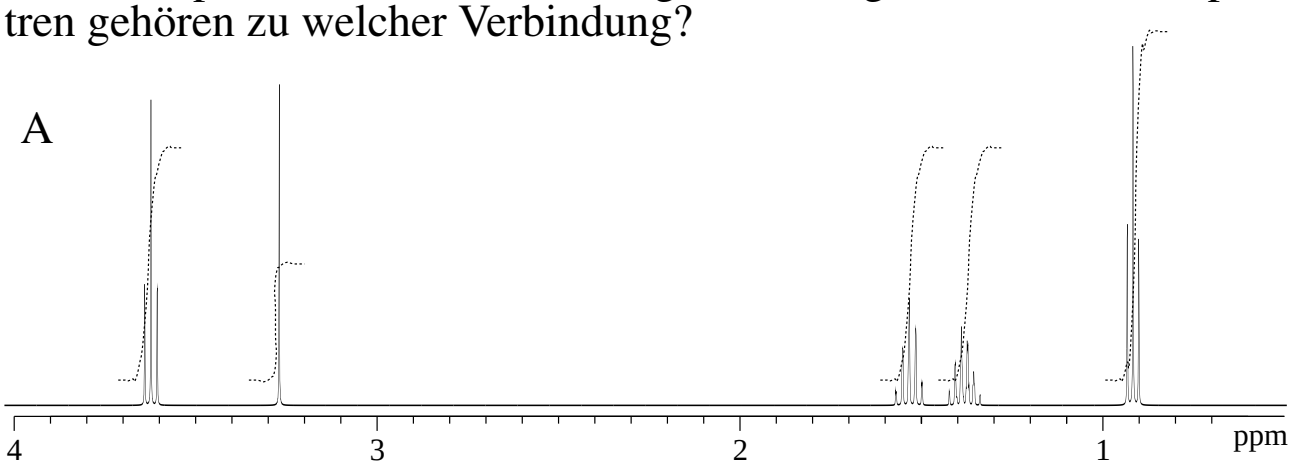
$\delta_b = -2.3 + 3 * 9.1 + 1 * 9.4 - 0 * 2.5 = 34.4$ (gem.: 29.7)

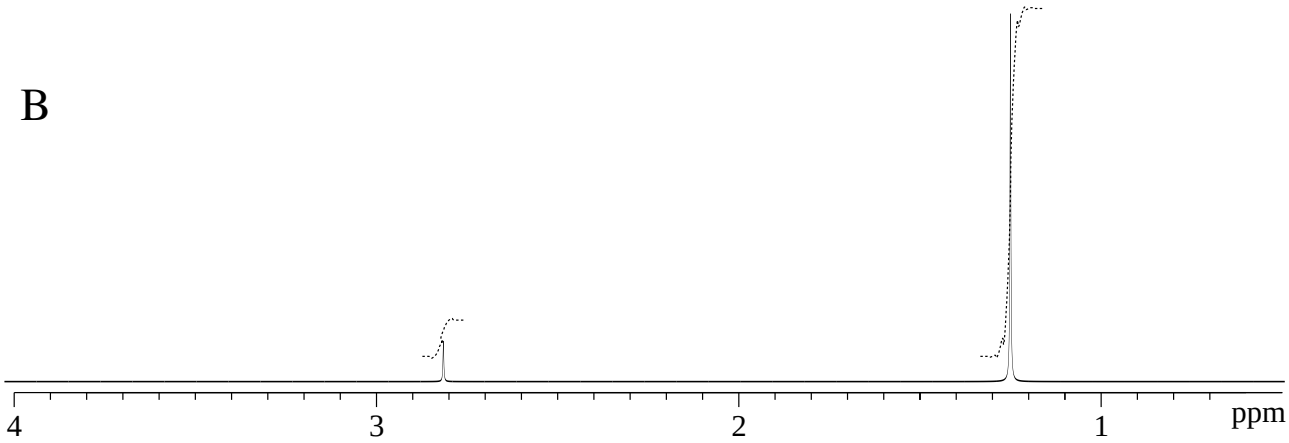
$\delta_c = -2.3 + 2 * 9.1 + 2 * 9.4 - 0 * 2.5 = 34.7$ (gem.: 31.7)

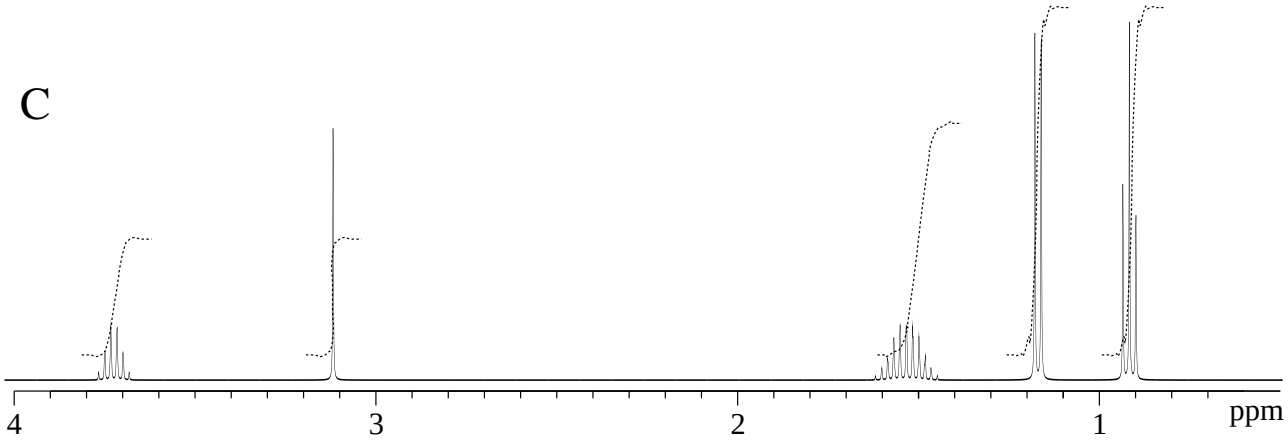
$\delta_d = -2.3 + 1 * 9.1 + 1 * 9.4 - 2 * 2.5 = 11.2$ (gem.: 11.4)

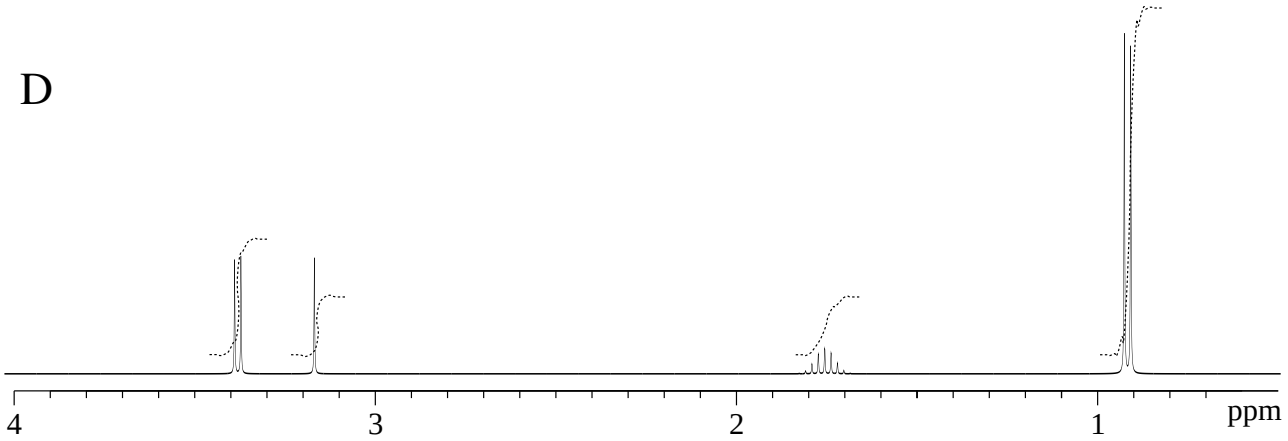
Übung 1

Es gibt 4 isomere Butanole mit der Summenformel $C_4H_{10}O$. Die ^1H- und ^{13}C-Spektren dieser Verbindungen sind abgebildet. Welche Spektren gehören zu welcher Verbindung?

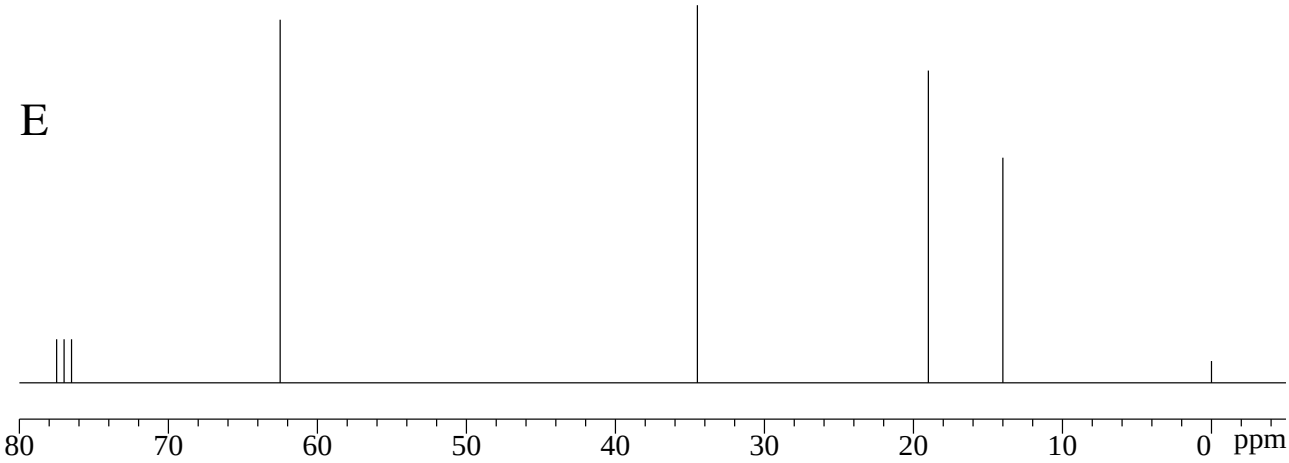




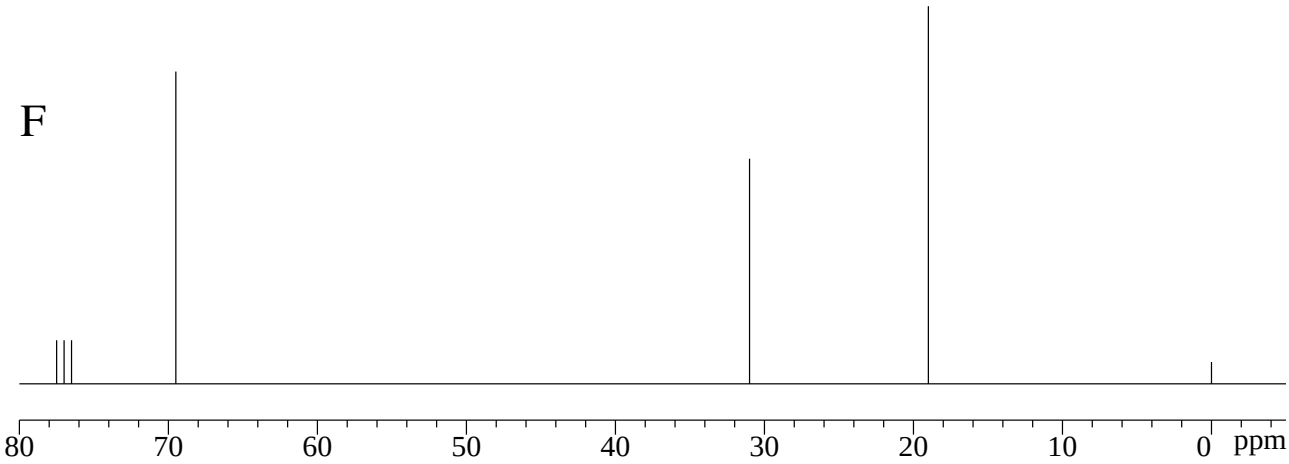




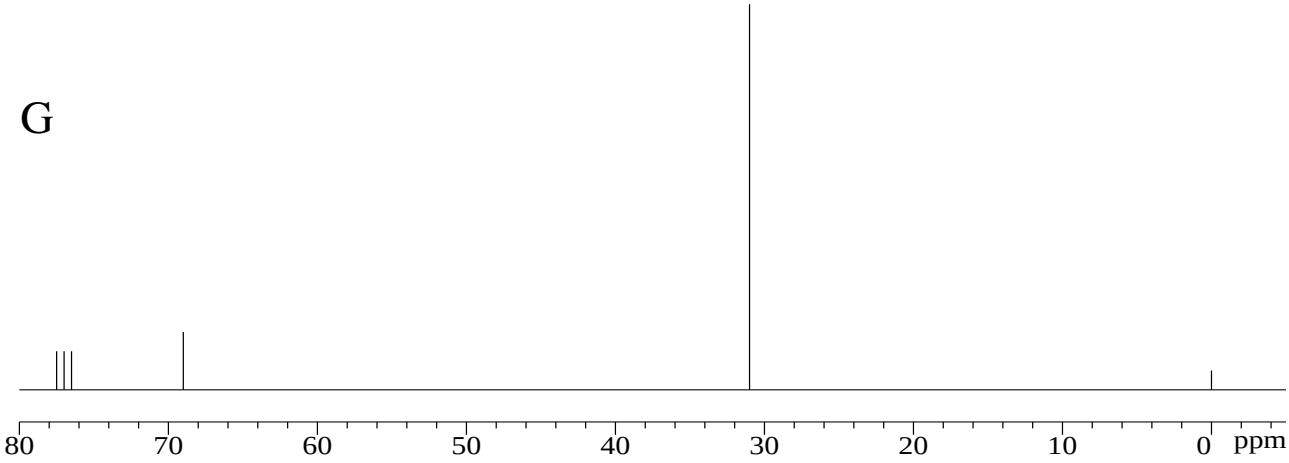
E


80
70
60
50
40
30
20
10
0
ppm

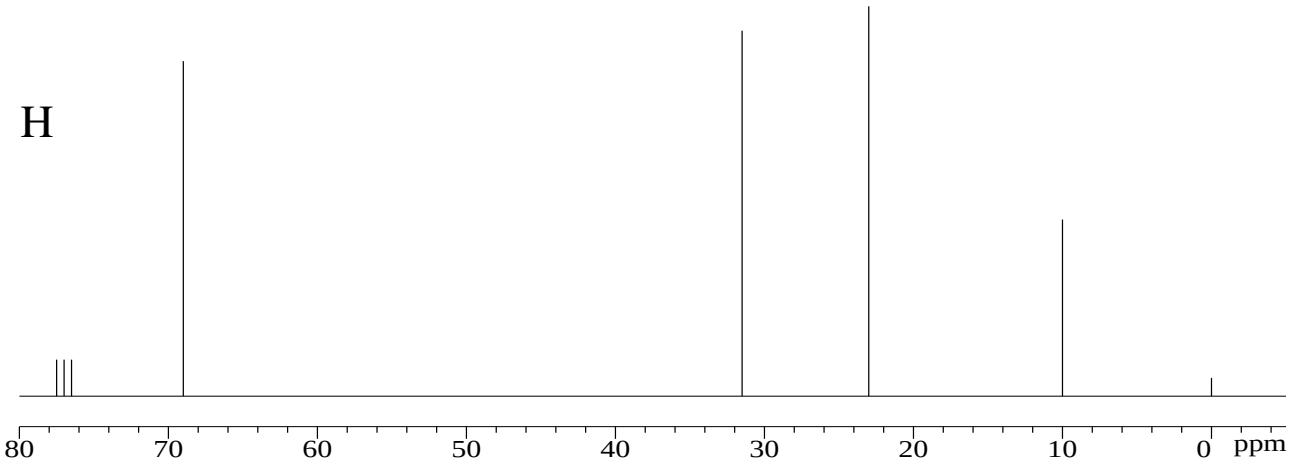
F


80
70
60
50
40
30
20
10
0
ppm

G

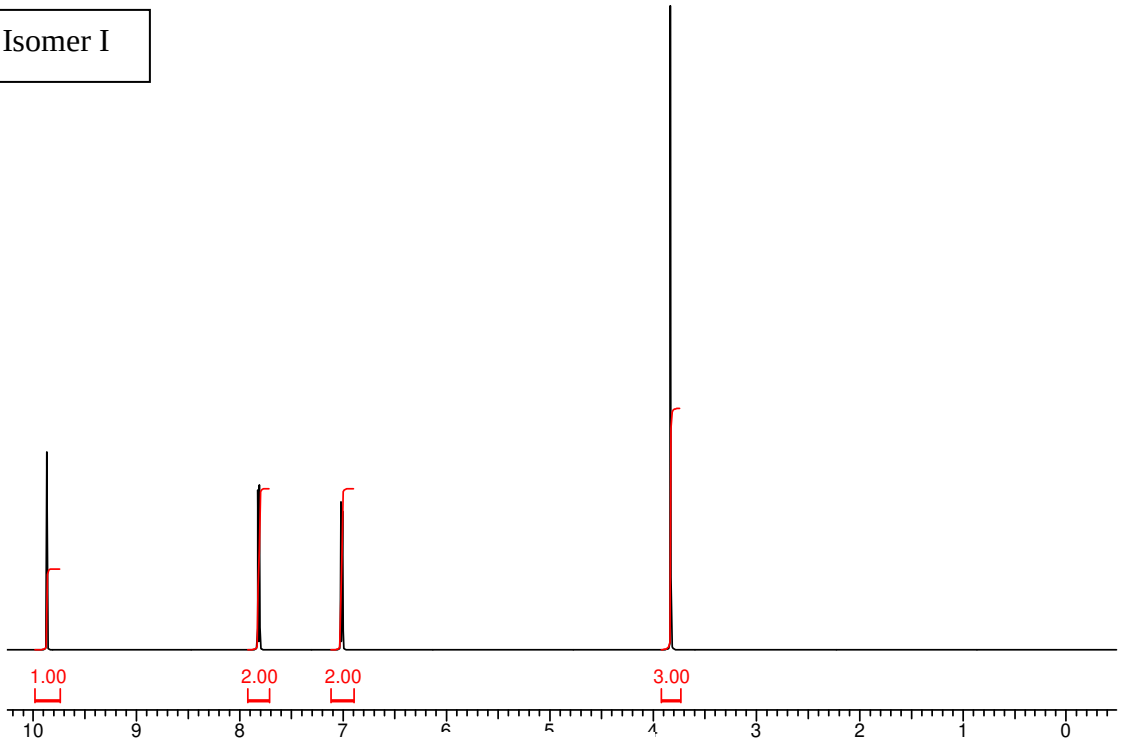

80
70
60
50
40
30
20
10
0
ppm

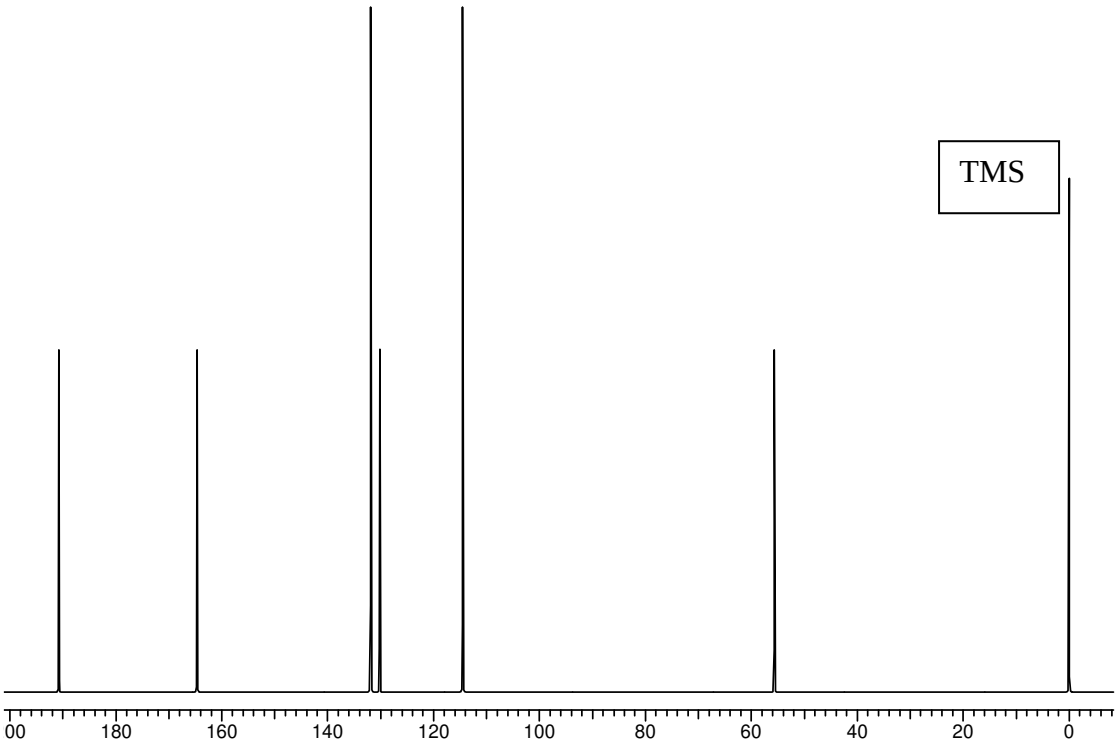
H

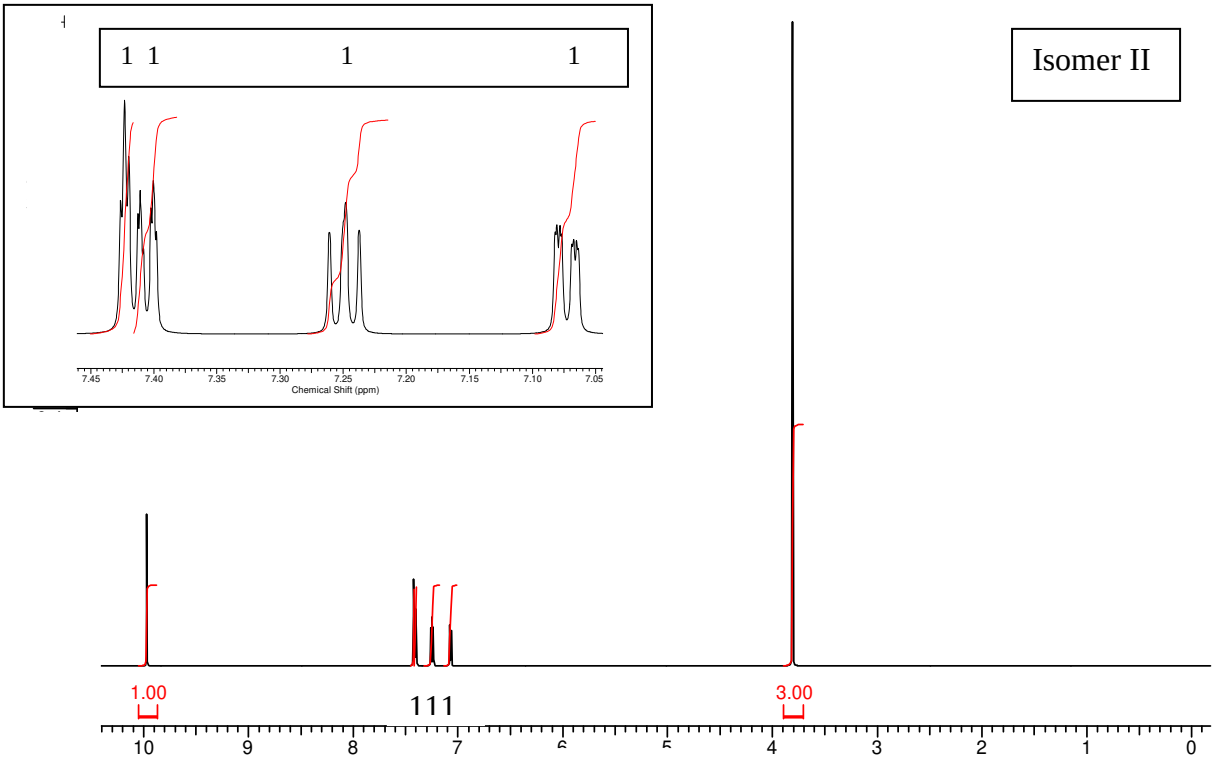

80
70
60
50
40
30
20
10
0
ppm

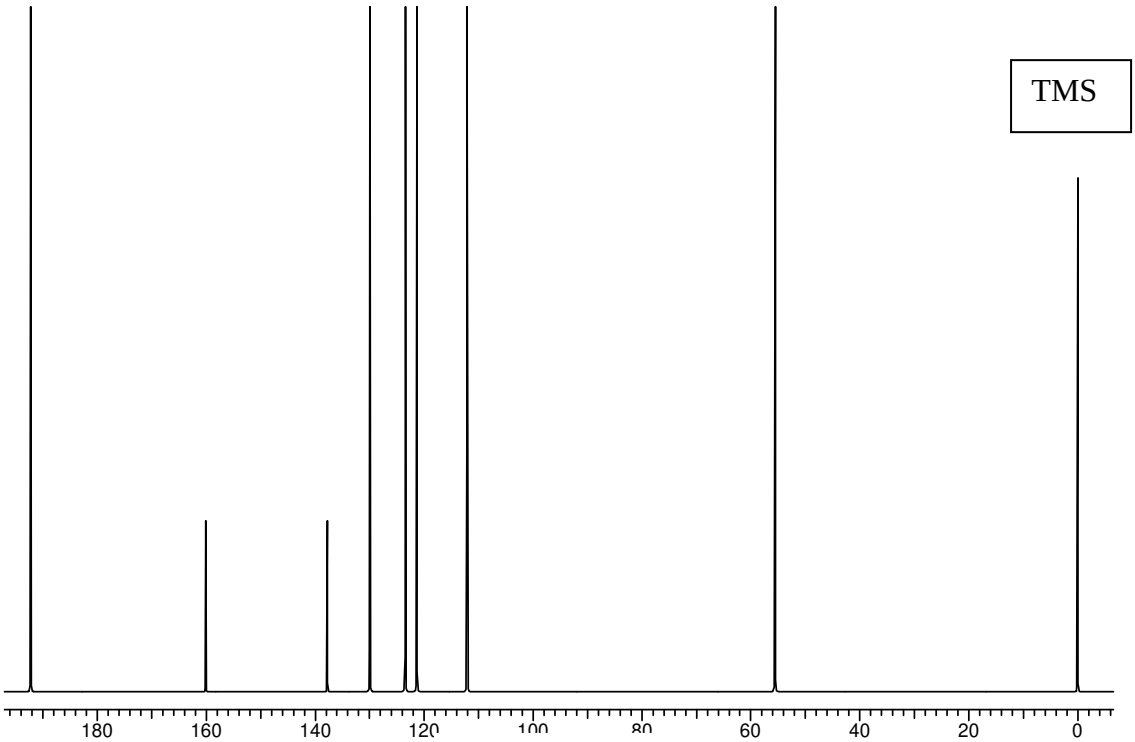
U2 Hier sind die Spektren von 2 Isomeren mit der Summenformel $C_8H_8O_2$.
Bestimmen Sie die Strukturen.

Isomer I



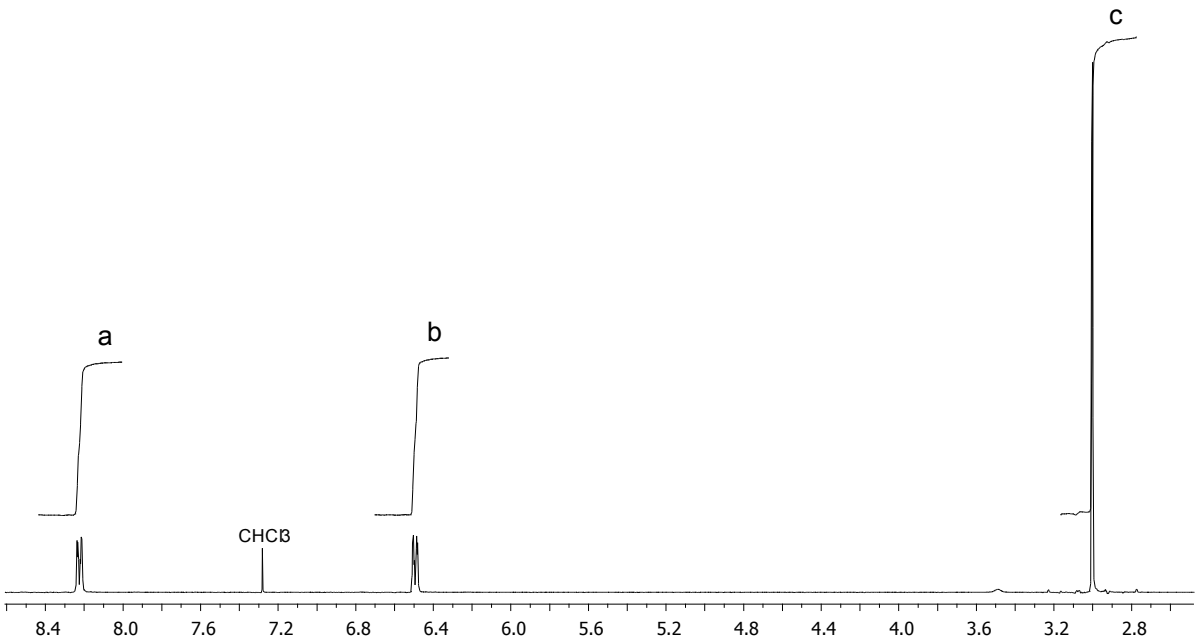


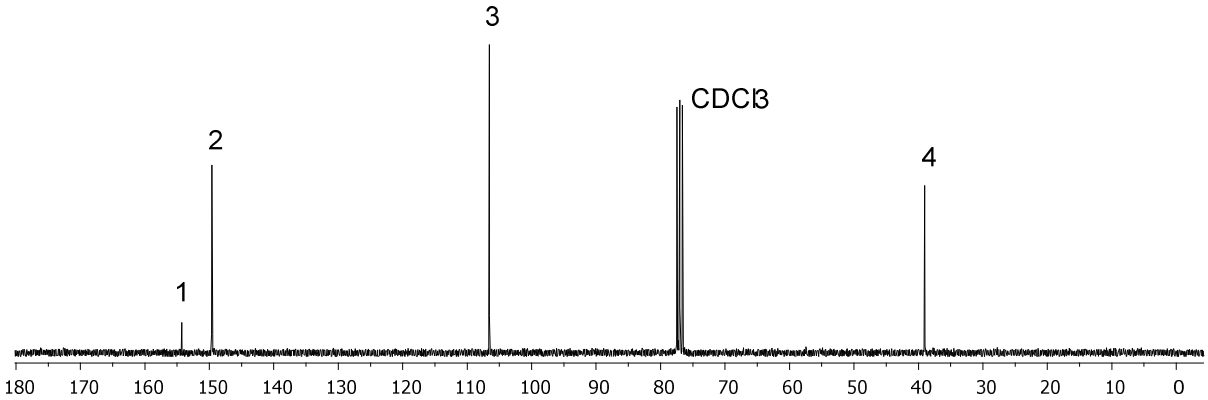

1 1
1
1
7.45
7.40
7.35
7.30
7.25
7.20
7.15
7.10
7.05
Chemical Shift (ppm)
Isomer II
1.00
111
3.00
10
9
8
7
4
3
2
1
0


TMS
180
160
140
120
60
40
20
0

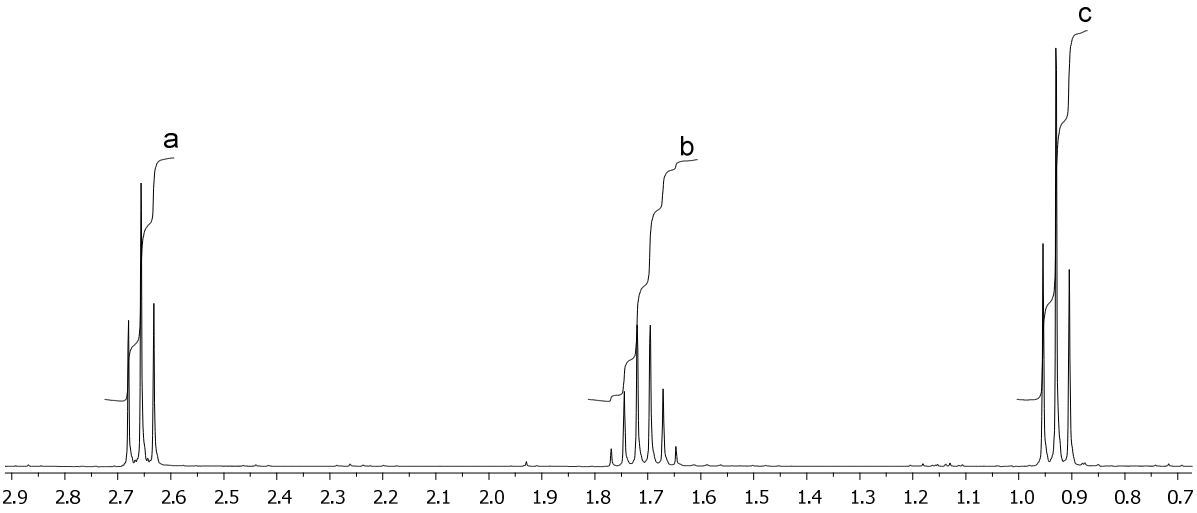
U3 $C_7H_{10}N_2$

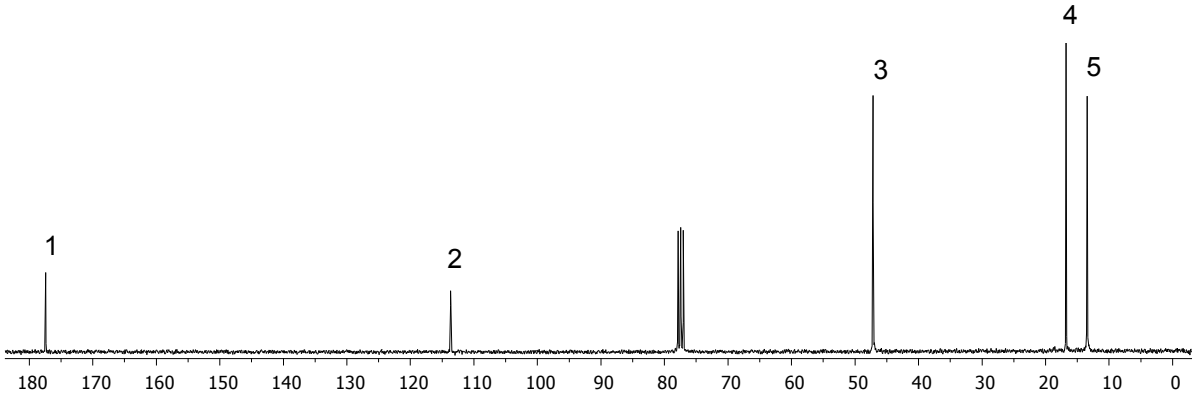
1. Bestimmen Sie die Struktur
2. Ordnen Sie die Signale zu.





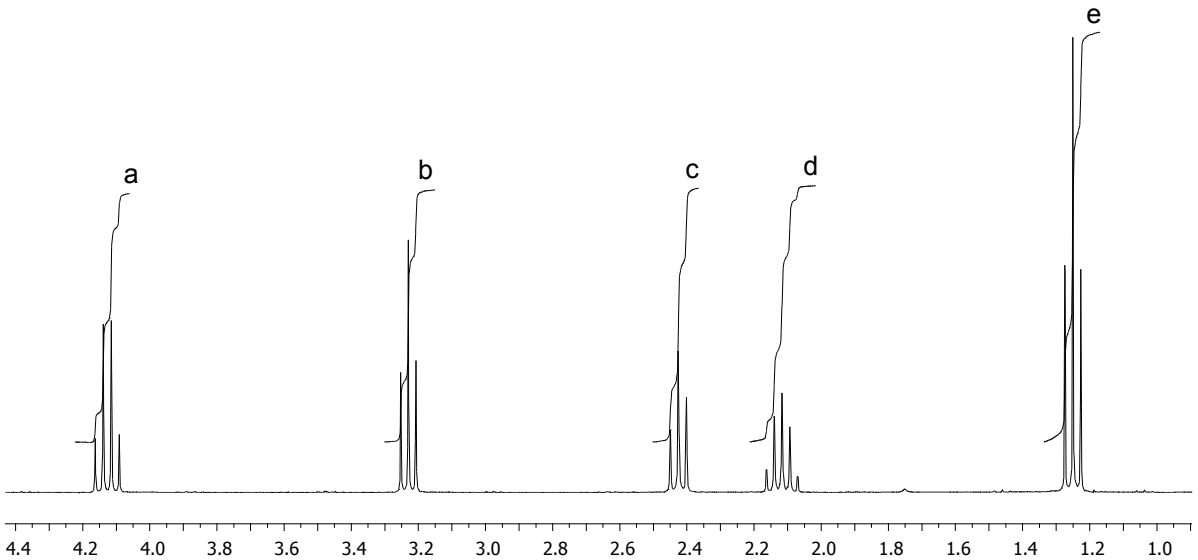
U 4 C_5H_7ON (N – 3bindig)

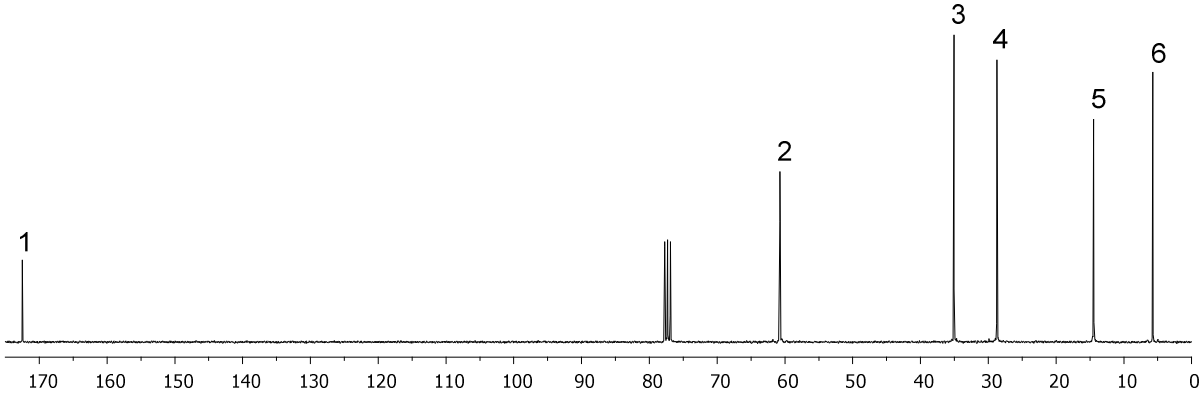


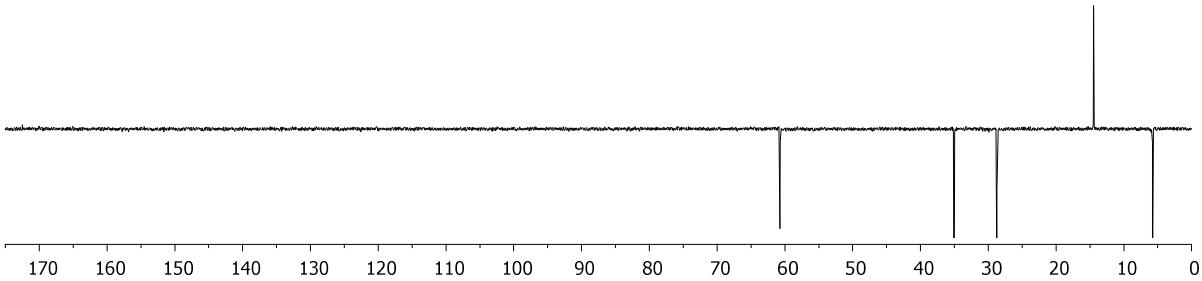


U 5 $C_6H_{11}IO_2$

1. Struktur ?



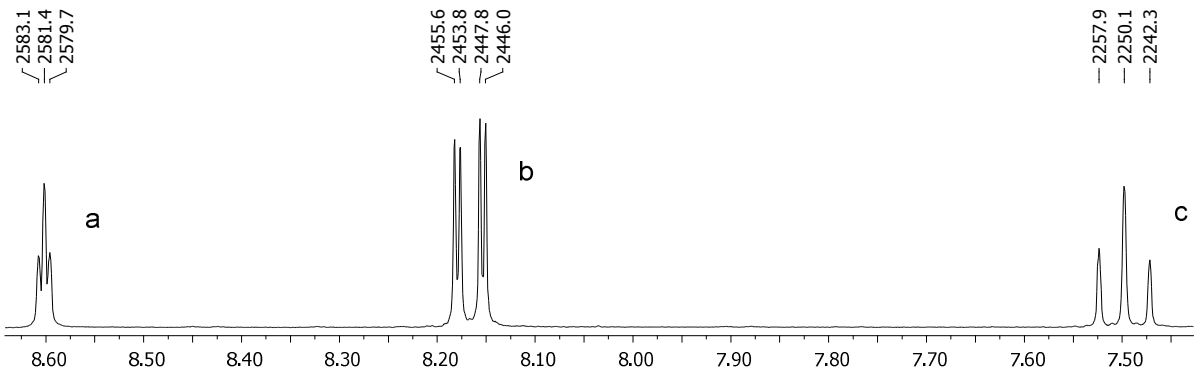


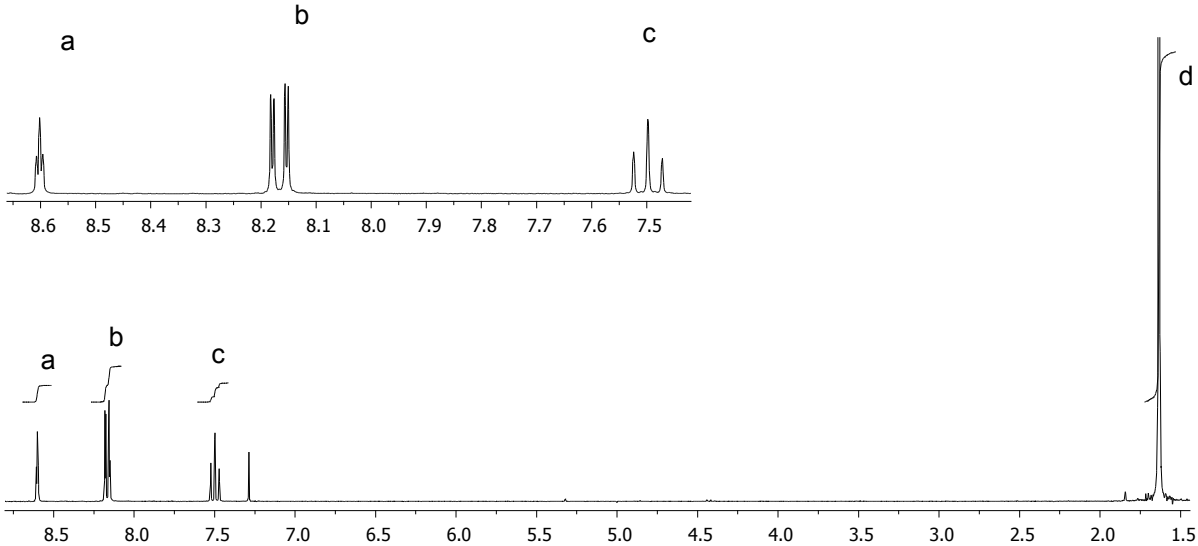


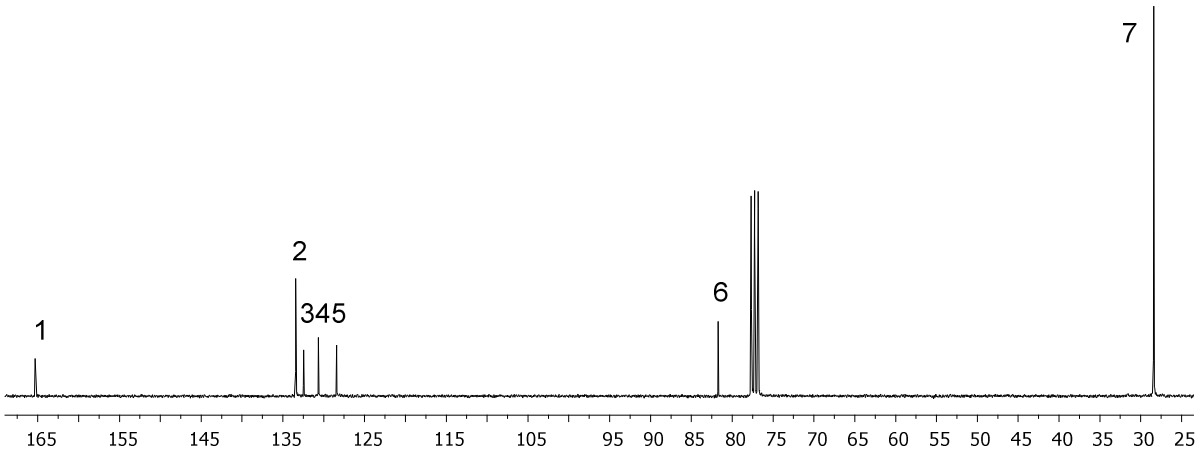
U6 $C_{16}H_{22}O_4$.

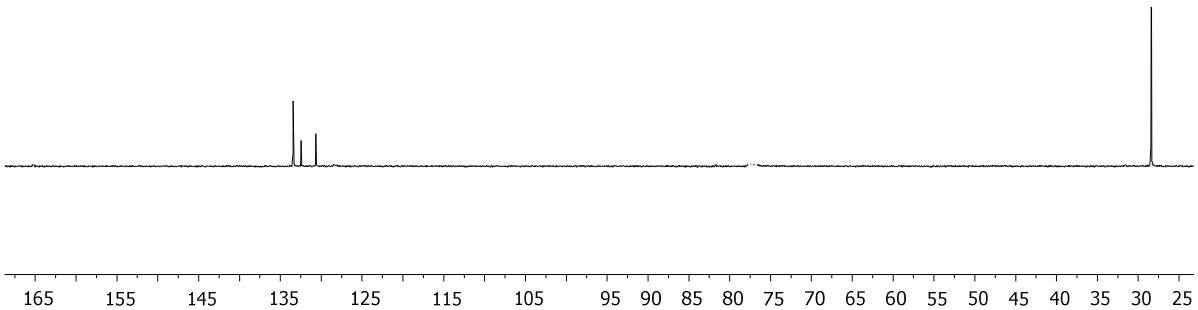
1. Struktur?
2. Zeichnen Sie den Splittingschlüssel für die aromatischen Protonen.
3. Auf welchem NMR-Gerät wurden diese Spektren aufgenommen? (200/300/400/600 MHz-Gerät)

   Hinweis: Der Name des NMR-Geräts hängt von der Protonen-Frequenz ab.
   Die 13C-Frequenz ist immer ¼ der Protonenfrequenz
   Die Achse (Frequenz in ppm) ist geräteunabhängig.
   Das Peakpicking (Frequenz in Hz) ist geräteabhängig (hier: 1 ppm = 300 Hz)
   Kopplungskonstanten (in Hz angegeben) sind geräteunabhängig
   Achten Sie auf die richtige Einheit Messfrequenz: MHz, Spektrum: Hz



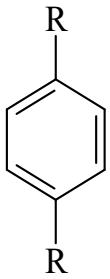

a
b
c
d
8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5

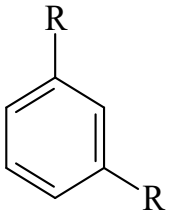

1
2
345
6
7
165 155 145 135 125 115 105 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25

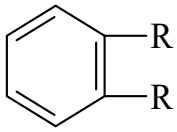

165 155 145 135 125 115 105 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25

U7

a) Wieviele Signale erhalten Sie im ^{1}H bzw. ^{13}C-Spektrum?
b) Geben Sie das Aufspaltungsmuster der Protonen an.

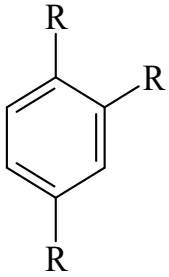


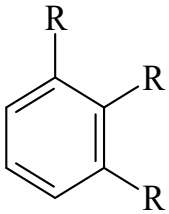




^{1}H-Signale

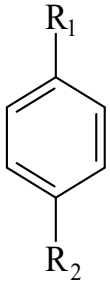
^{13}C-Signale

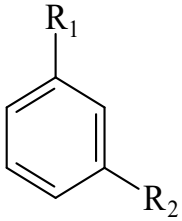


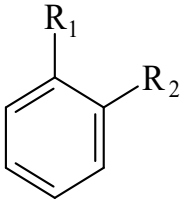


^{1}H-Signale

^{13}C-Signale

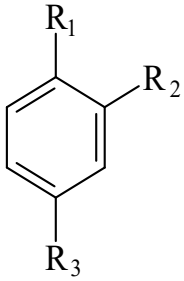


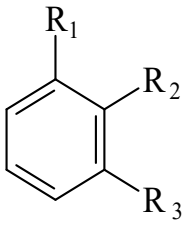


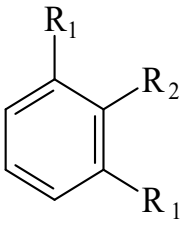


^{1}H-Signale

^{13}C-Signale



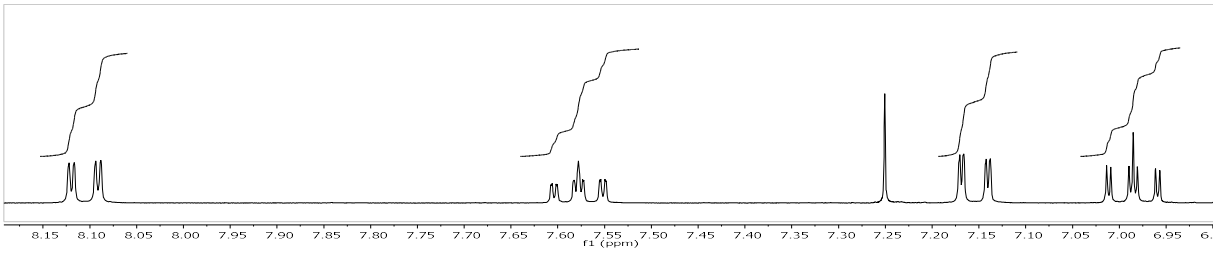


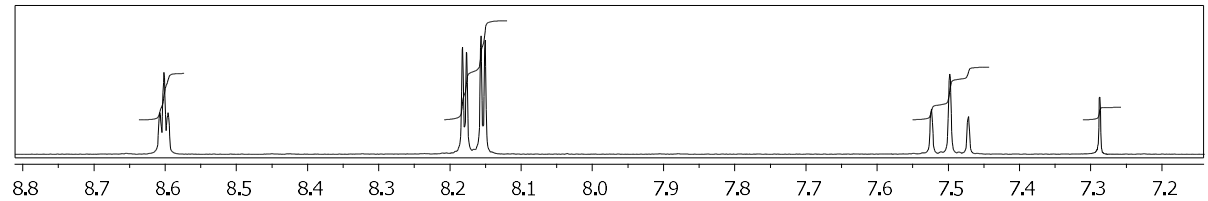


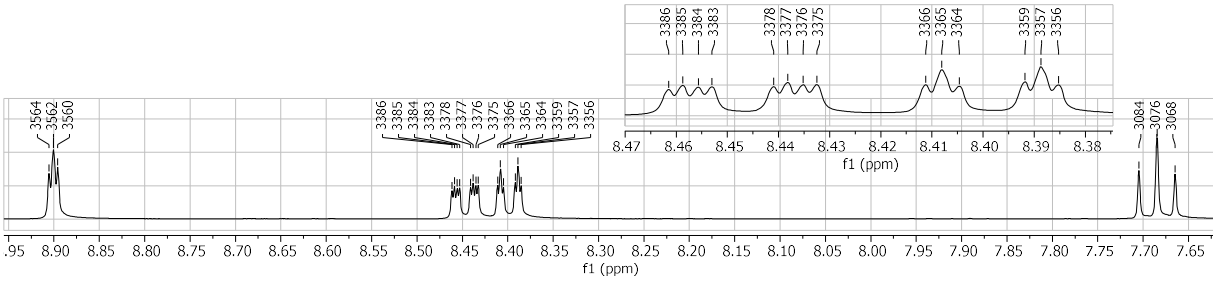
^{1}H-Signale

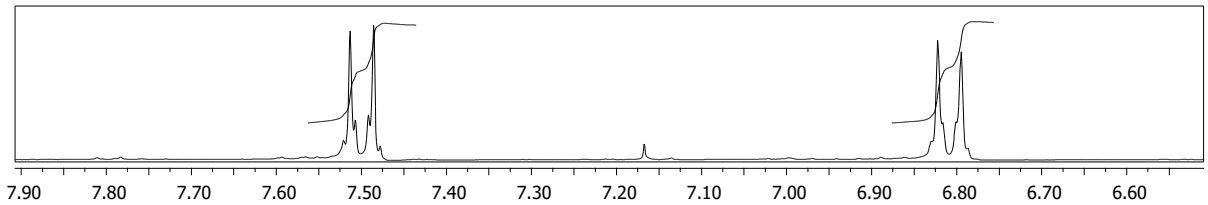
^{13}C-Signal

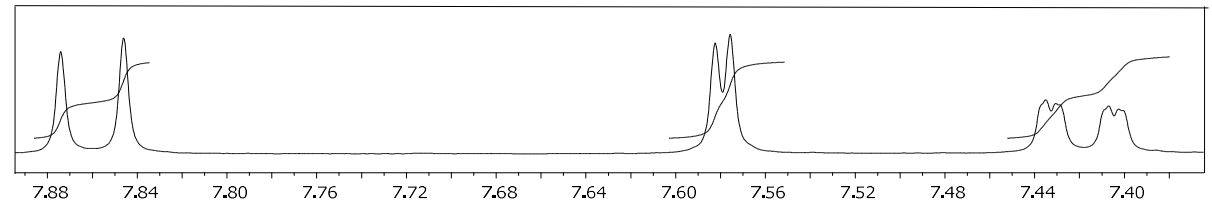
Wie sind die Aromaten in folgenden Spektren substituiert? U7/2

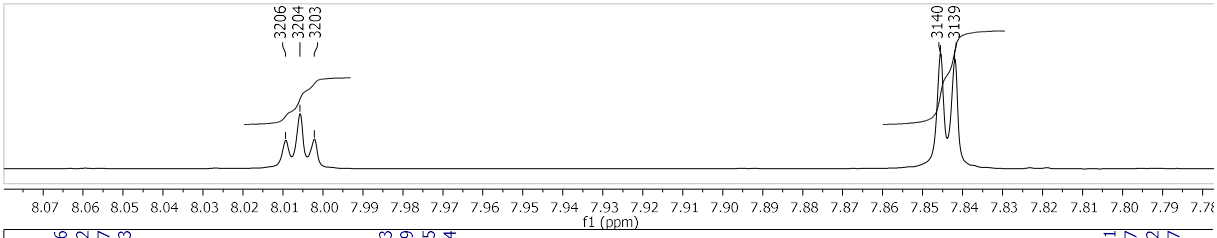


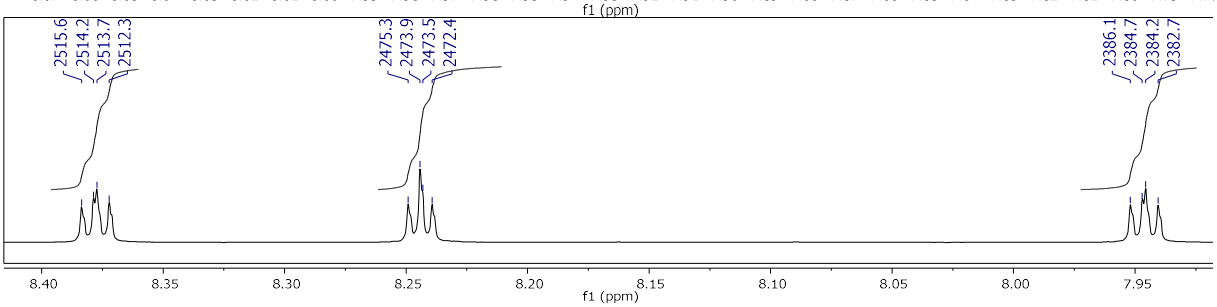










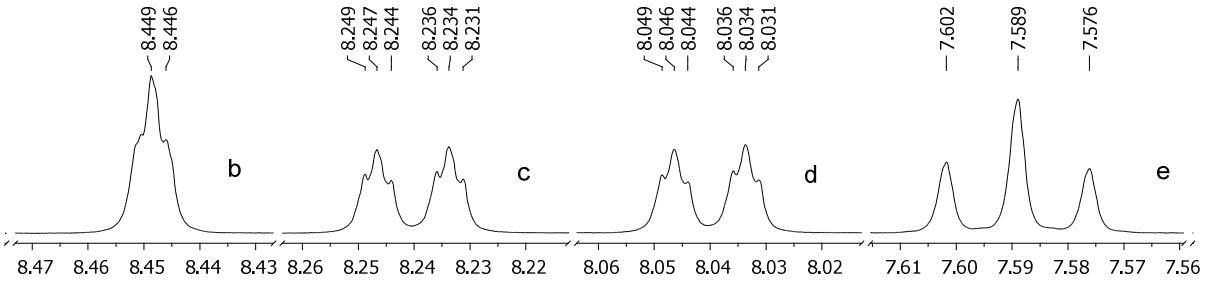


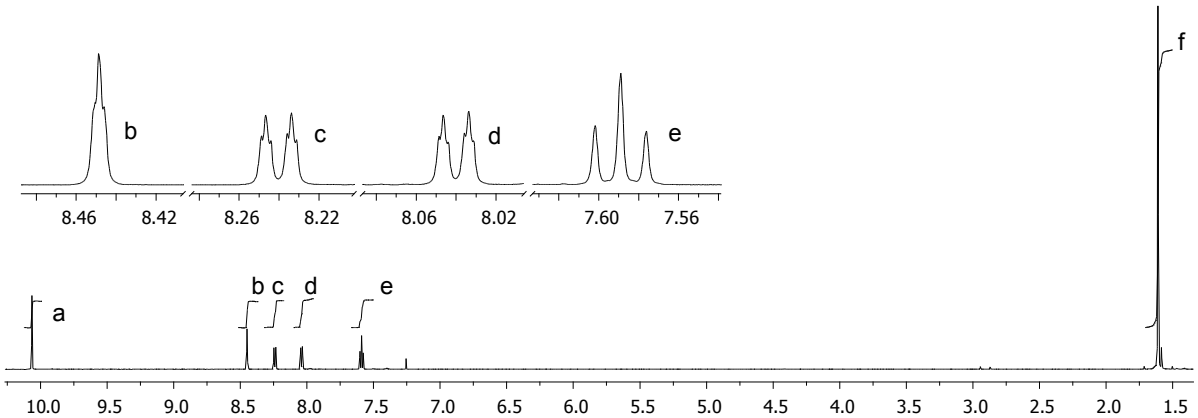
U 8 $C_{12}H_{14}O_3$

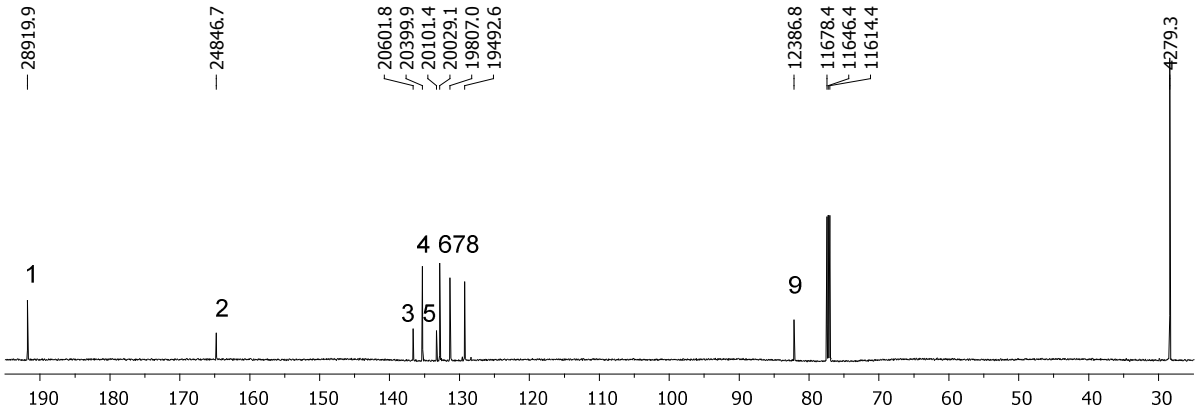
1. Struktur?

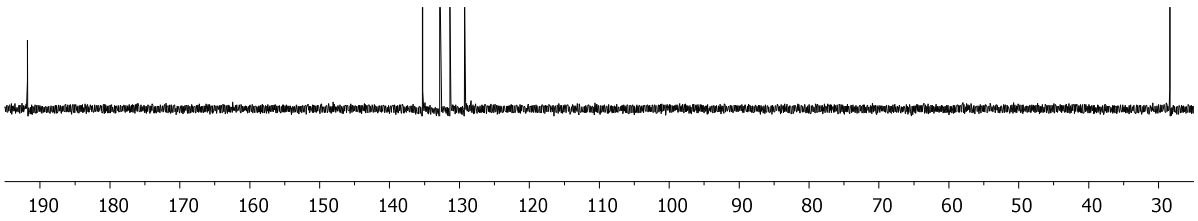
2. Auf welcher Maschine wurden die Spektren gemessen?

3. Zeichnen Sie den Splittingschlüssel für alle arom. Protonen incl. allen Kopplungskonstanten.




b
c
d
e
f
a
8.46
8.42
8.26
8.22
8.06
8.02
7.60
7.56
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5

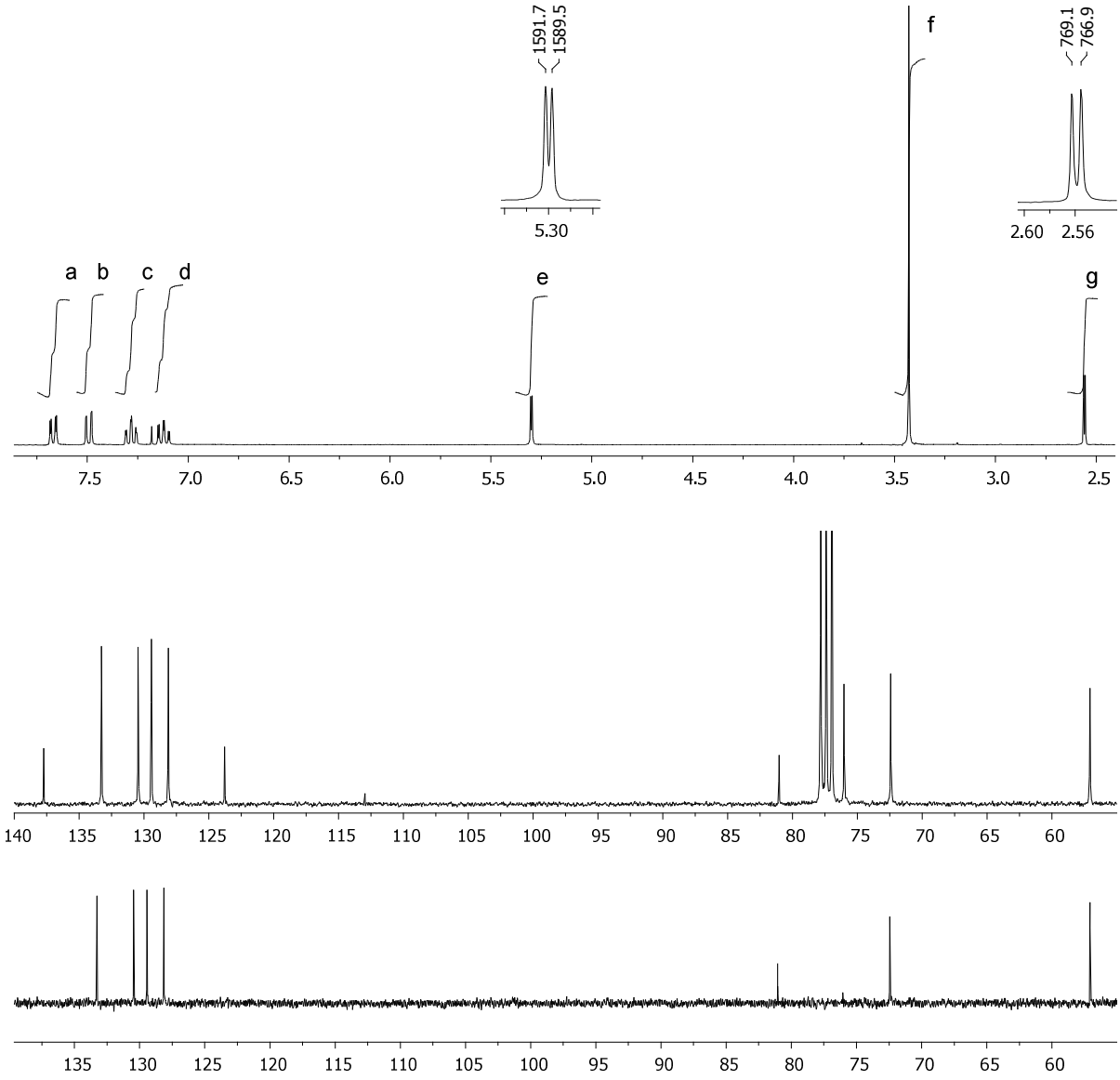

28919.9
24846.7
20601.8
20399.9
20101.4
20029.1
19807.0
19492.6
12386.8
11678.4
11646.4
11614.4
4279.3
1
2
3
4
5
678
9
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30


190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30

U9 $C_{10}H_9OBr$

Hinweis: δ (Acetylen, ^{1}H) = 1,8 ppm , δ(Acetylen, ^{13}C) = 71,9 ppm

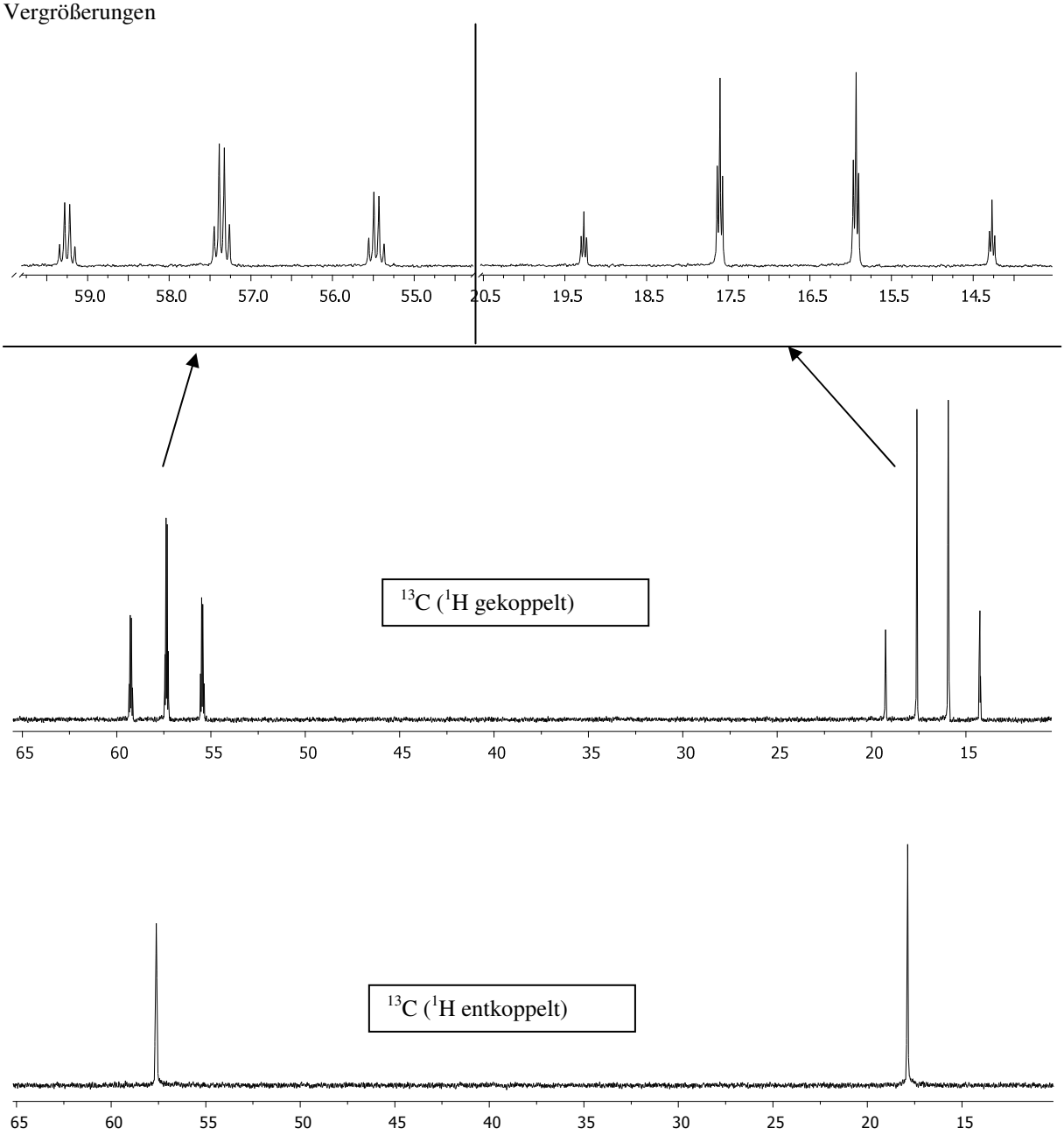
1. Struktur?
2. Im Protonenspektrum haben die 2 Peaks bei 5,3 ppm und 2,56 ppm die gleiche Kopplungskonstante. Was schließen Sie daraus?



U 10: Entkopplung

- Um welchen Alkohol handelt es sich?
- Erklären Sie das Kopplungsmuster
- Warum entkoppelt man normalerweise das ^{13}C-Spektrum?
- Wenn man nicht entkoppelt, sieht man in ^{13}C-Spektren die Protonenkopplungen. Warum sieht man im ^{1}H-Spektrum keine ^{13}C-Kopplungen?

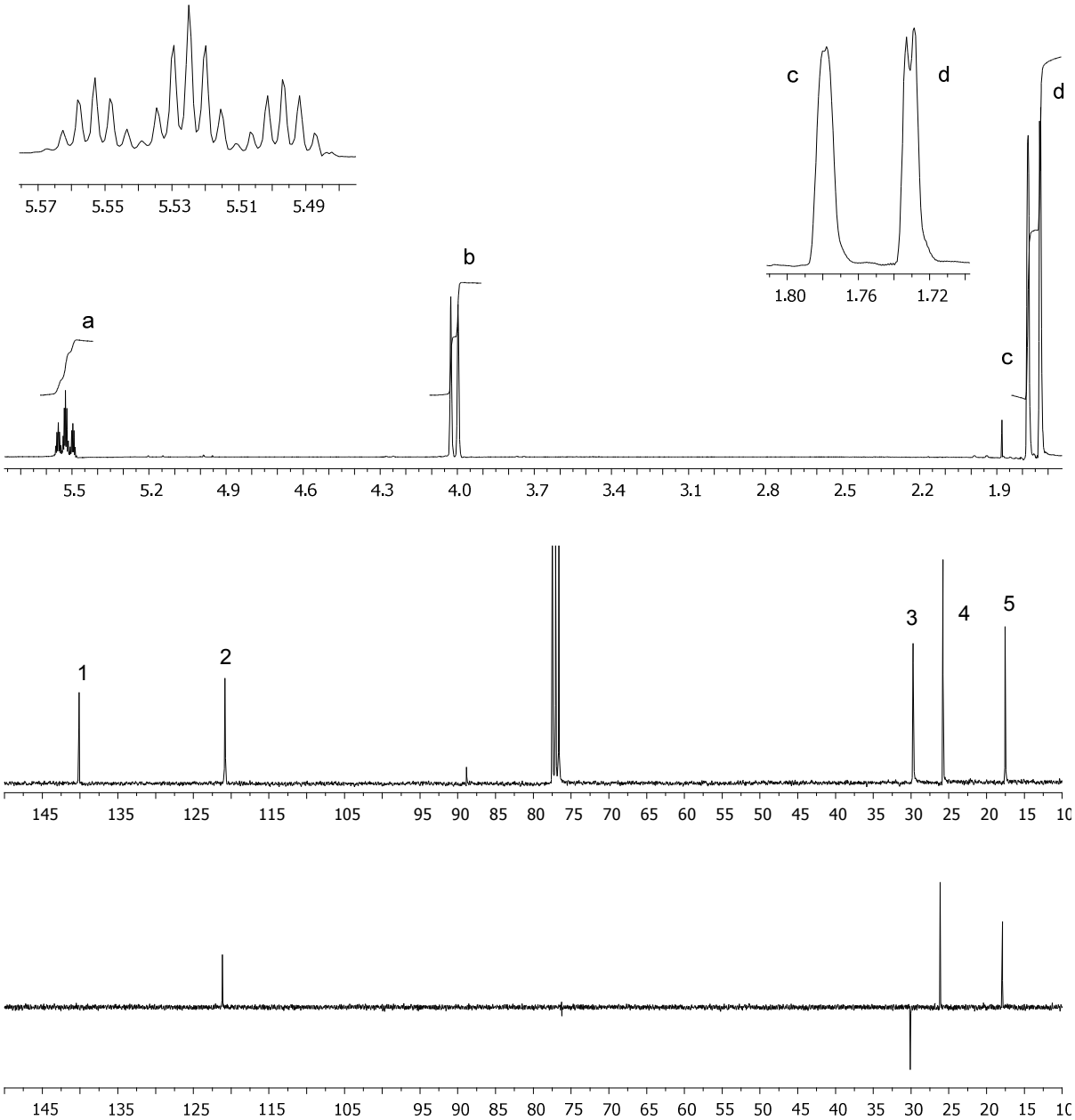
Vergrößerungen



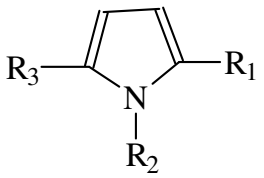
U 11 C_5H_9Br

1. Struktur ?

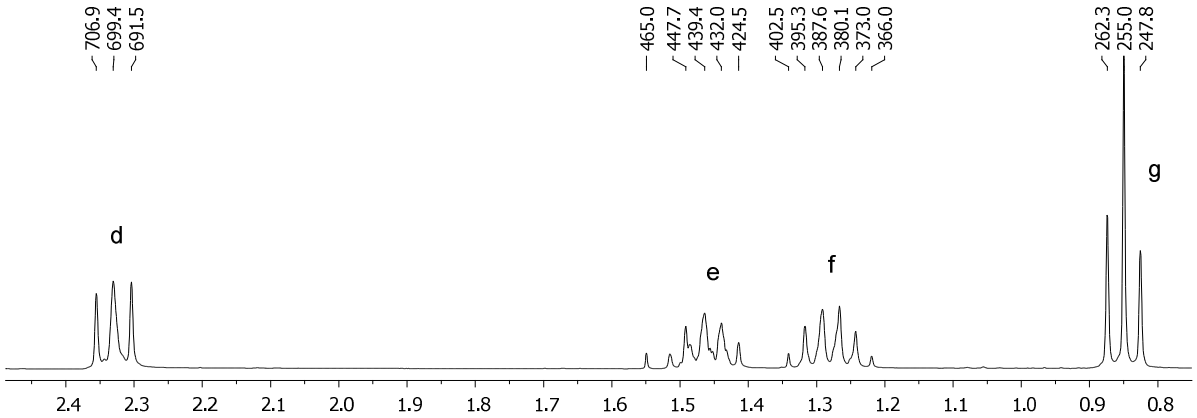
2. Zeichnen Sie den Splittingschlüssel für alle ^{1}H-Signale.

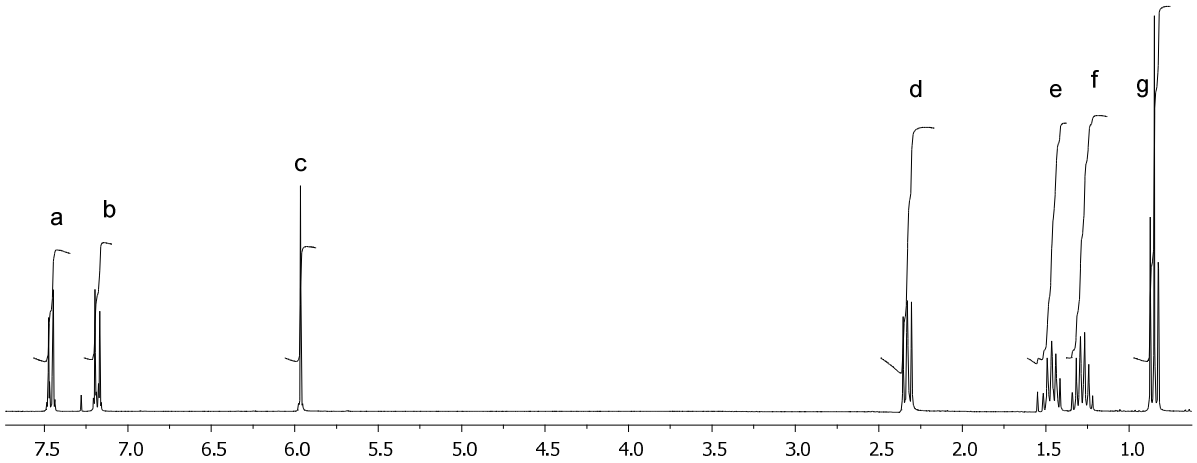


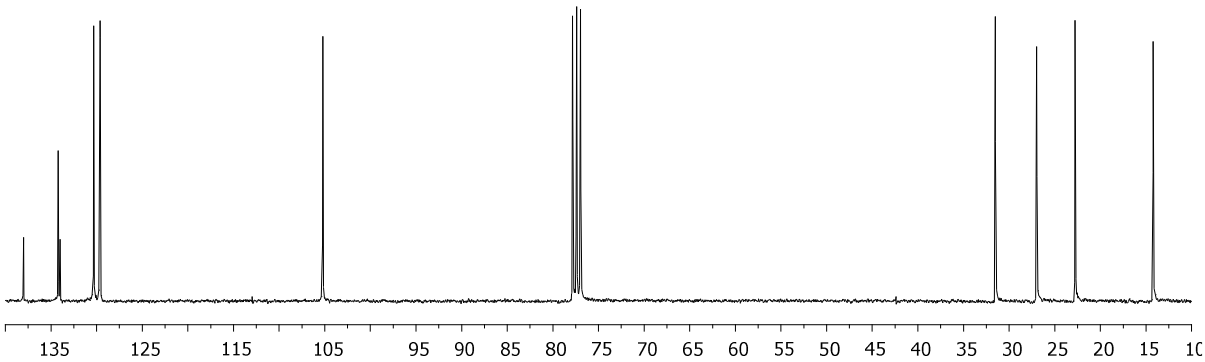
U 12 $C_{18}H_{24}NCl$

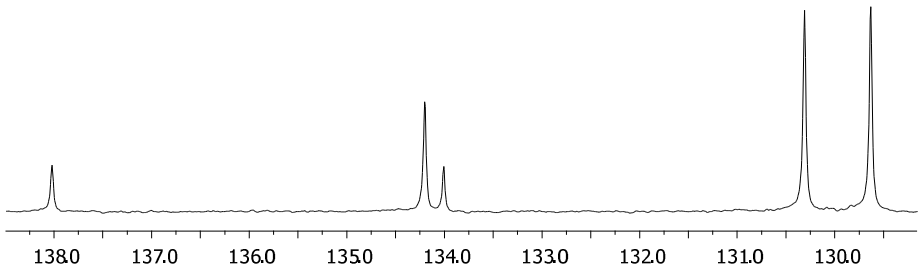


1. Struktur – bestimmen Sie die 3 Reste
2. Zeichnen Sie den Splittingschlüssel für die aliphatischen Protonen. Bezeichnen Sie die Aufspaltungen mit den jeweiligen Kopplungenkonstanten. (z. B. J_{AB}, J_{AC} usw.)
3. Auf welchem NMR-Gerät wurden diese Spektren aufgenommen?
4. Wie würde das Spektrum unten auf dieser Seite ausschauen, wenn es auf einem 600 MHz-Gerät gemessen worden wäre?

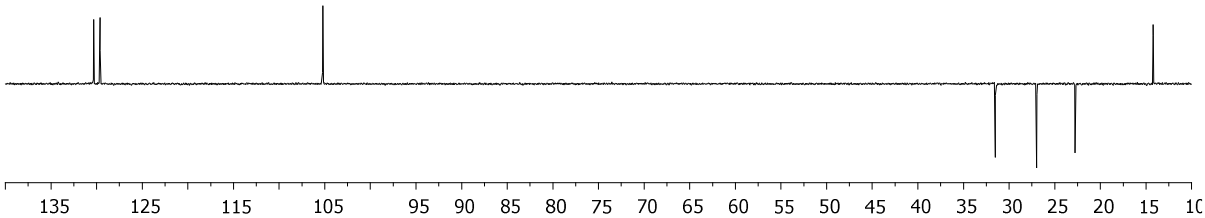






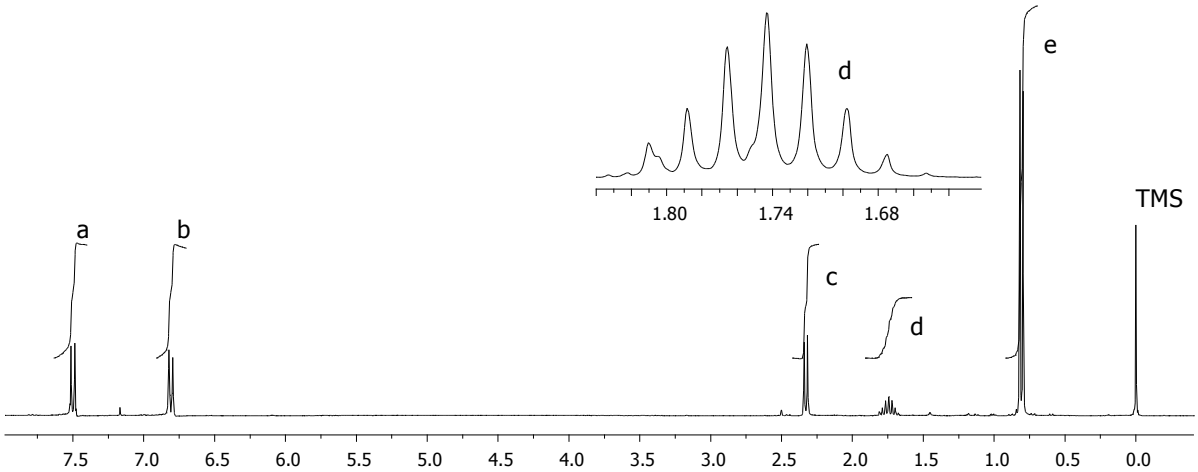


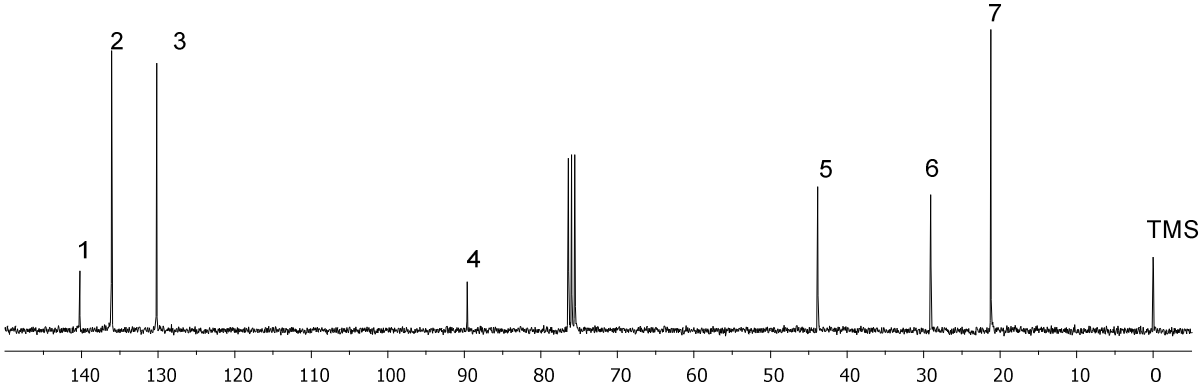
Vergrößerung

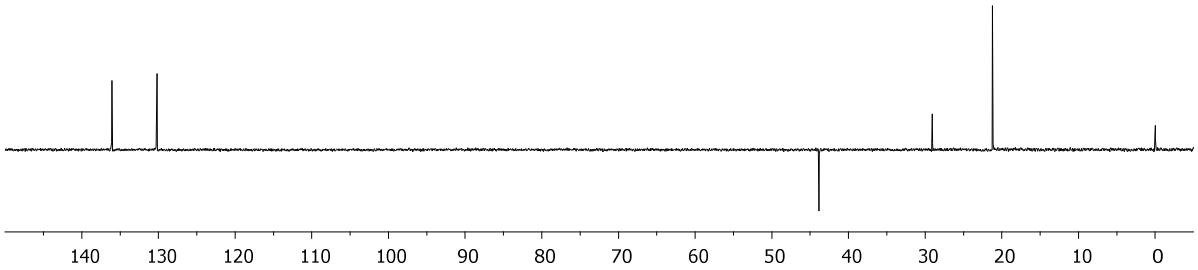


U13: $C_{10}H_{13}J$

Struktur?

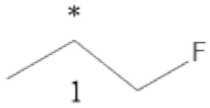


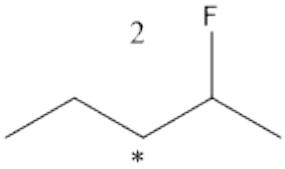


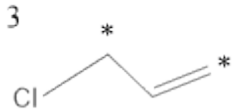


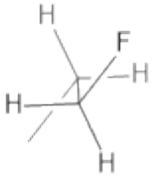
U14

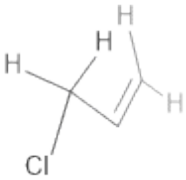
homotop -	Rotation
enantiotop -	Spiegelebene
diastereotop -	nichts, chirales Zentrum

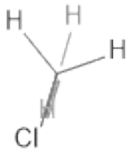


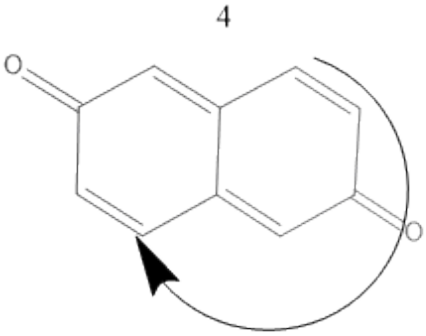


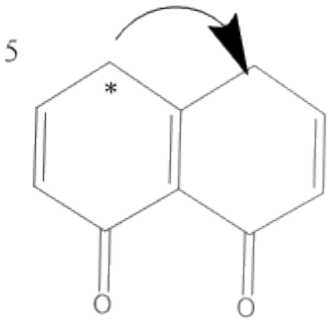


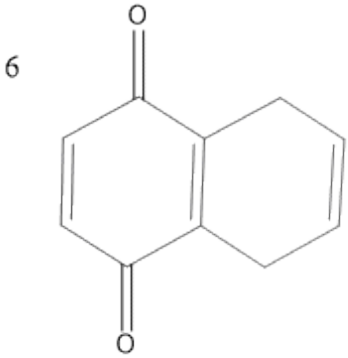


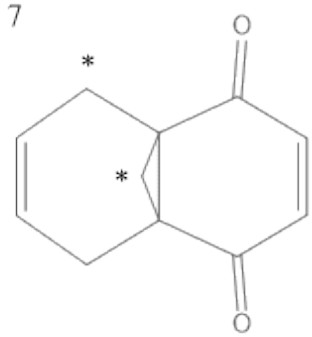


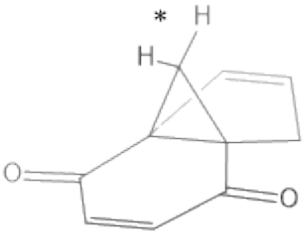


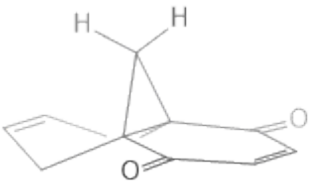


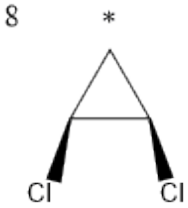


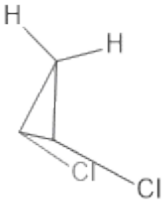


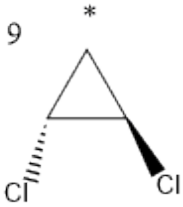


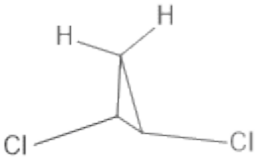




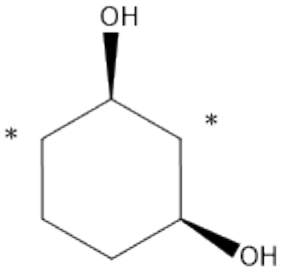


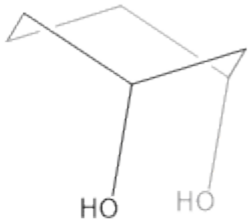




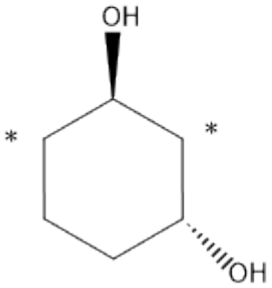


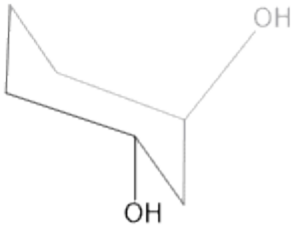
10



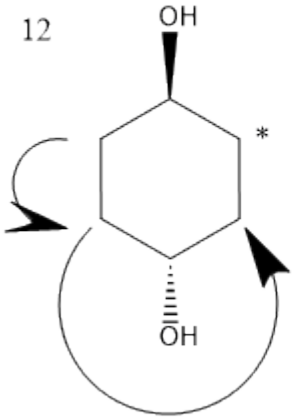


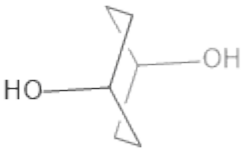
11

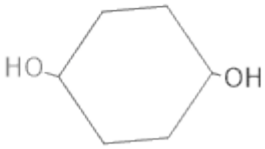




12



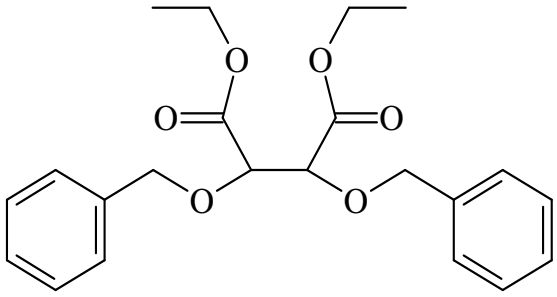




1. Bestimmen Sie, ob die 2 Protonen der markierten Methylen-Gruppen (*) homotop, enantiotop oder diastereotop sind.
2. Bestimmen Sie, ob die markierten Gruppen (Pfeile) homotop, enantiotop oder diastereotop sind.
3. Wieviele Signale erwarten Sie im ^{1}H-Spektrum?
4. Bestimmen Sie das Spinsystem.

5. Geben Sie je ein Beispiele für ein AB, AB2, ABC, ABCDE und AA'BB'-System an.

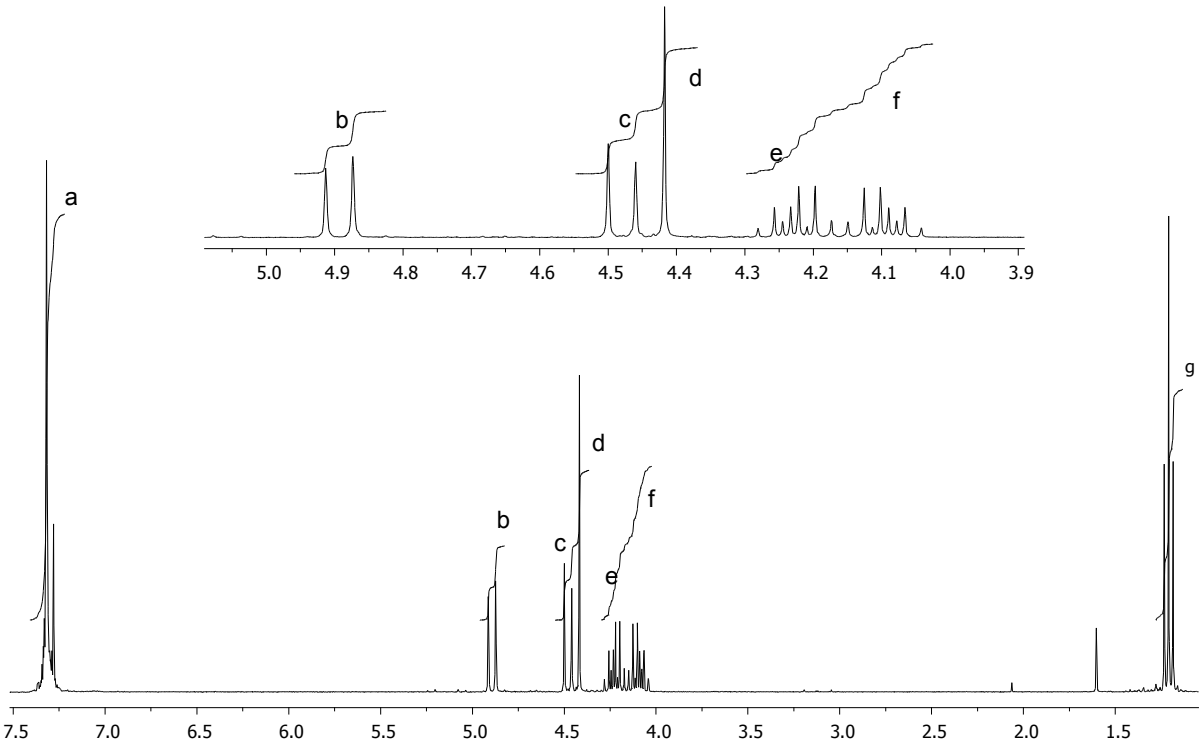
U 15

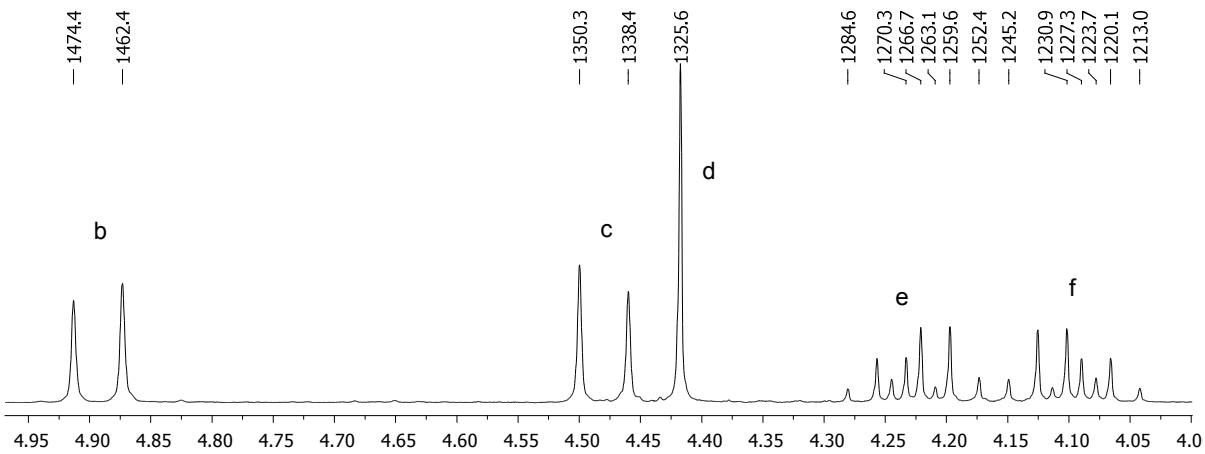


1. Ordnen Sie alle Protonen-Signale zu.

2. Zeichnen Sie einen Splittingschlüssel für die Protonen zwischen 4 und 5 ppm incl. allen Kopplungskonstanten in Hz (z.B. J_{ab}= 8 Hz) (Seite 2)

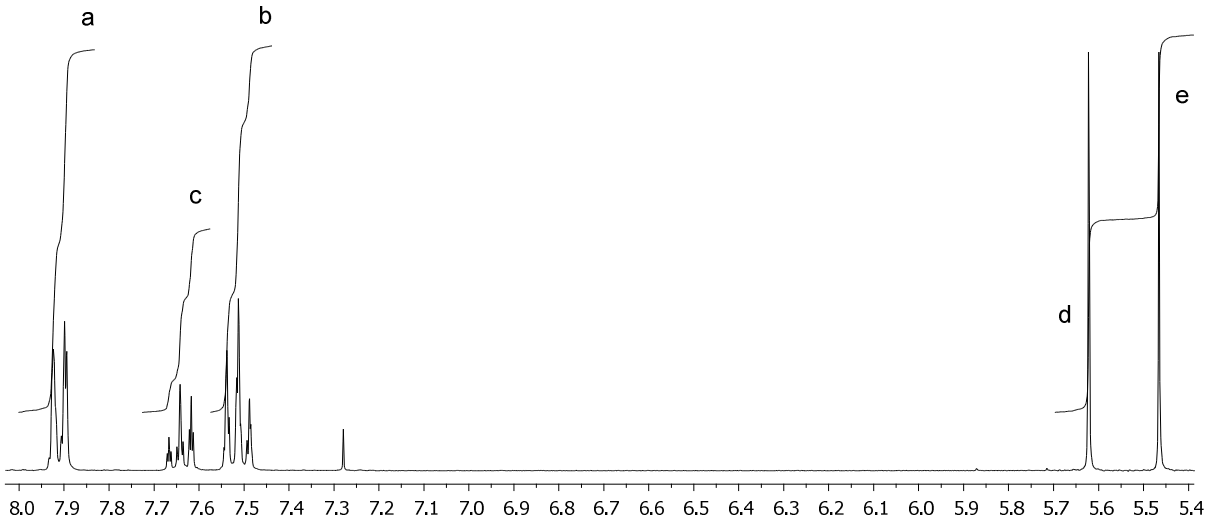
3. Erklären Sie die Protonen-Signale zwischen 4.4 und 5 ppm genau. (Warum ist b und c ein Duplett? Warum ist d ein Singulett?)

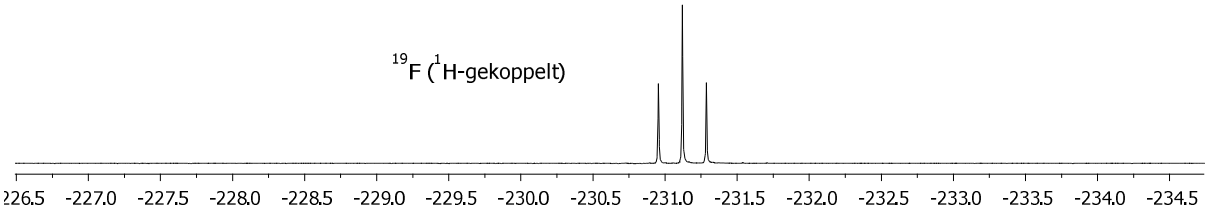


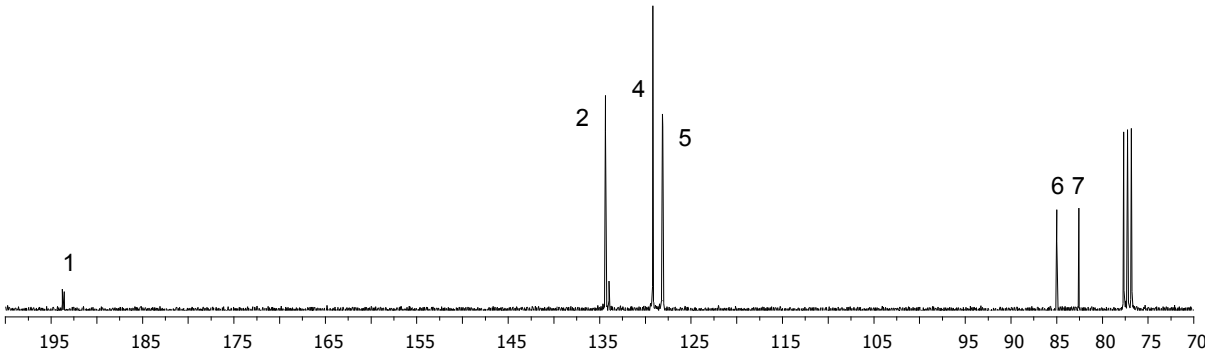

1474.4
1462.4
1350.3
1338.4
1325.6
1284.6
1270.3
1266.7
1263.1
1259.6
1252.4
1245.2
1230.9
1227.3
1223.7
1220.1
1213.0
b
c
d
e
f
4.95
4.90
4.85
4.80
4.75
4.70
4.65
4.60
4.55
4.50
4.45
4.40
4.35
4.30
4.25
4.20
4.15
4.10
4.05
4.0

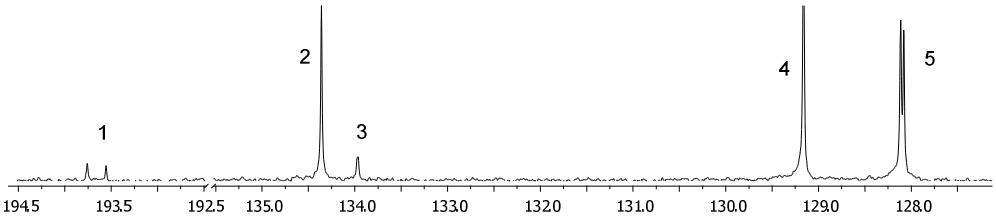
U16 C_8H_7OF.

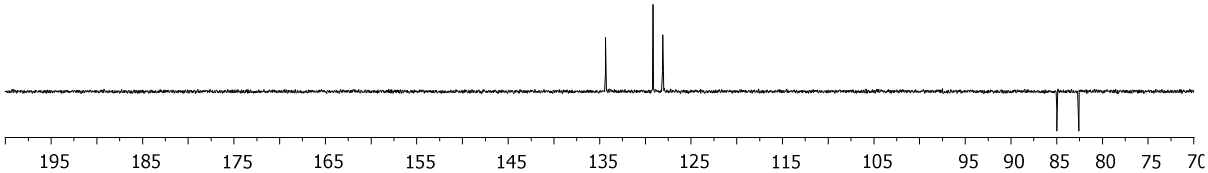
1. Struktur?
2. Erklären Sie die Signale bei ca. 82 und 86 ppm. (2 P)



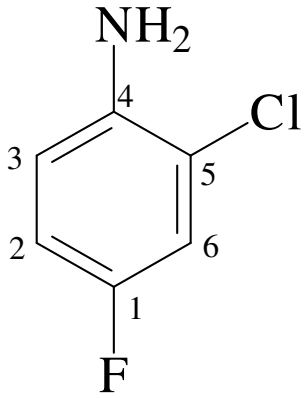




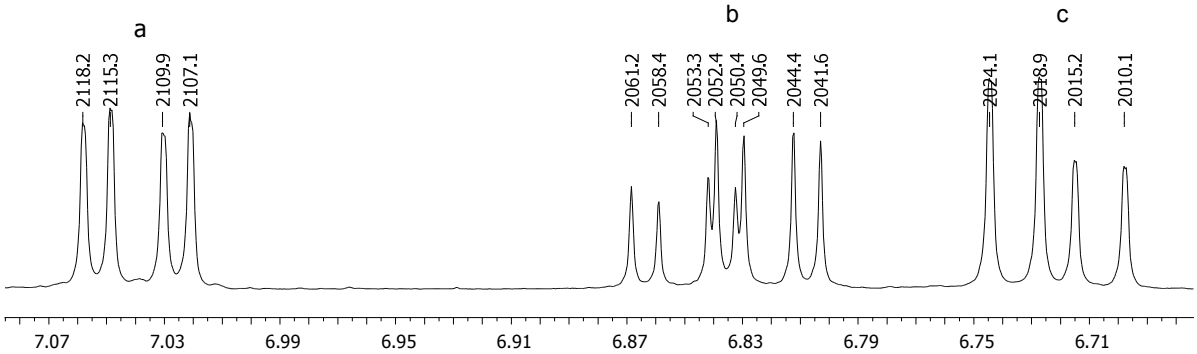




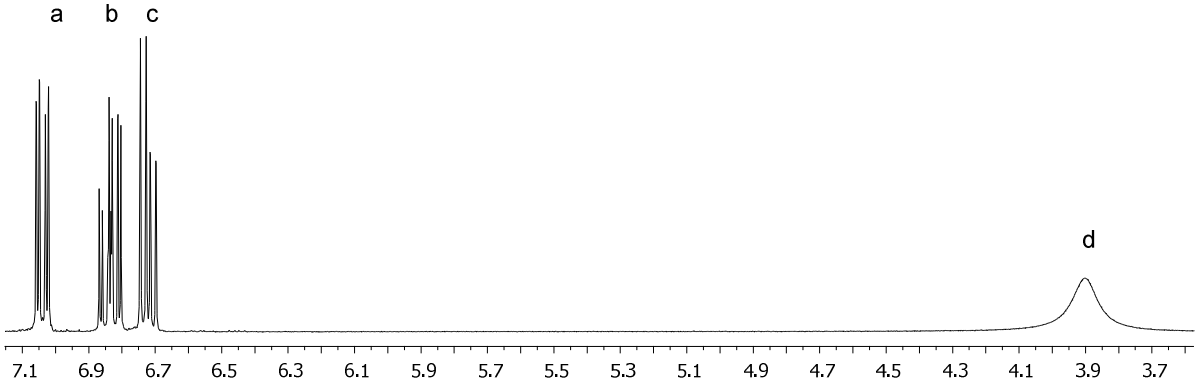
U17

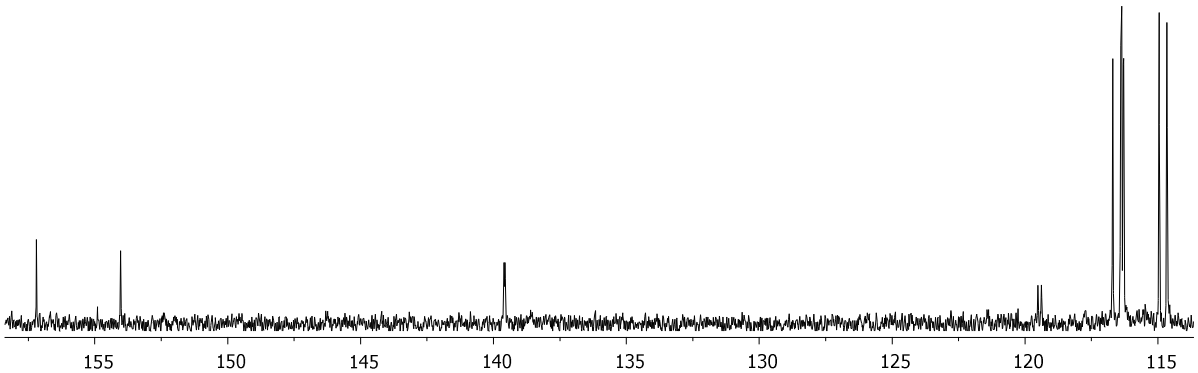


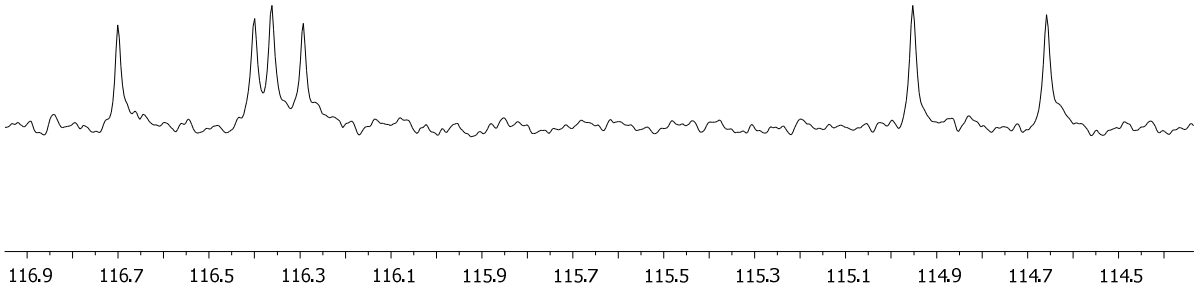
1. Ordnen Sie die Protonen zu. (Für die genaue Zuordnung der 13C-Signale lernen Sie später das HSQC-Spektrum kennen)
2. Zeichnen Sie einen Splittingschlüssel für die Protonen (1 Hz = 1mm). Bestimmen Sie alle Kopplungskonstanten.



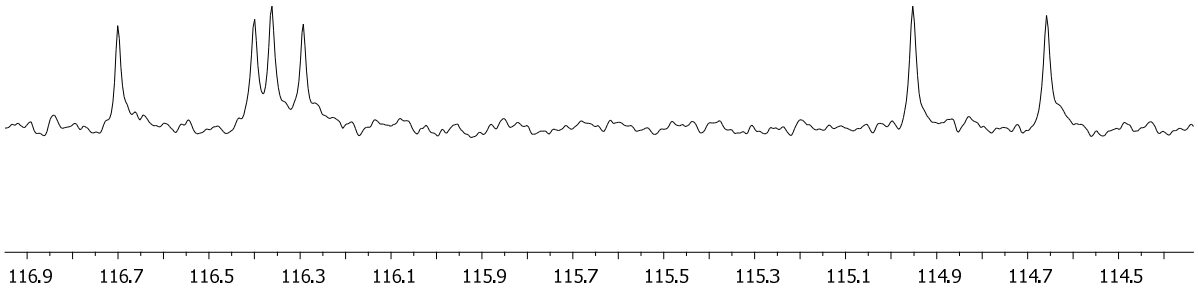
3. Zeichnen Sie das F-Spektrum (Ohne und mit Protonen-Entkopplung, δ=-130 ppm)
   → 2 Spektren zeichnen. Geben Sie auch hier die Kopplungskonstanten an.
4. Zeichnen Sie das Protonen-Spektrum, wenn bei dessen Aufnahme ^{19}F entkoppelt wäre.
5. Warum sind im 13C-Spektrum so viele Signale zu sehen, obwohl nur 6 Cs im Molekül sind? Können Sie einige Signale zuordnen?







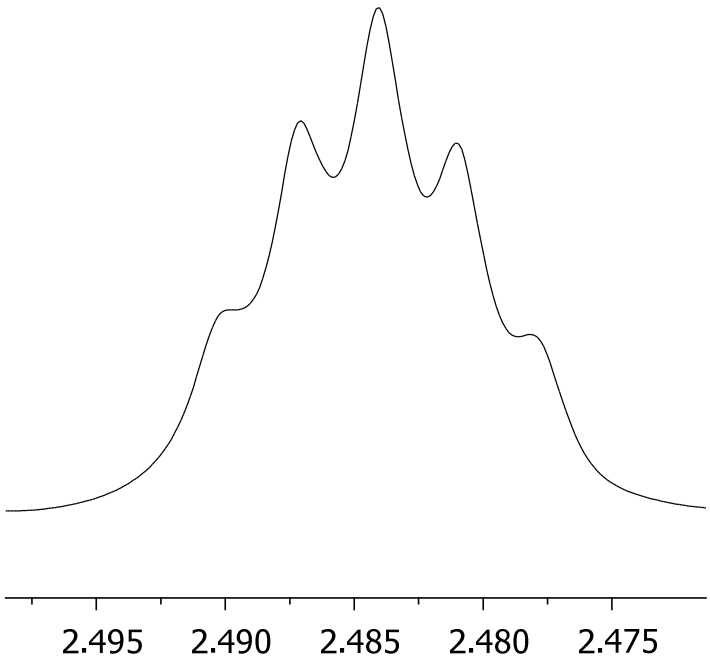
^{13}C-Vergrößerung

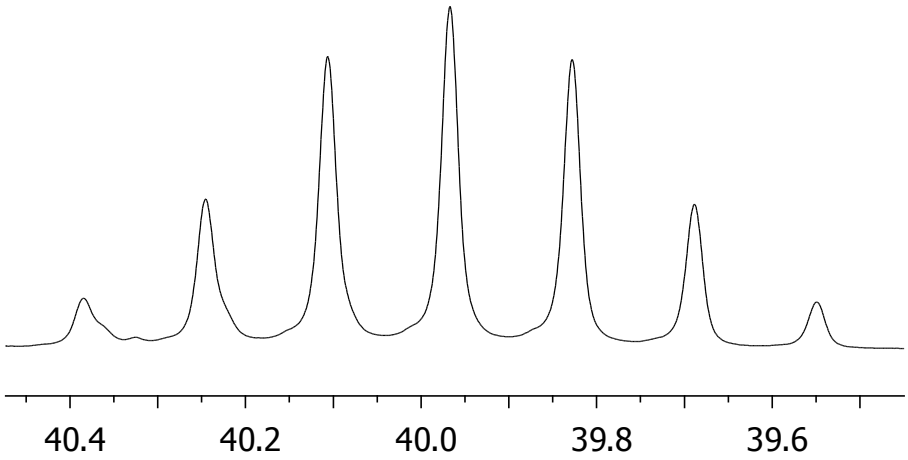


Dept

U18

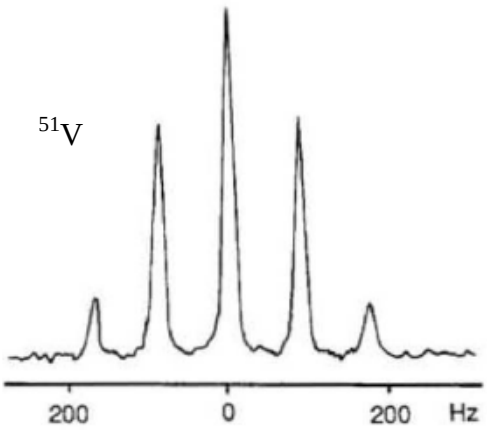
1. Erklären Sie das Kopplungsmuster von d6-DMSO (99 %)
2. Wie würden die Spektren ausschauen, wenn Sie d6-DMSO (100 % deuteriert) hätten?
3. Wie würden die Spektren ausschauen, wenn Sie d5-DMSO hätten? (^{1}H, ^{13}C (1H-entk.), ^{13}C (1H-gek.))

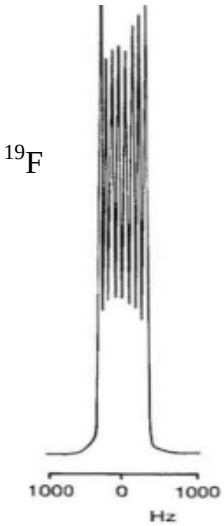




U19

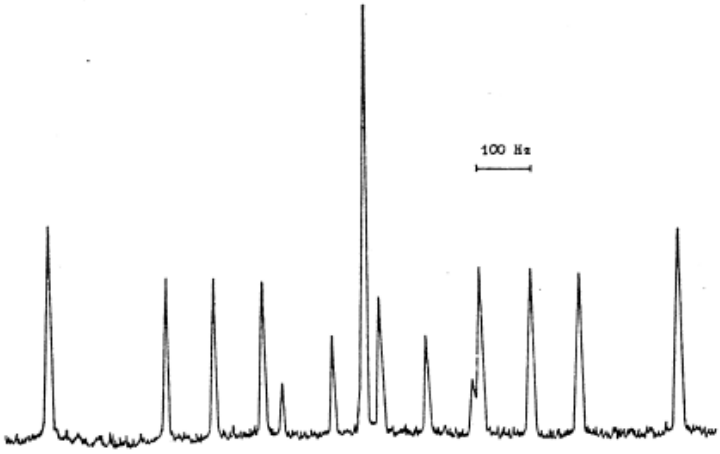
Erklären Sie die Aufspaltung des ^{51}V- und des ^{19}F-NMR-Spektrums des Anions VOF_4^-.
51V: I=7/2, Nat. Häufigkeit: 99.76 %
19F: I=1/2, Nat. Häufigkeit: 100 %
Was sagen Ihnen diese beiden Spektren über die Struktur des Anions aus?





U20

Erklären Sie in folgendem 31P-Spektrum die Aufspaltung von partiell deuterierter hypophosphoriger Säure $H_2PO(OH)$



^{31}P–N.M.R. spectra of partially deuterated H_2POOH

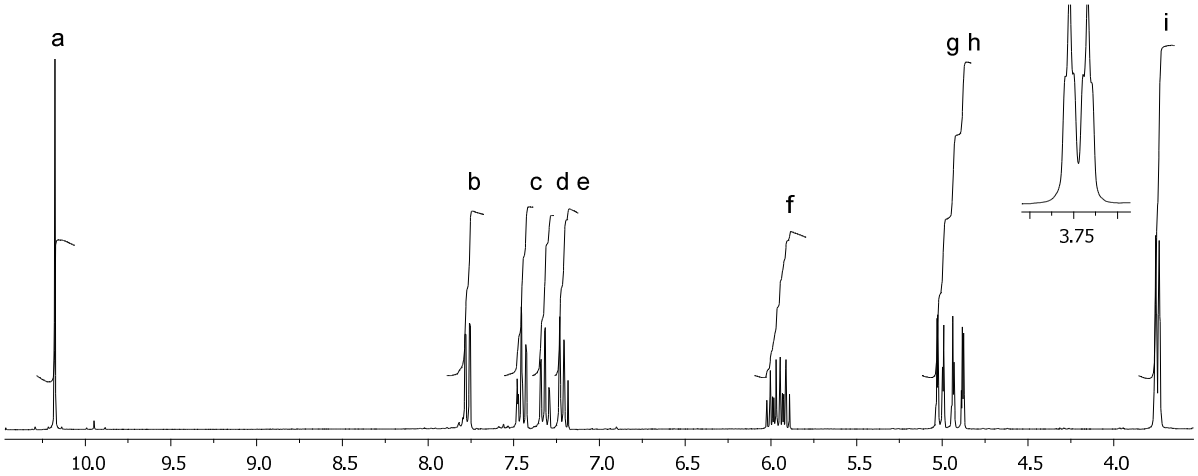
$H_2PO(OH)$

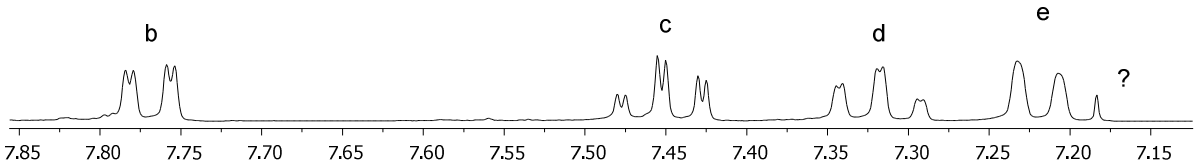
$HDPO(OH)$

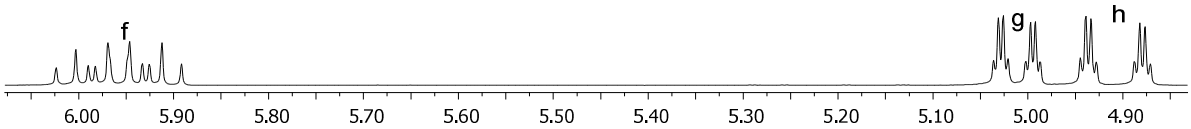
$D_2PO(OH)$

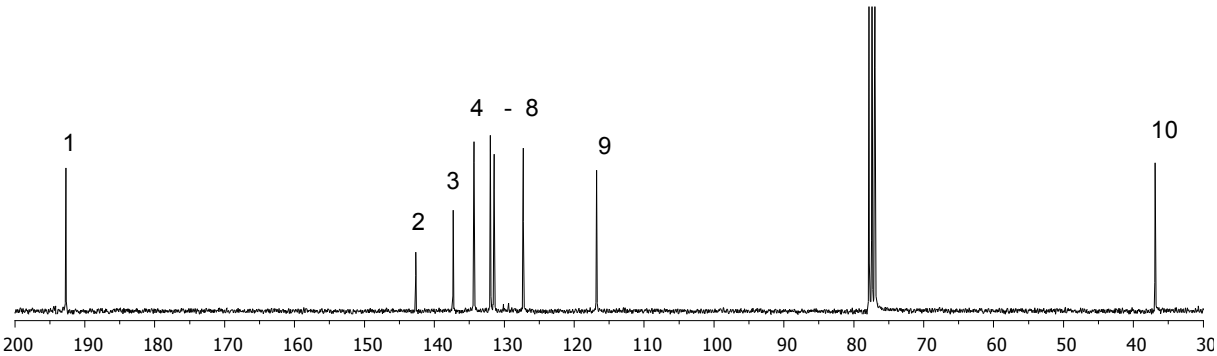
U21 $C_{10}H_{10}O$

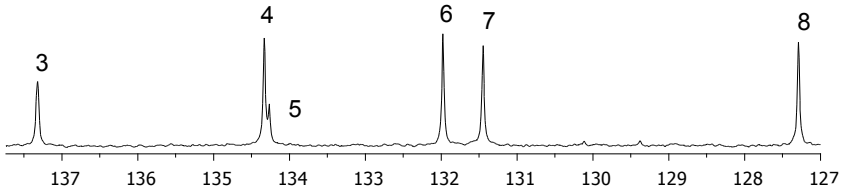
- Strukturen ?
- Splittingschlüssel mit Kopplungskonstanten

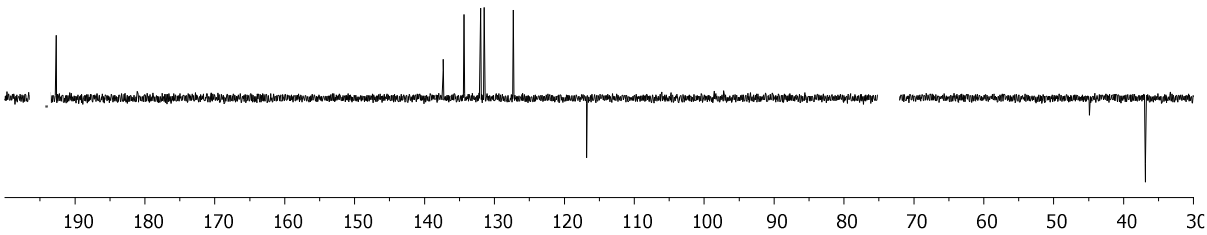




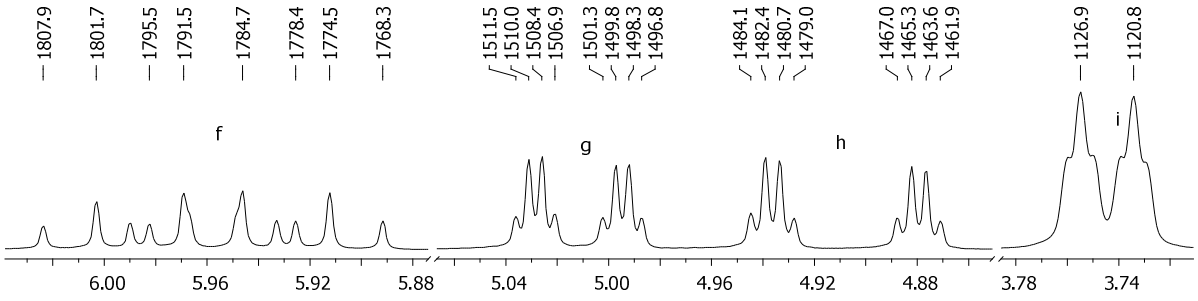








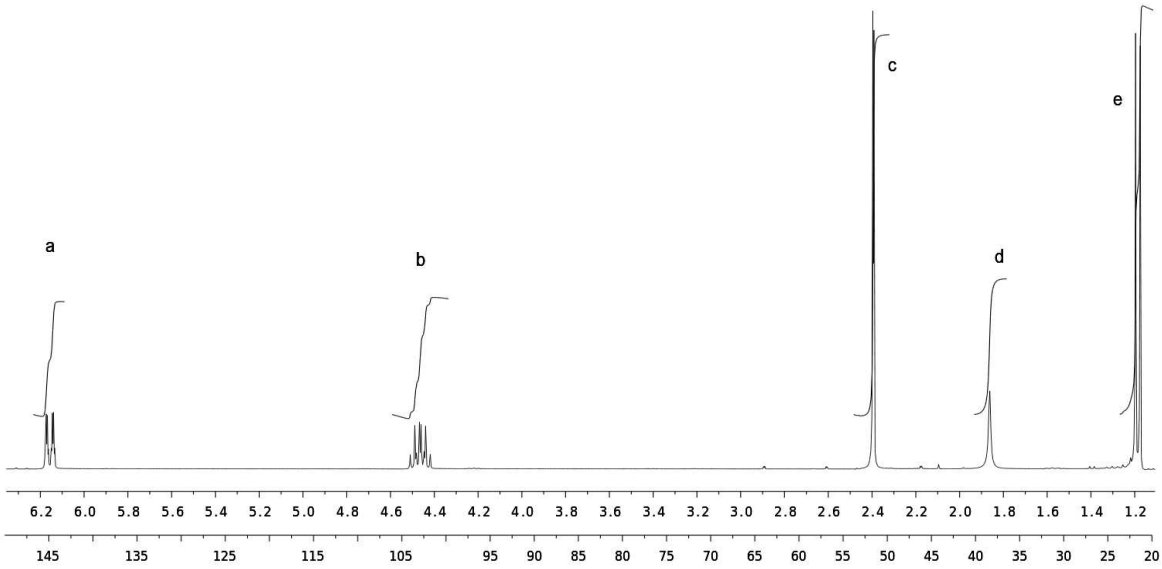
Zeichnen Sie einen Splittingschlüssel incl. allen Kopplungskonstanten.
Der Rechner zeigt nicht alle Kopplungskonstanten an. → Selber zufügen!

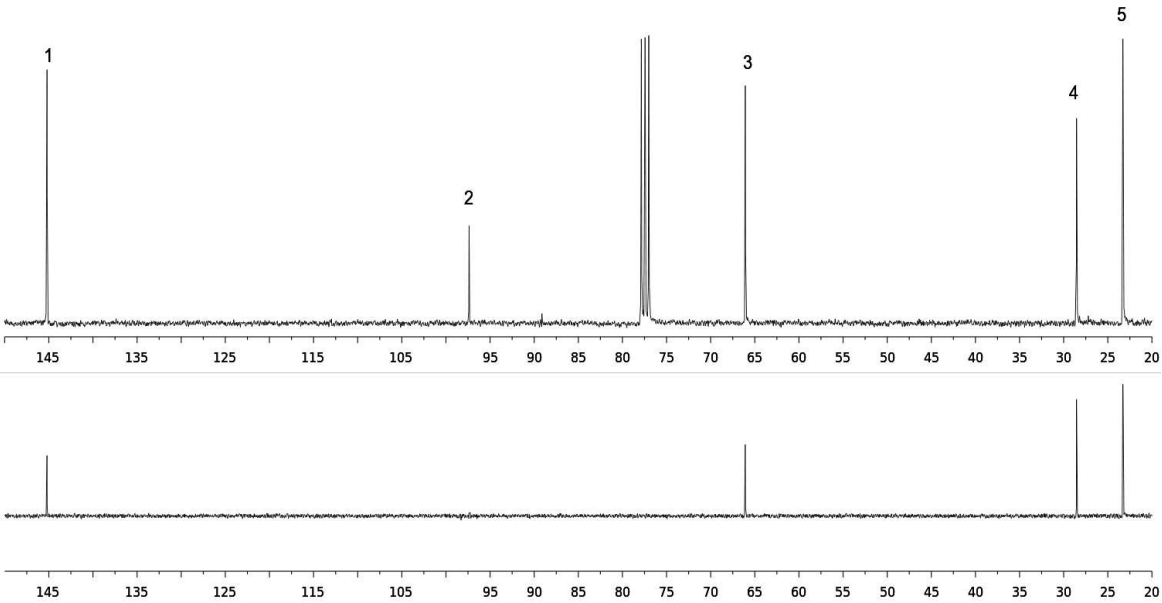


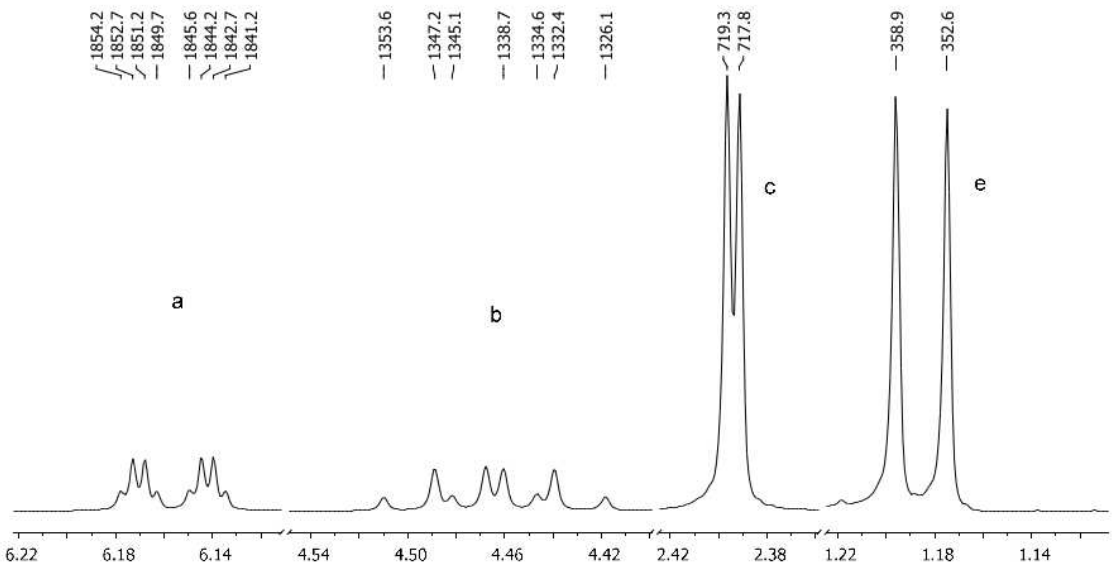
U22 SF: C_5H_9OI

1. Struktur ?

2. Erklären Sie das Kopplungsmuster der Signale bei 4.45 ppm und 6.15 ppm. Bestimmen Sie die Kopplungskonstanten. (Seite 2)






1854.2
1852.7
1851.2
1849.7
1845.6
1844.2
1842.7
1841.2
1353.6
1347.2
1345.1
1338.7
1334.6
1332.4
1326.1
719.3
717.8
358.9
352.6
a
b
c
e
6.22
6.18
6.14
4.54
4.50
4.46
4.42
2.42
2.38
1.22
1.18
1.14

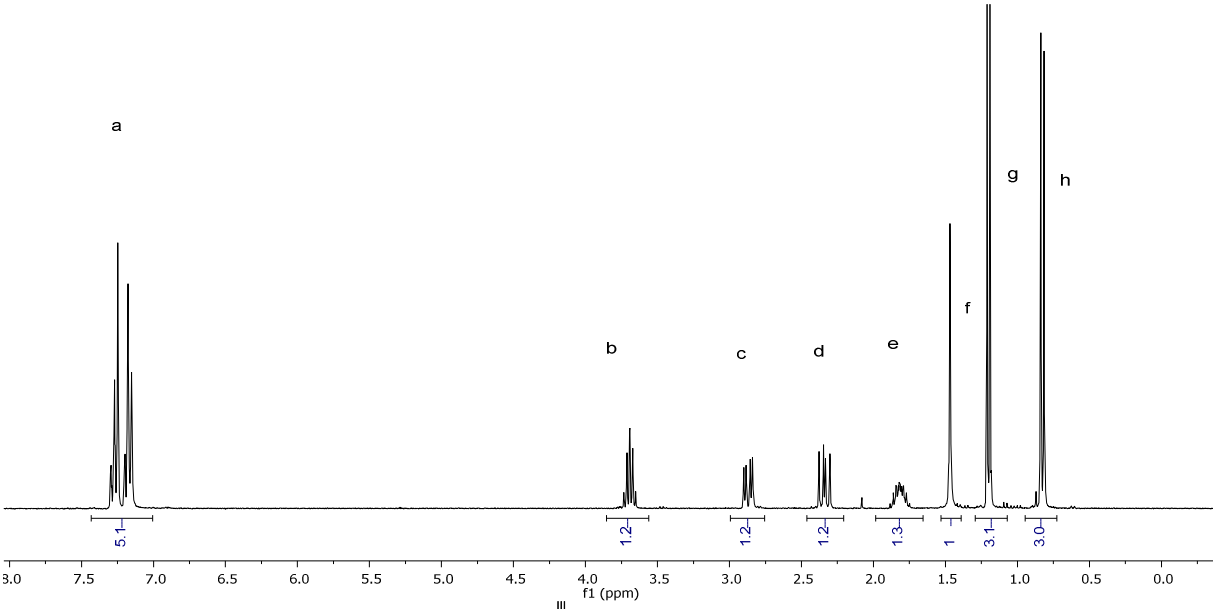
U23

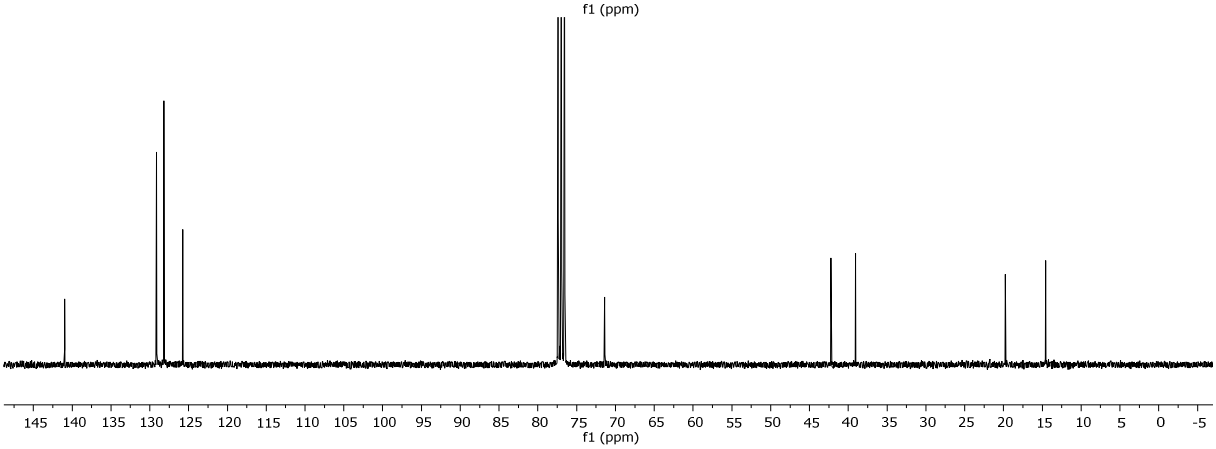
Auf folgenden Seiten sind die NMR-Spektren einer Verbindung mit folgender Summenformel abgebildet: $C_{11}H_{16}O$.

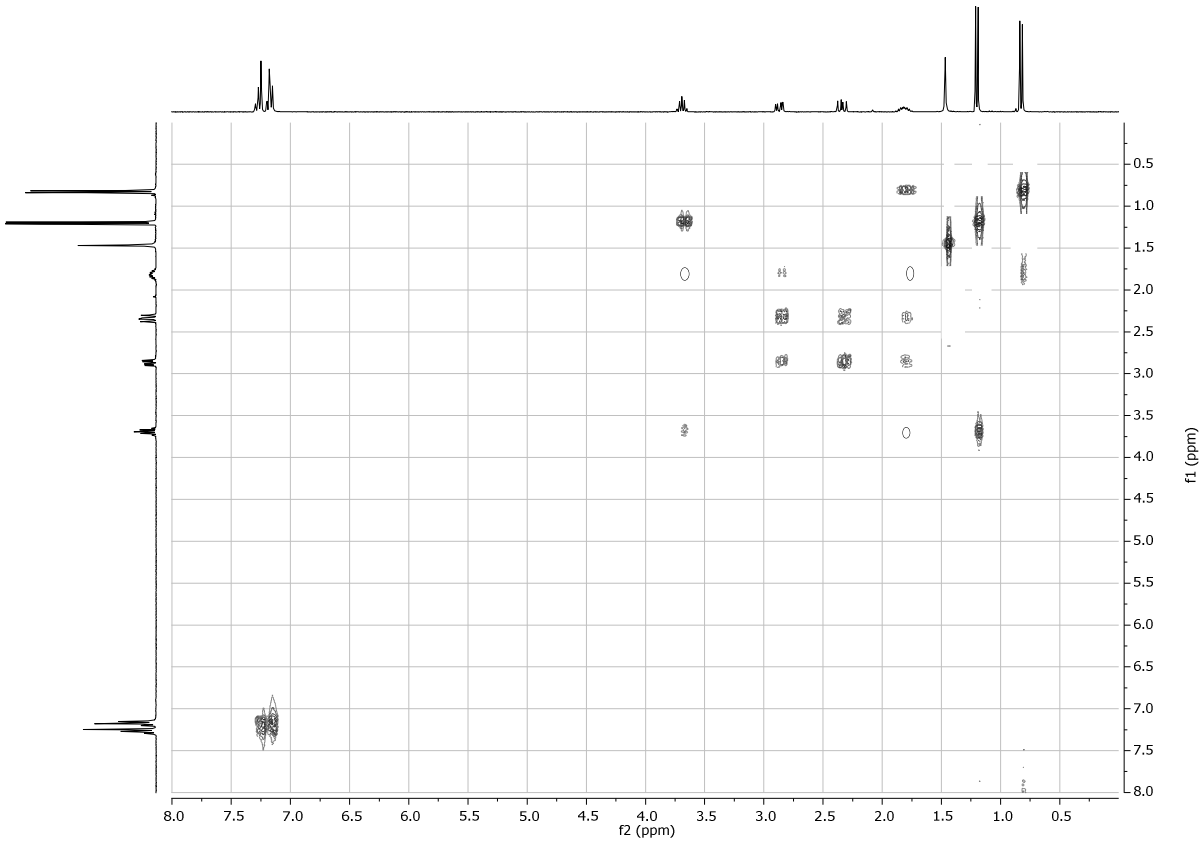
1. Geben Sie eine sinnvolle Struktur an. (5 P)

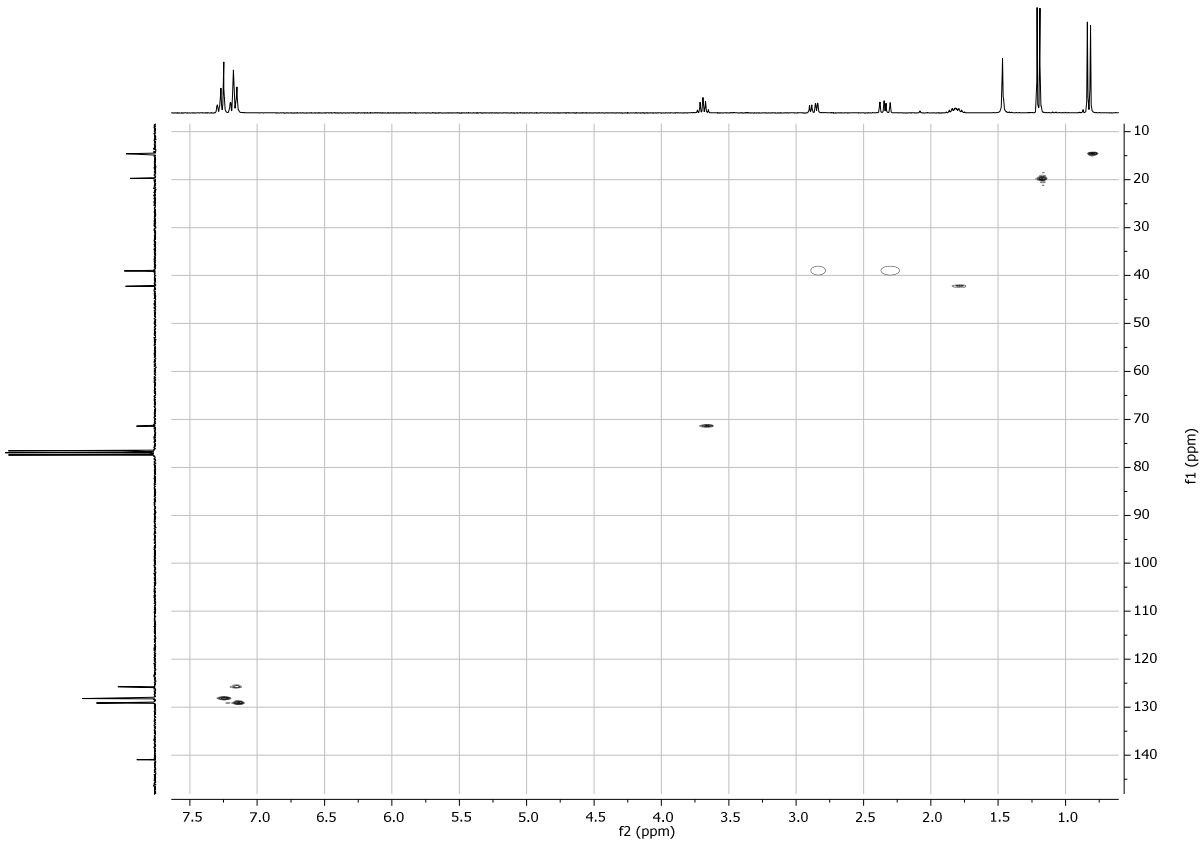
2. Bestimmen Sie das Spinsystem der Protonen (1 P)

3. Zeichnen Sie für den Aliphaten-Teil einen Splittingschlüssel. (6 P)





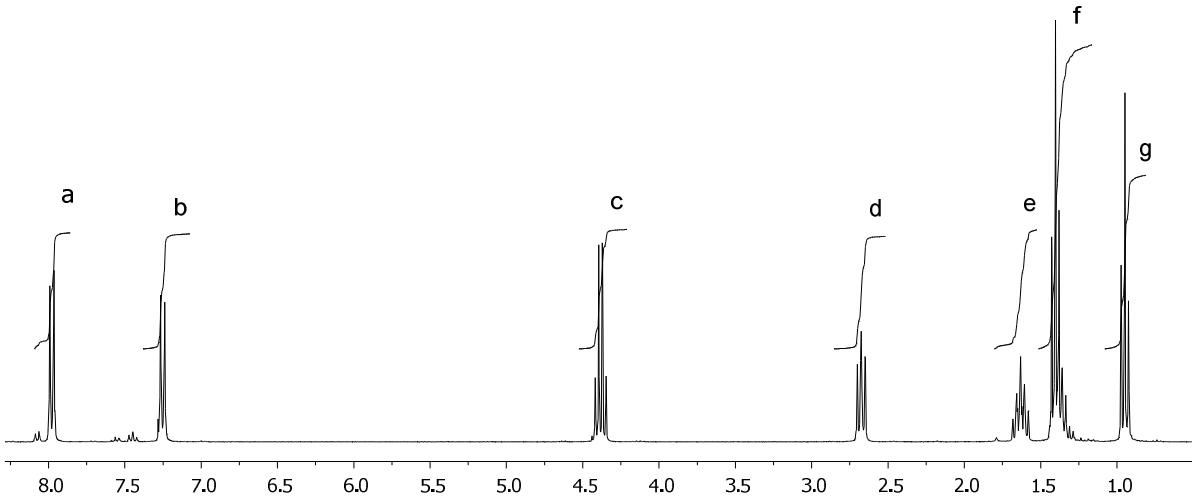

f2 (ppm)
f1 (ppm)

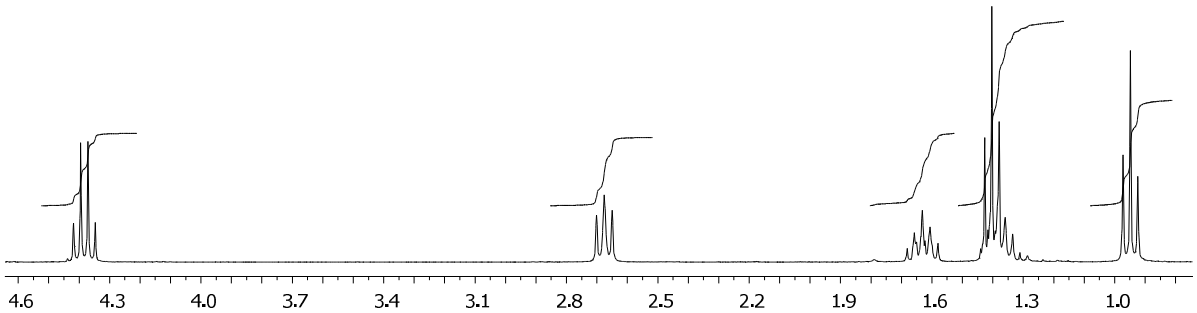

f2 (ppm)
f1 (ppm)

U24

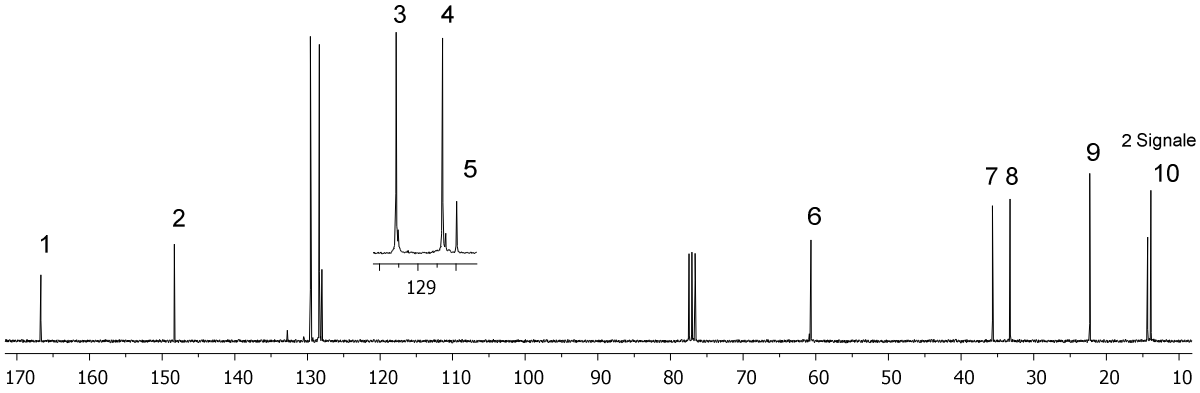
SF: $C_{13}H_{18}O_2$

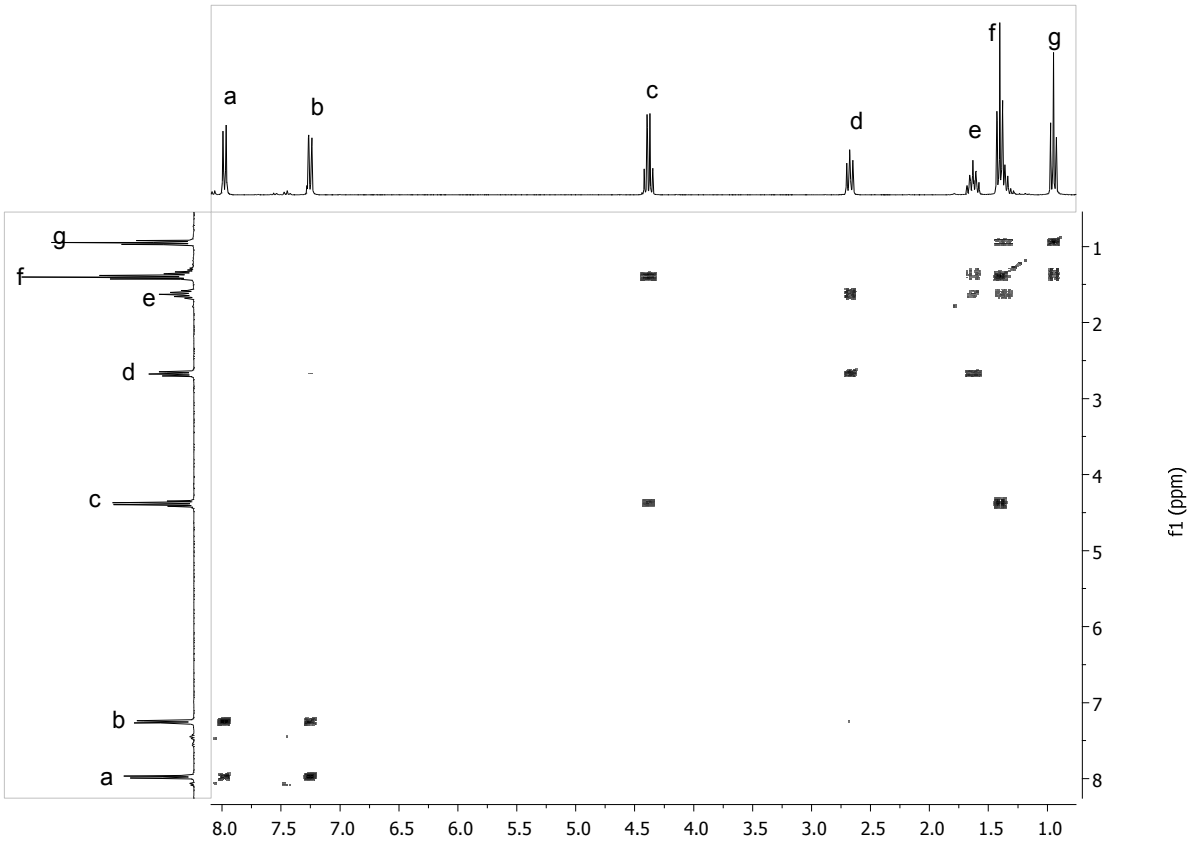
1. Bestimmen Sie die Struktur
2. Erklären Sie das Signal f.

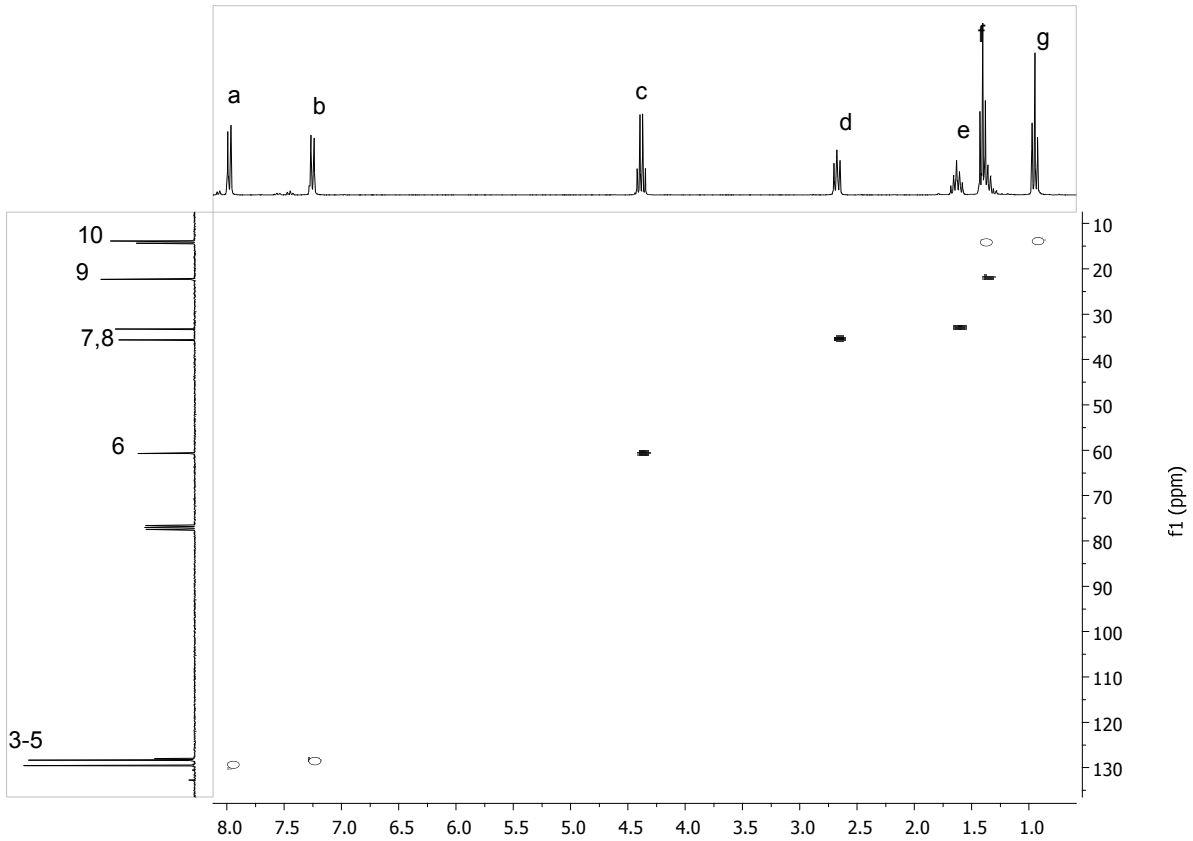




Vergrößerung







HSQC: phasensensitiv

○ → CH oder CH_3

● → CH_2

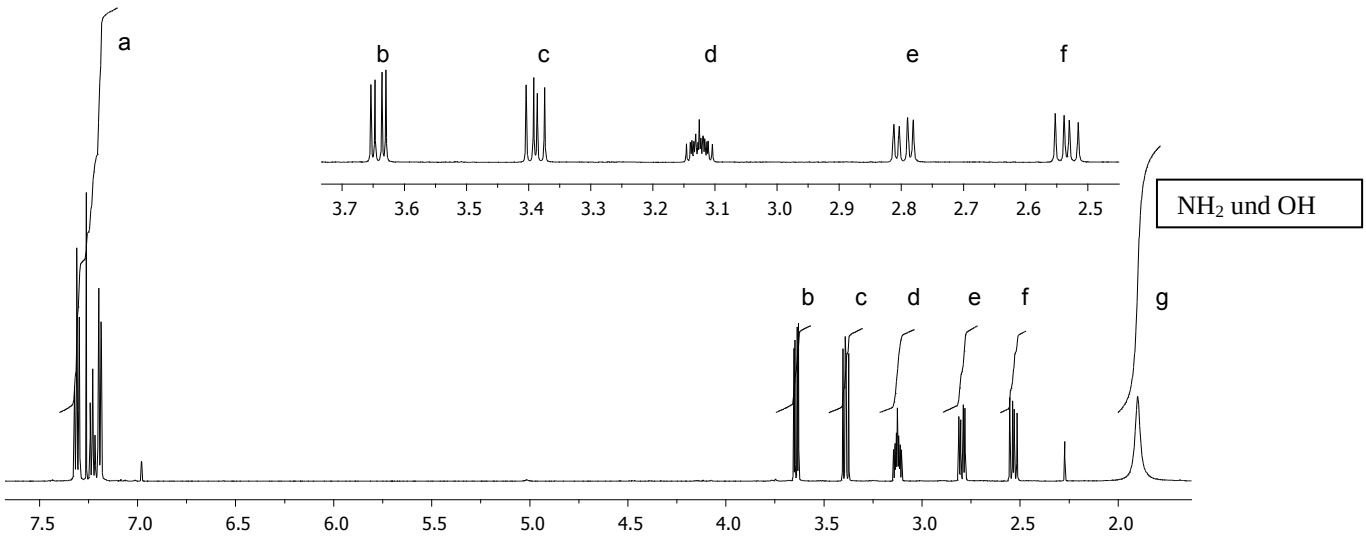
U25 $C_9H_{13}NO$

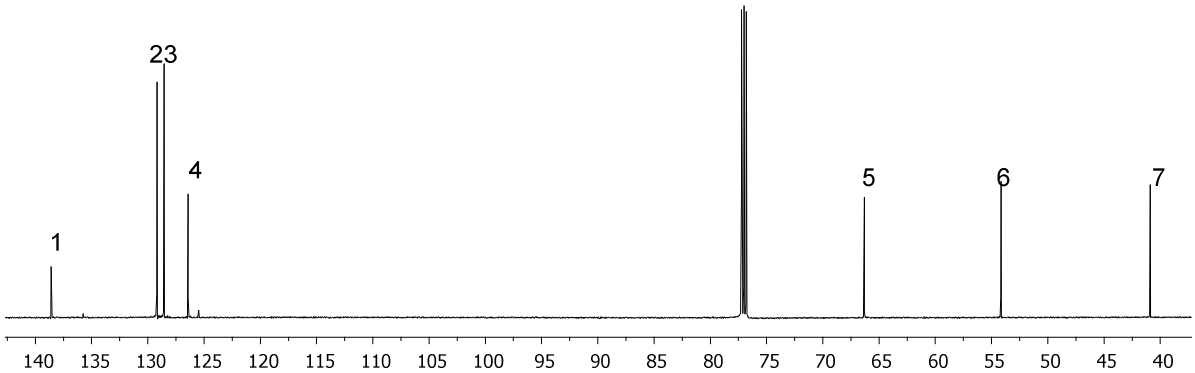
Hinweis: O ist elektronegativer als N !!

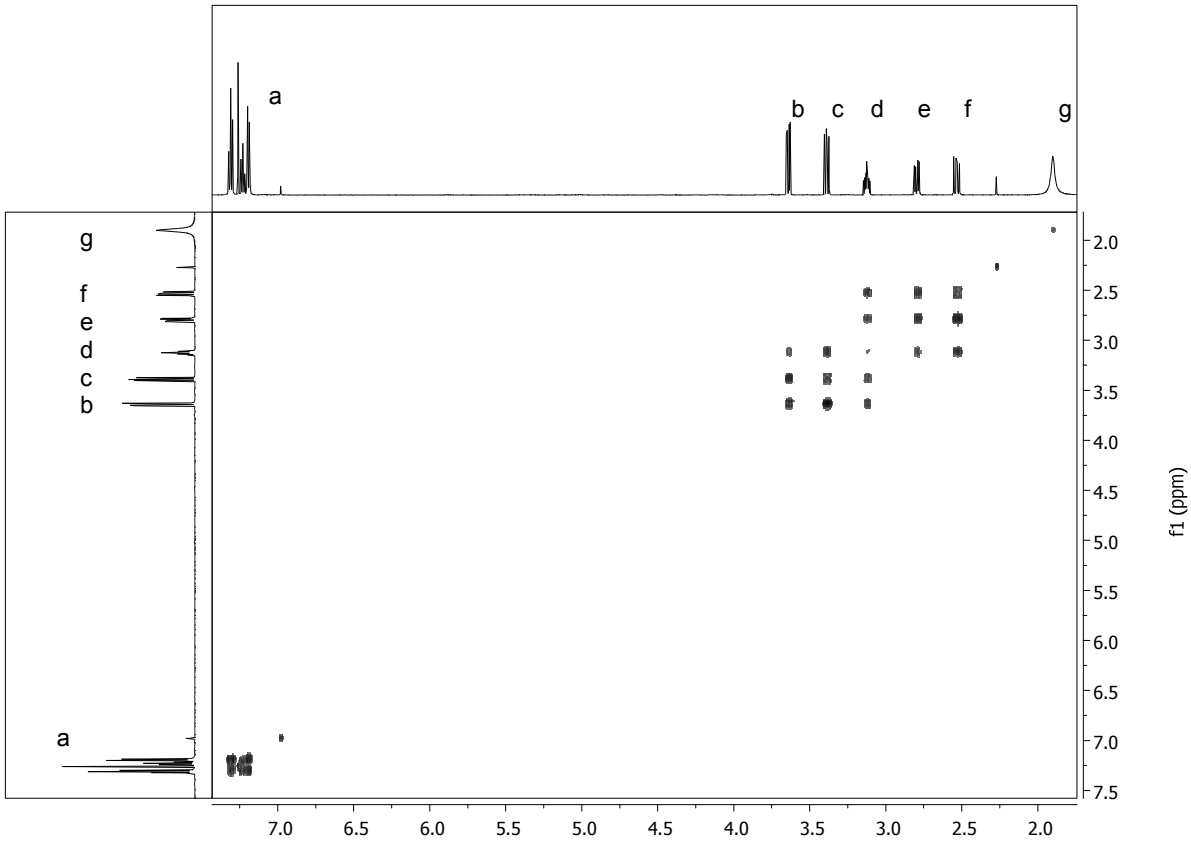
1. Bestimmen Sie die Struktur

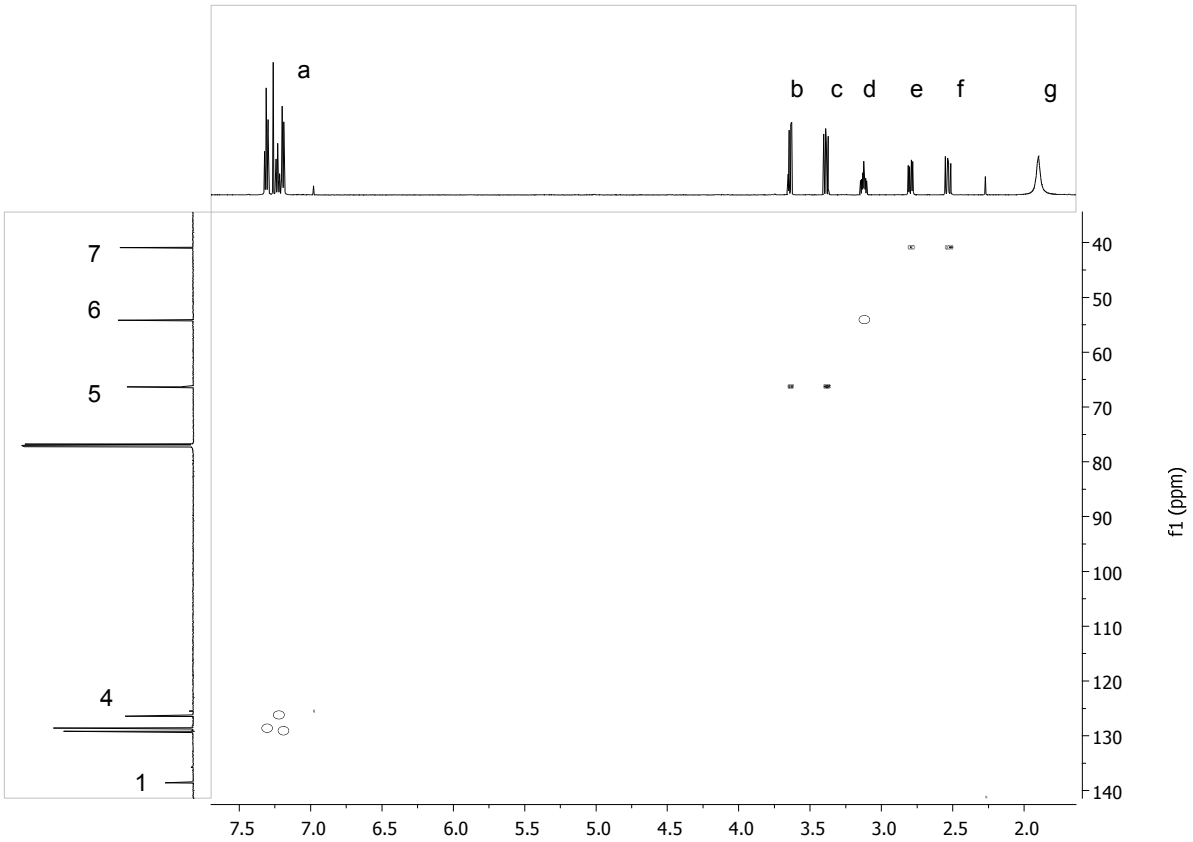
1. Bestimmen Sie das Spinsystem der Protonen.

2. Im HSQC sehen Sie, dass an einem C-Atom 2 verschiedene H-Atome sitzen können.
   a) Welche Eigenschaft haben diese Protonen? Kurze Erklärung.
   b) Wie nennt man diese Protonen auf Grund dieser Eigenschaft?
   c) Welche Auswirkung hat diese Eigenschaft auf das Spinsystem?

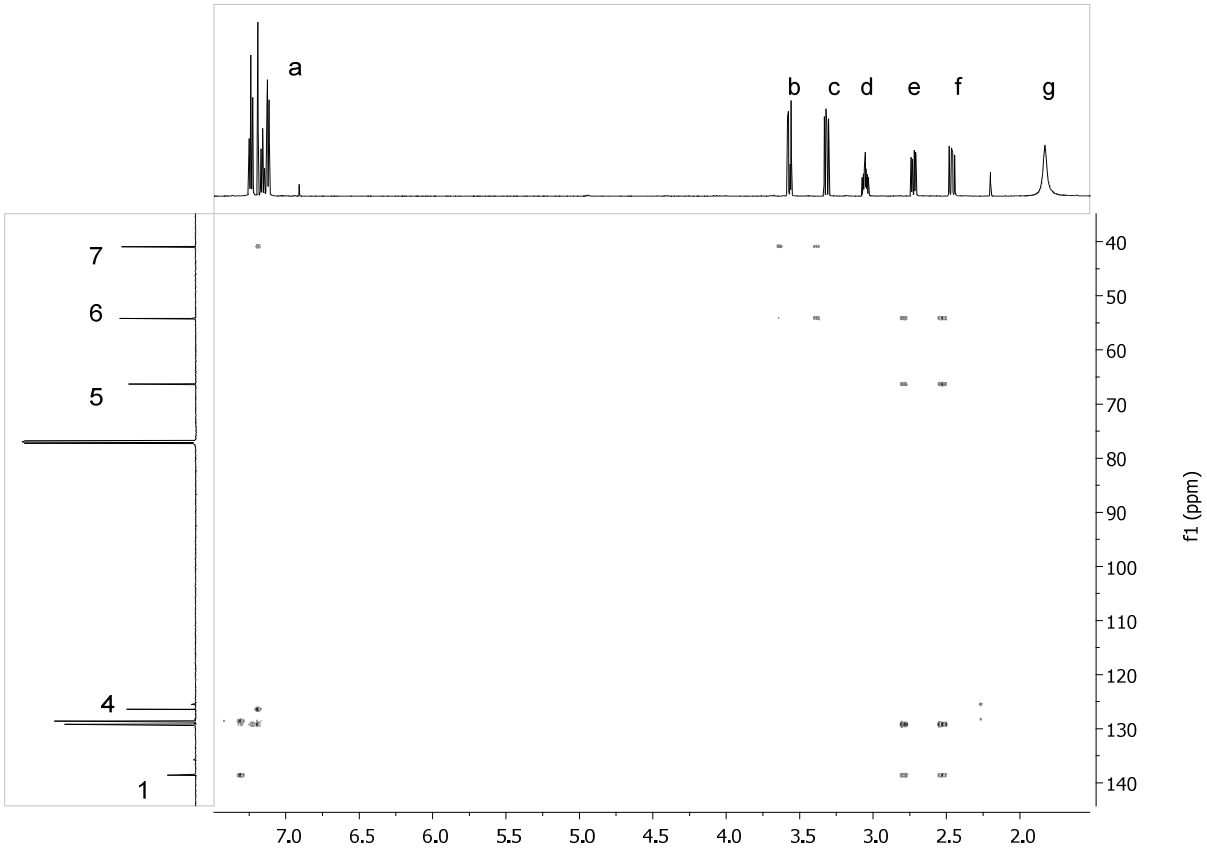

a
b
c
d
e
f
g
NH2 und OH


1
23
4
5
6
7


a
b
c
d
e
f
g
f1 (ppm)

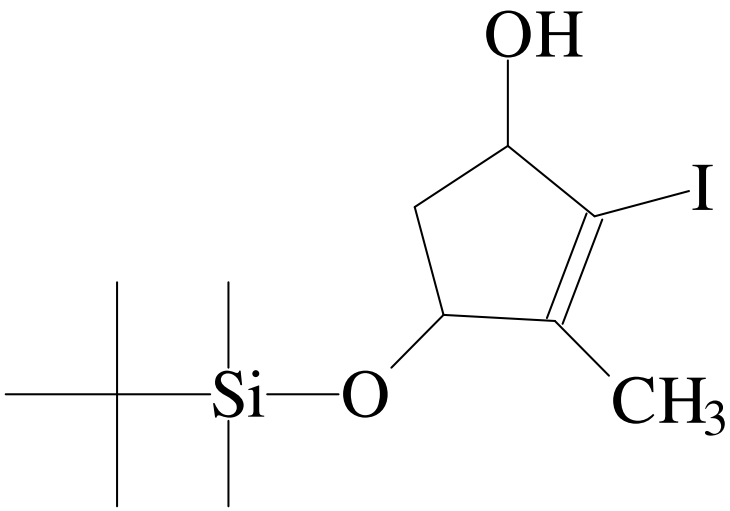


HSQC: $^{1}J_{CH}$ phasensensitiv ○ → CH oder CH_3
● → CH_2

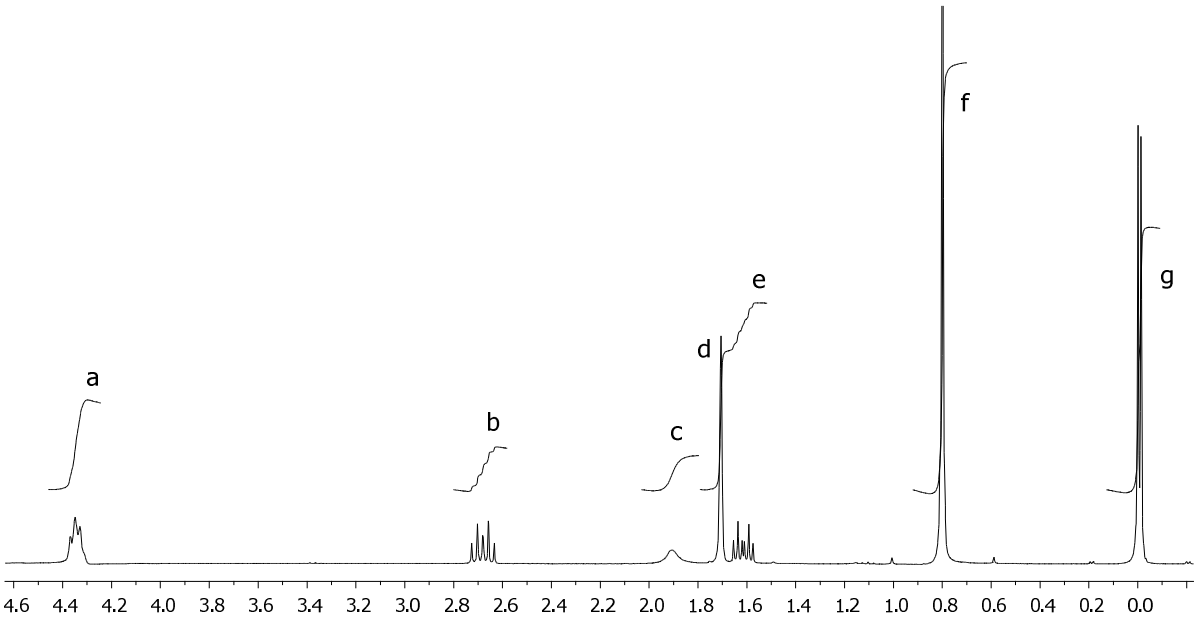


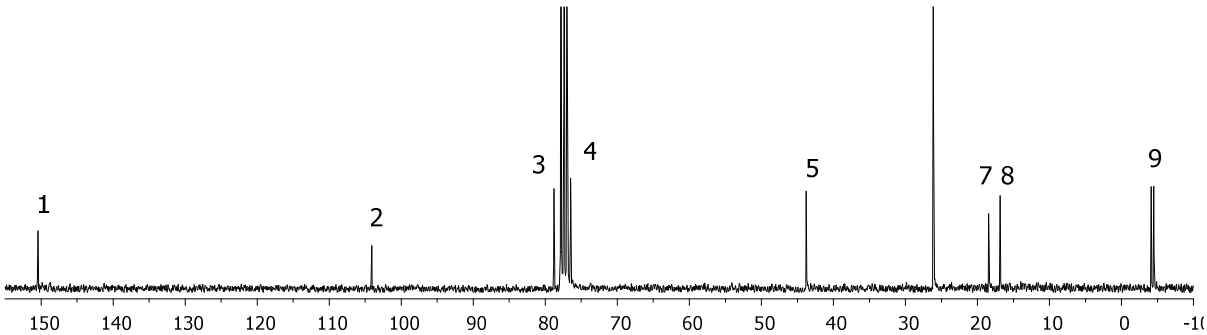
HMBC $^{3}J_{CH}$ und $^{2}J_{CH}$

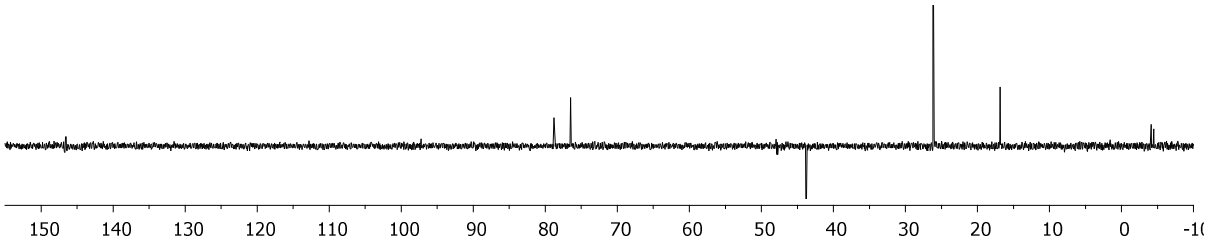
U26

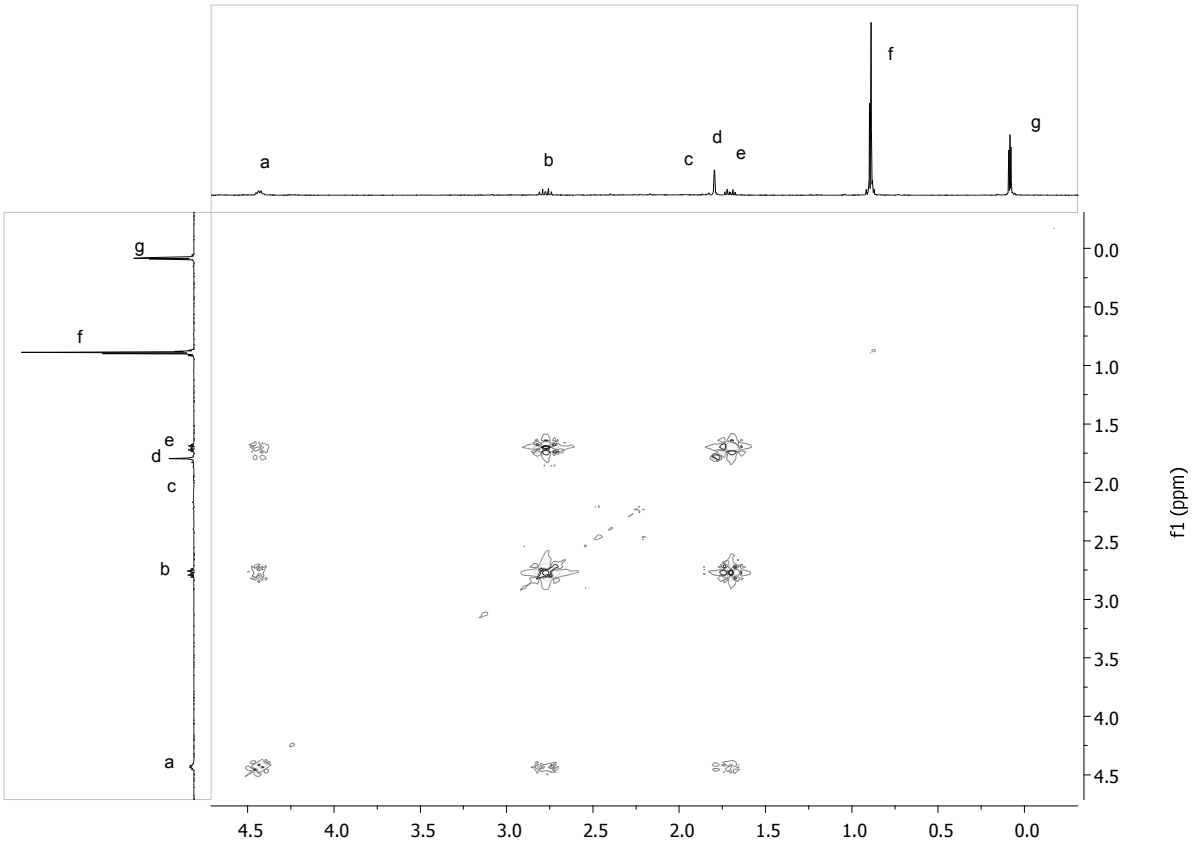


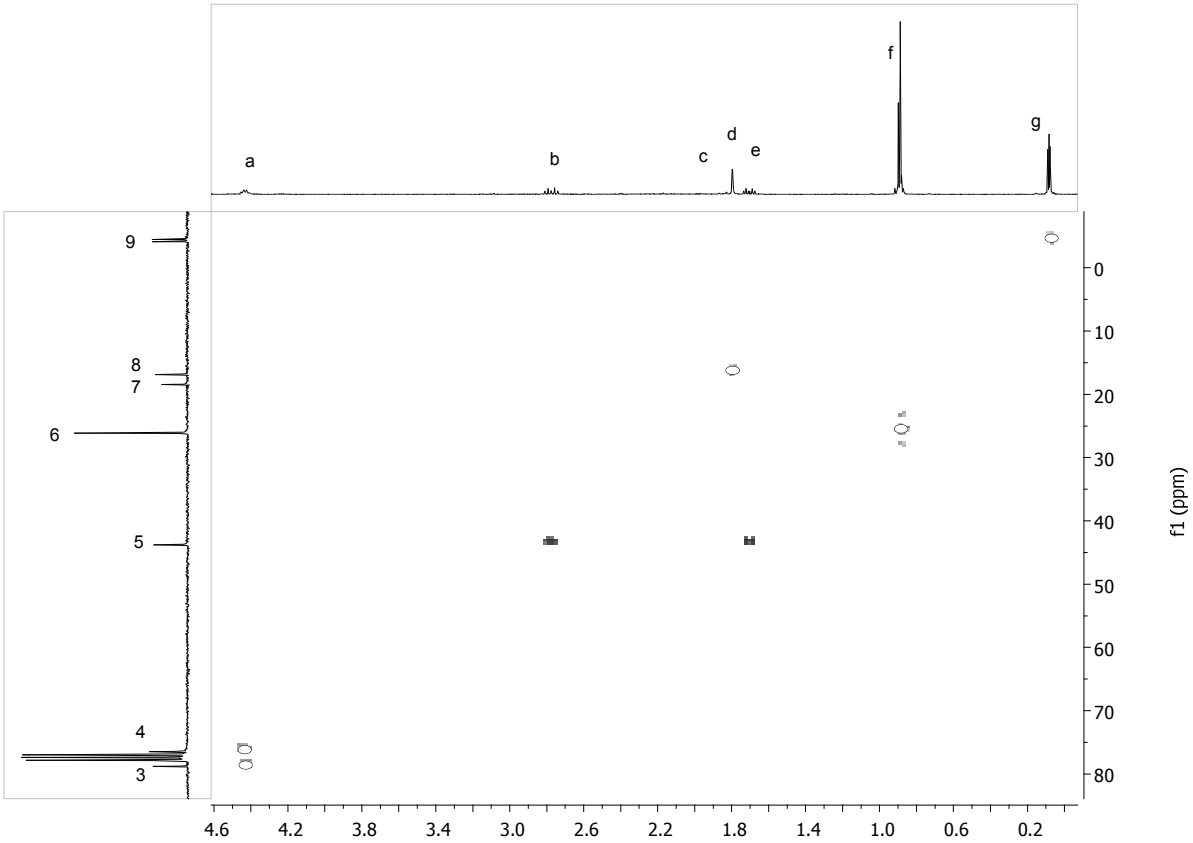
1. Ordnen Sie alle Signale soweit möglich zu.
2. Warum ist das 13C-Signal bei ca. -5 ppm ein Dublett? (Zwei Signale)
3. Zeichnen Sie einen Splittingschlüssel für die 4 Protonen am Ring (nicht für OH)
4. Geben Sie das Spinsystem an. Beachten Sie Punkt 2!


a
b
c
d
e
f
g
4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0 0.8 0.6 0.4 0.2 0.0

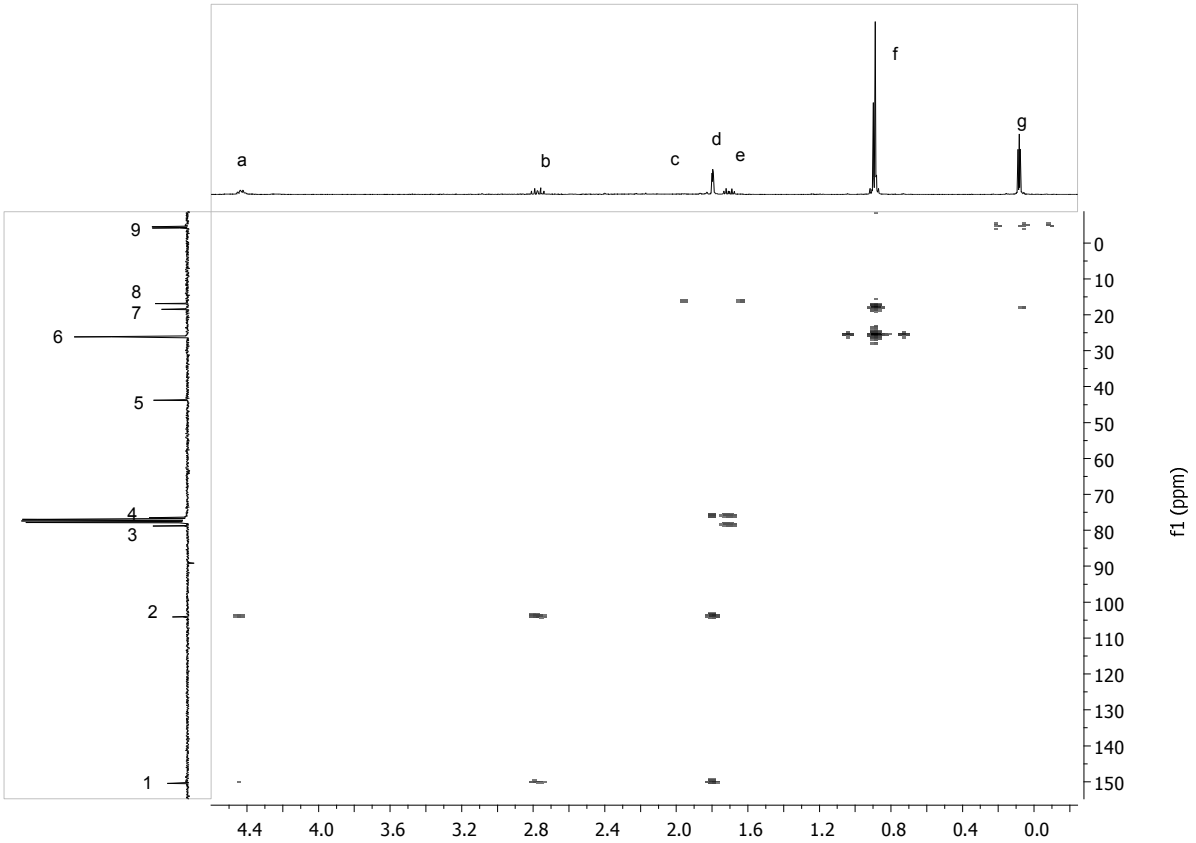

1
2
3
4
5
7 8
9
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10


150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

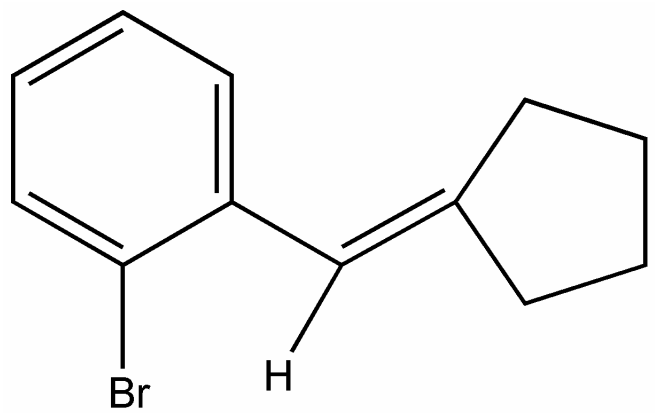

a
b
c
d
e
f
g
f1 (ppm)


a
b
c
d
e
f
g
3
4
5
6
7
8
9
f1 (ppm)

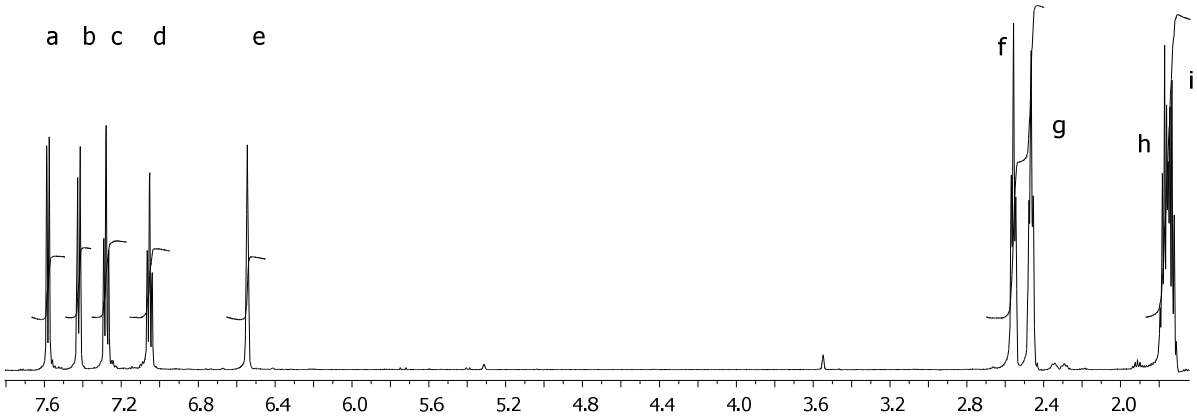
HMBC: vorwiegend $^{3}J_{CH}$-Kopplungen. (d. h. zwischen C und H liegen 3 Bindungen)
gelegentlich $^{2}J_{CH}$-Kopplungen

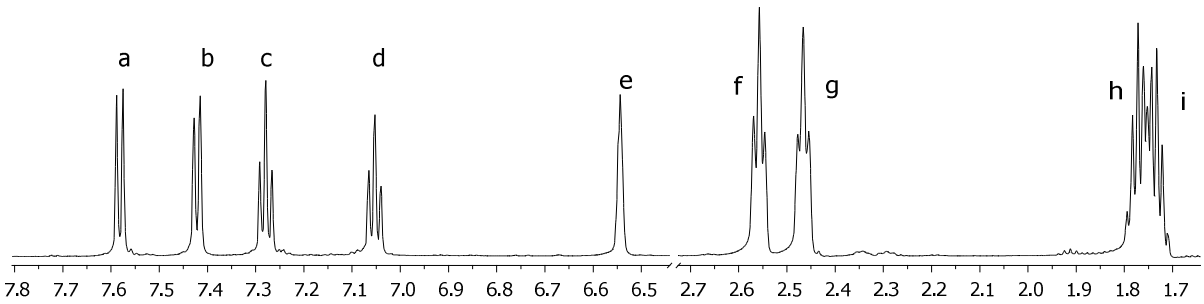


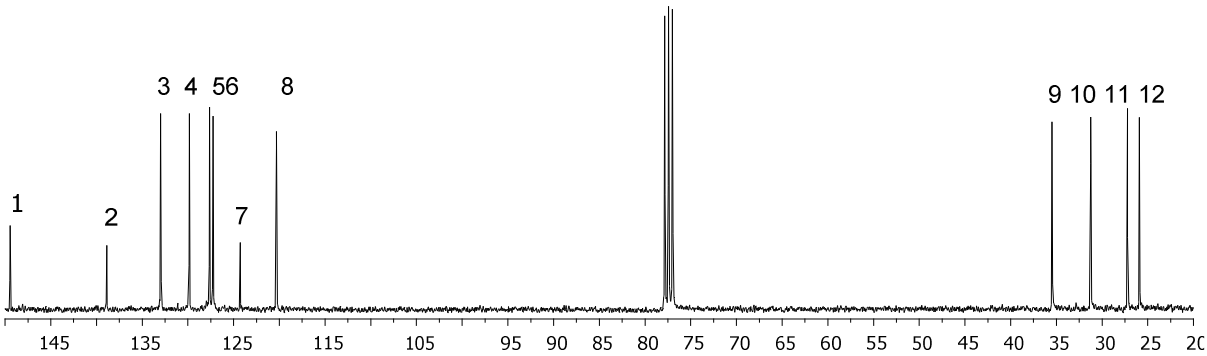
U27

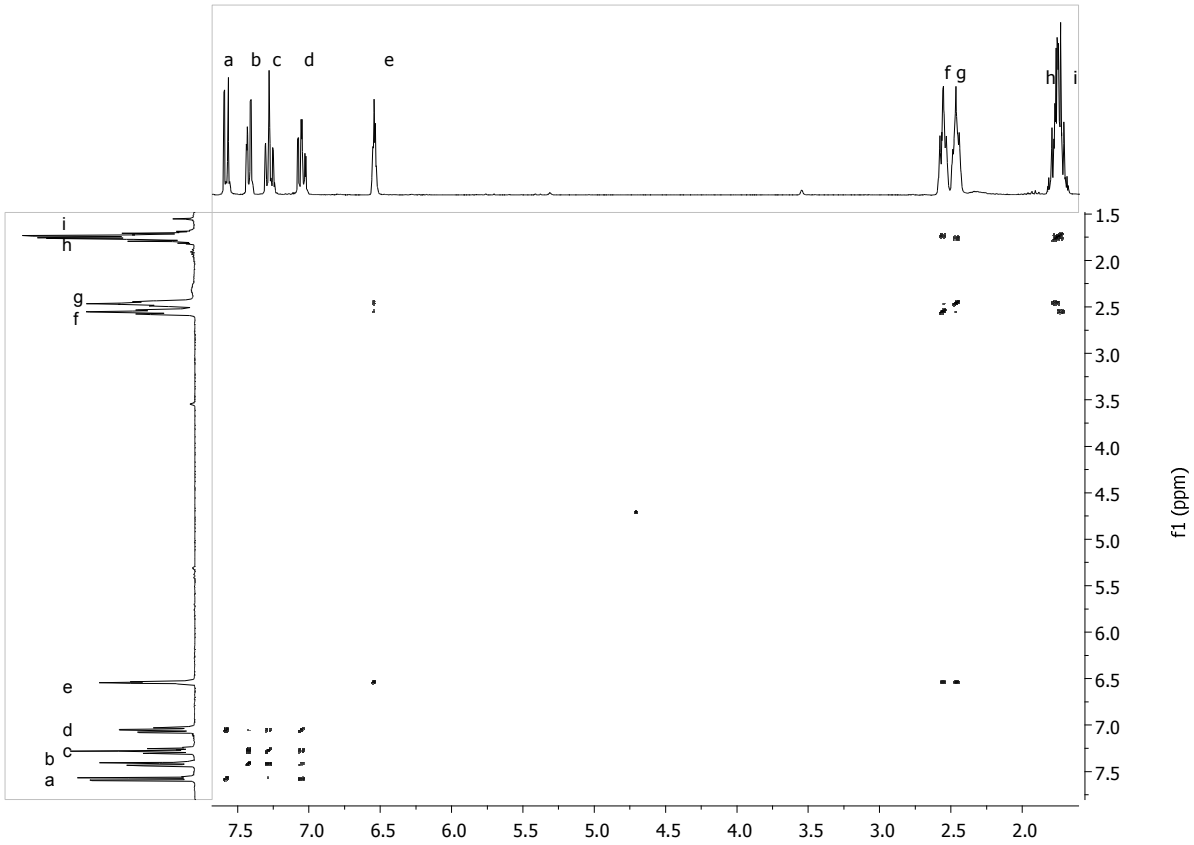


1. Ordnen Sie die Signale aus dem ^{1}H und ^{13}C -Spektrum obiger Strukturformel zu.

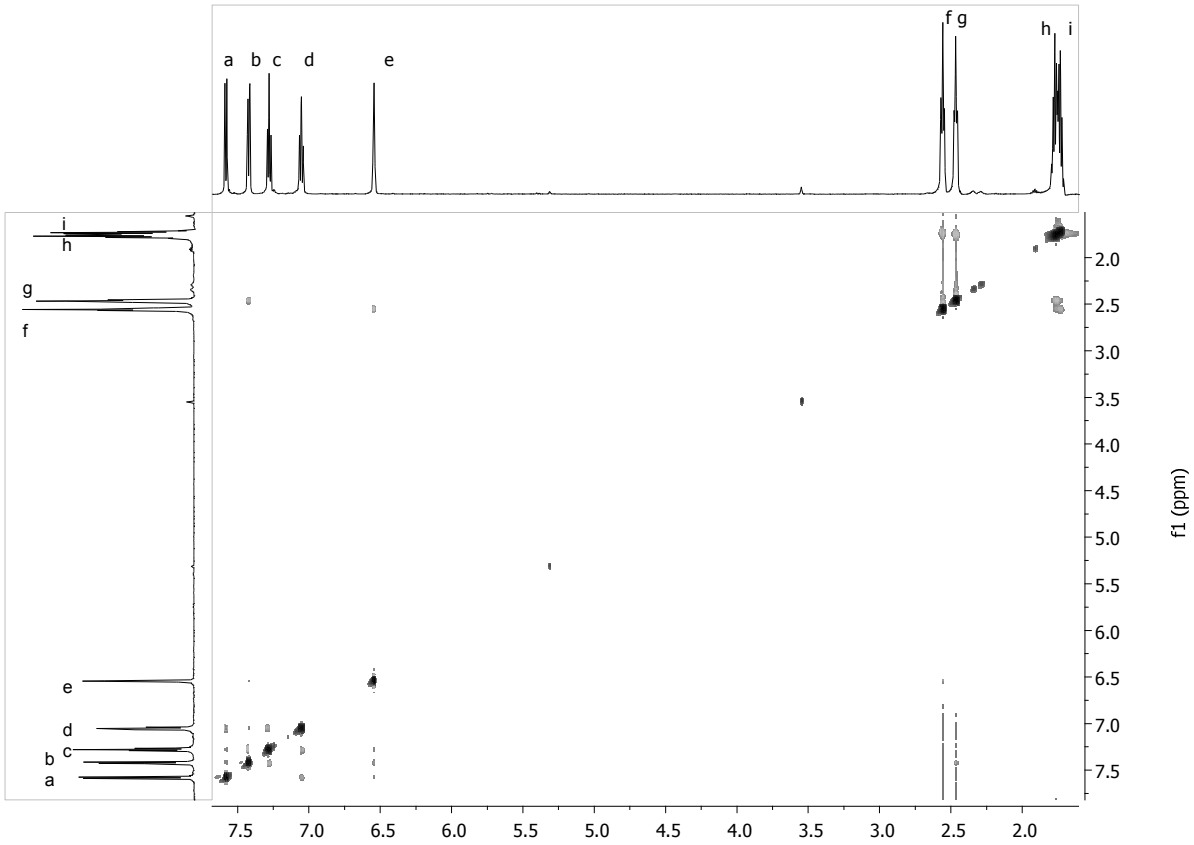

a b c d e
f
g
h
i
7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0


a b c d e f g h i
7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 2.7 2.6 2.5 2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7

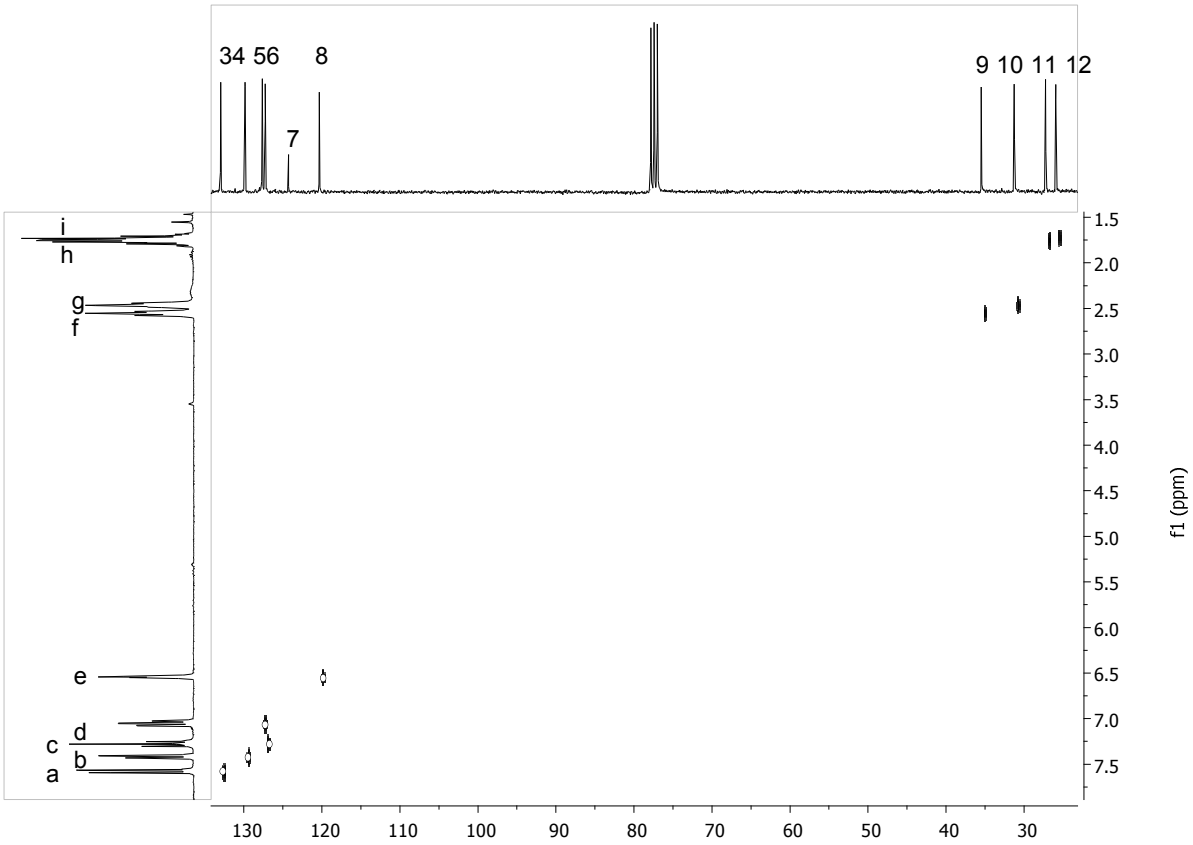

1 2 3 4 56 7 8 9 10 11 12
145 135 125 115 105 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20

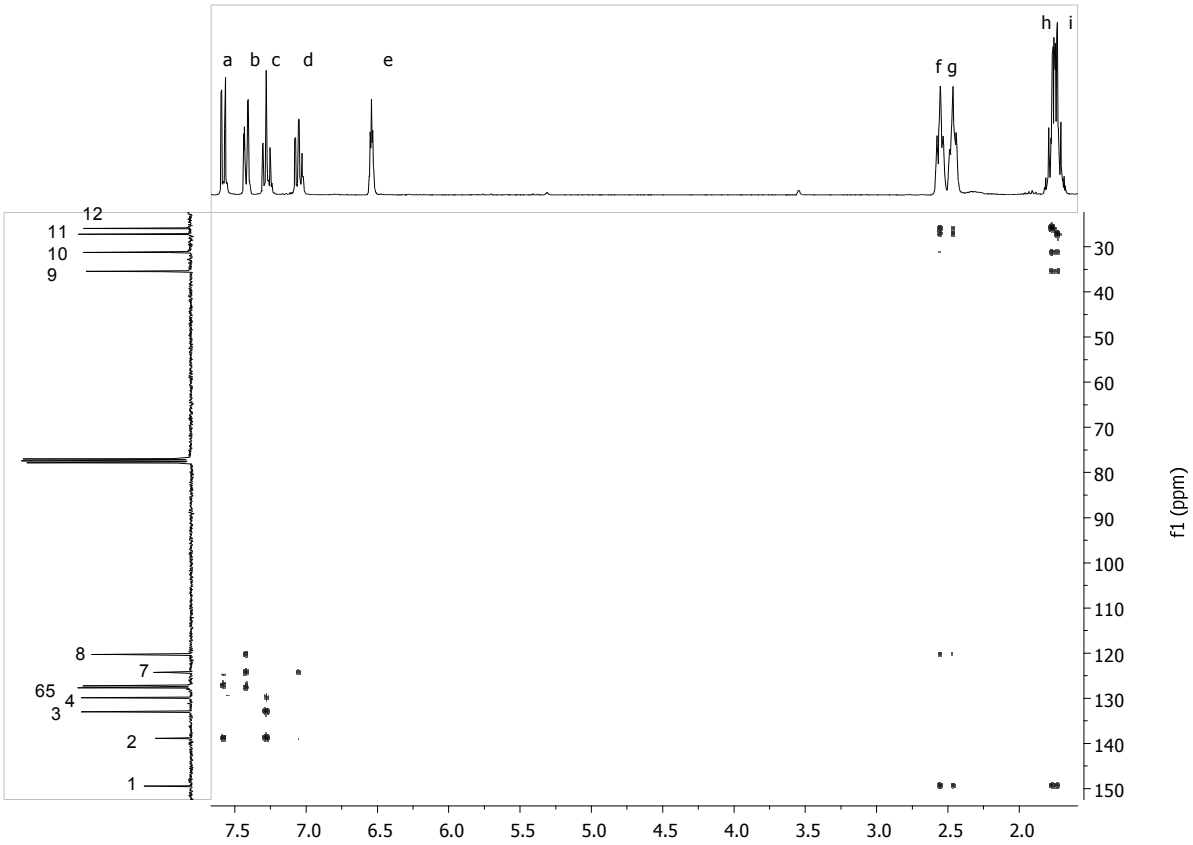


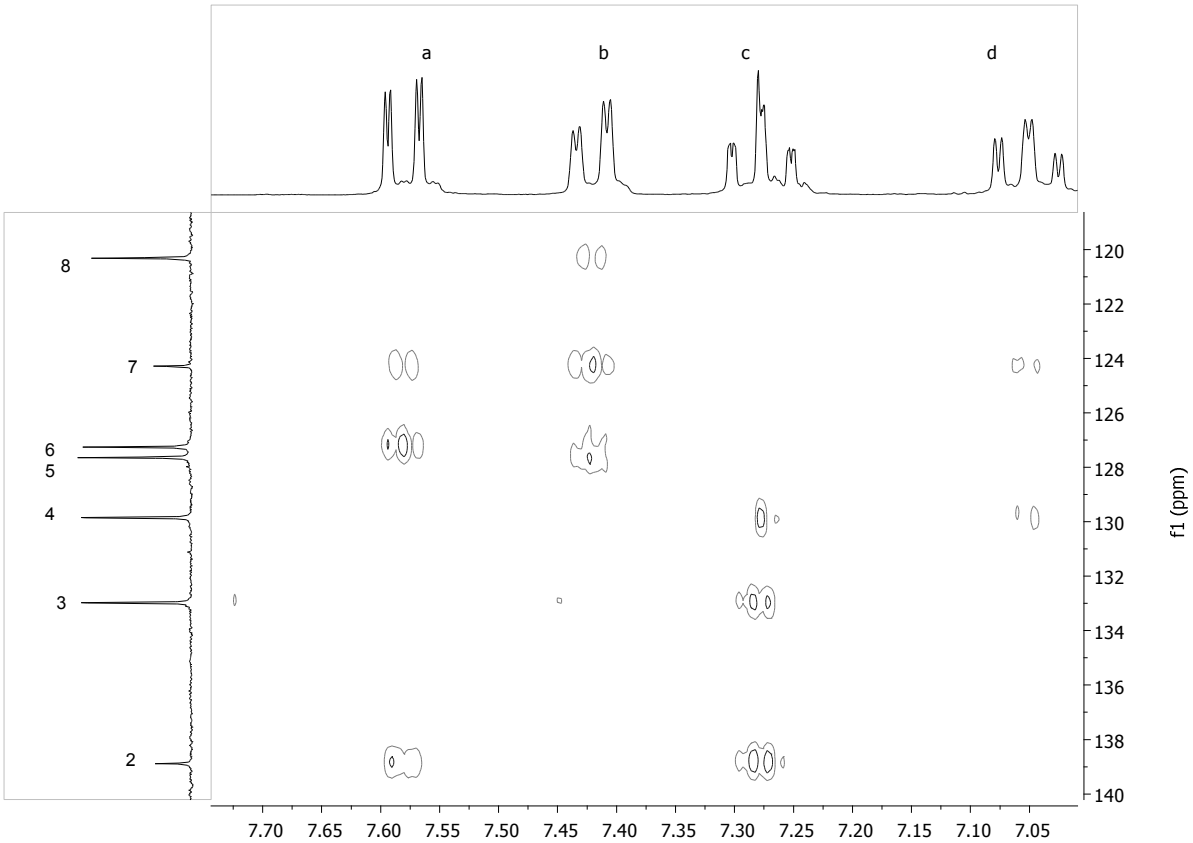
cosy



noesy


34 56
8
7
9 10 11 12
i
h
g
f
e
d
c
b
a
f1 (ppm)


a b c d
e
f g
h i
12
11
10
9
8
7
65
4
3
2
1
f1 (ppm)



Vergrößerung des HMBCs

2. Geben Sie alle im obigen Spektrum (Vergrößerung des HMBCs) sichtbaren Kopplungen in folgender Tabelle an und bestimmen Sie deren Art (^{1}J, ^{2}J, ^{3}J, ^{4}J usw.) (3 P)

^{13}C	^{1}H	Kopp.
8	b	^{3}J

U 28 $C_{13}H_{18}O_2$

1. Welche Fragmente finden Sie auf Grund der Spektren? (3 P)

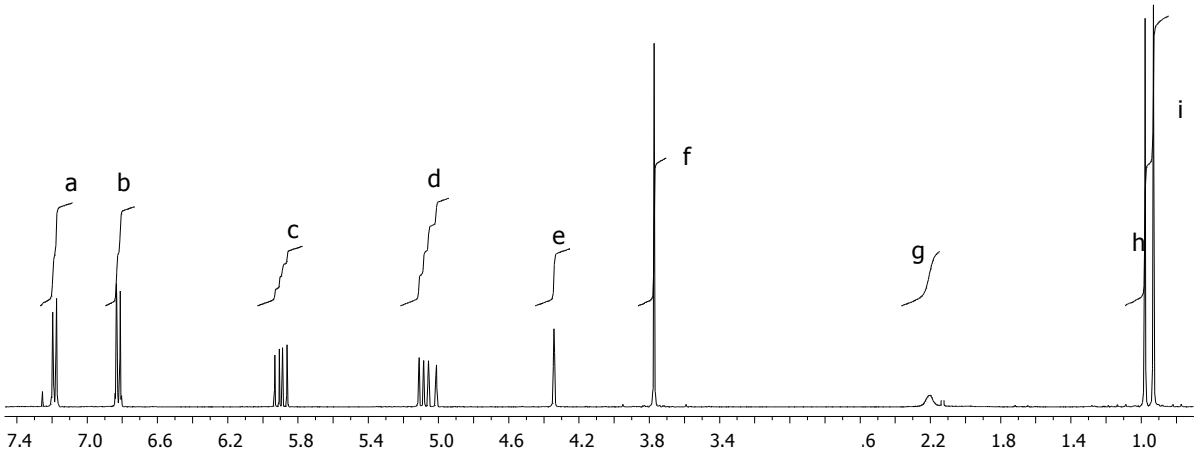
2. Ordnen Sie die Signale so gut wie möglich zu, um Frage 3 beantworten zu können.
3. Geben Sie eine sinnvolle Struktur an. (2 P)

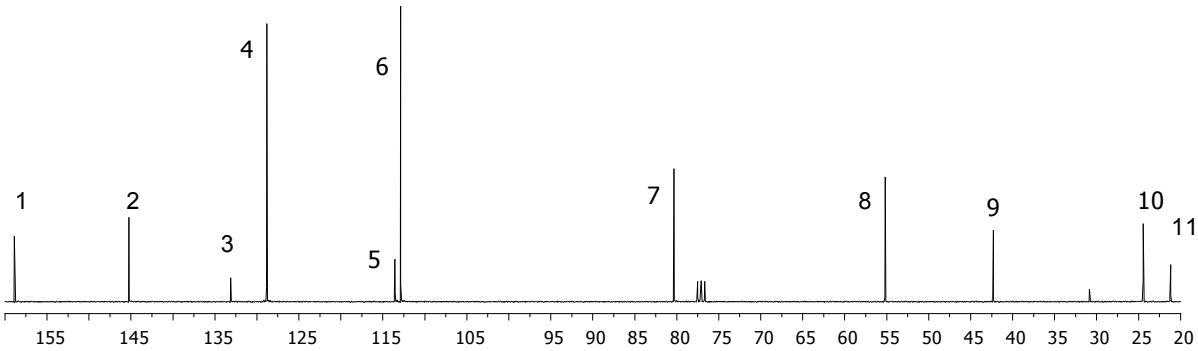
4. Ordnen Sie alle Signale zu (^{1}H und ^{13}C). (4 P)

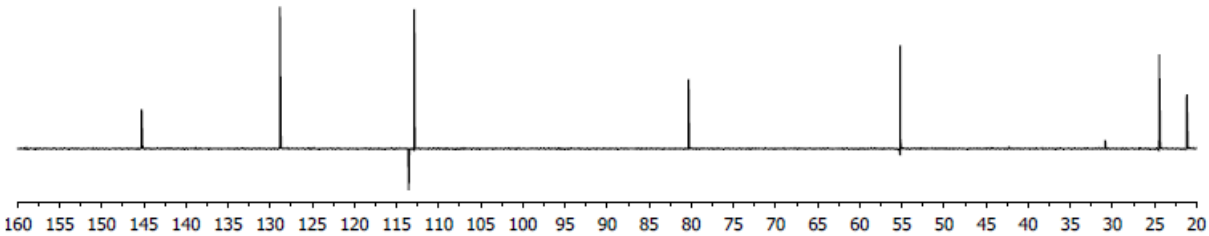
5. Zeichnen Sie die im HMBC sichtbare Kopplung der C-Atome 1, 2, 3, 4, 5 und 6 in Ihr gefundenes Molekül ein. Verwenden Sie Farbstifte (nicht rot!). Füllen Sie nachfolgende Tabelle aus.(4 P)

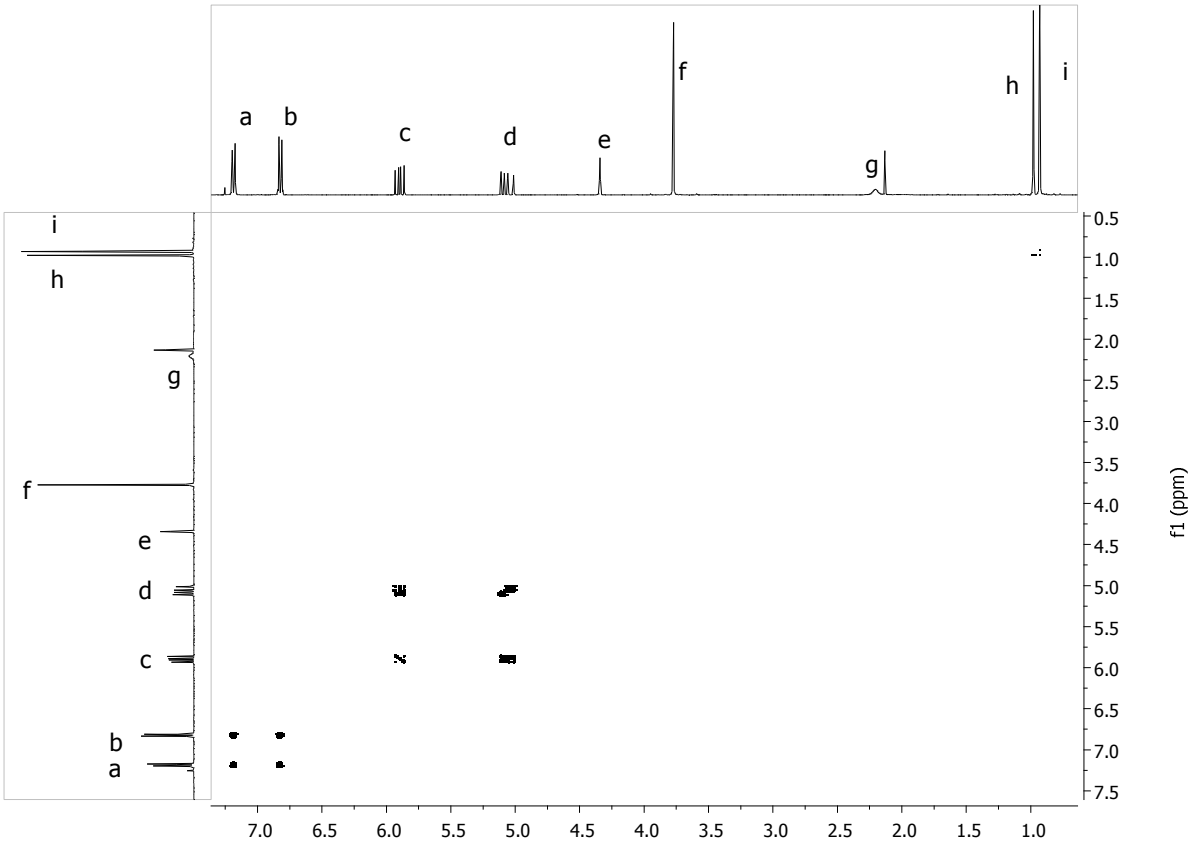
C-Atom	H-Atom	Kopplung
1	f	$^{3}J_{CH}$

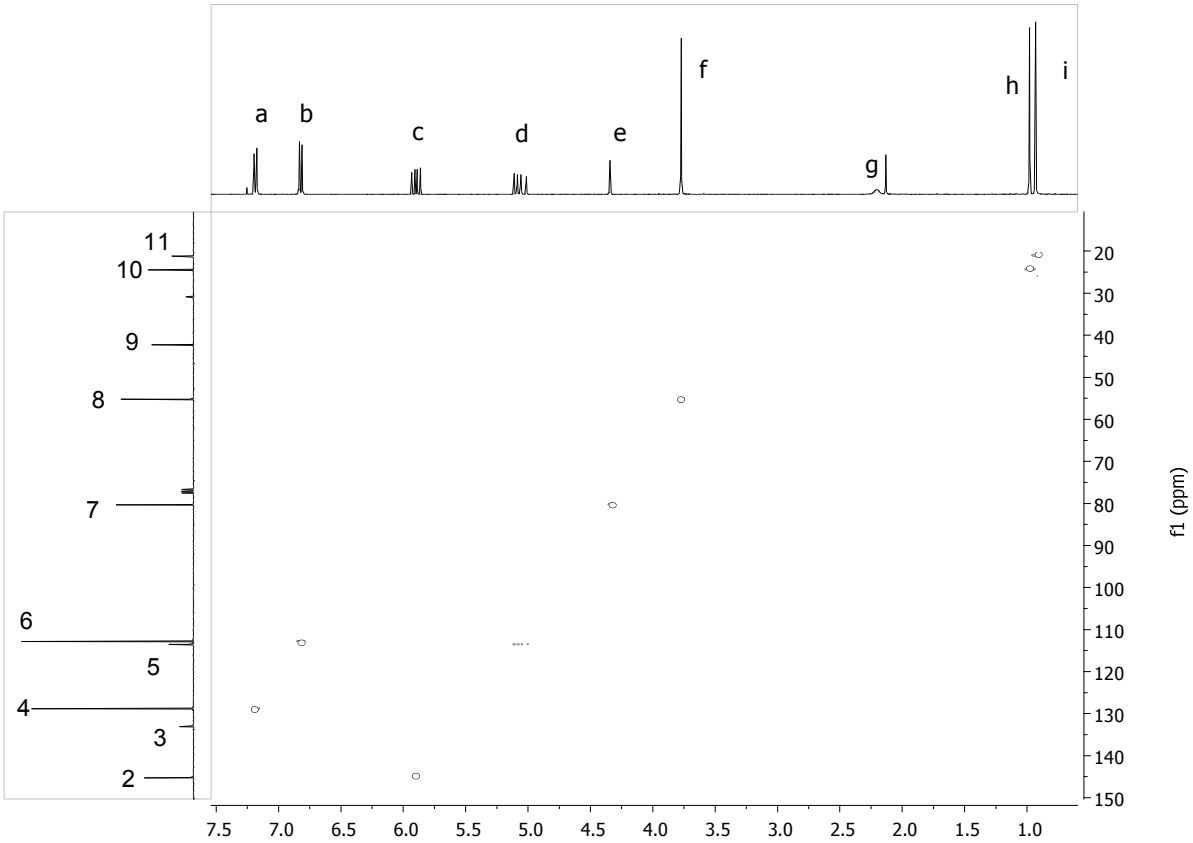
usw.

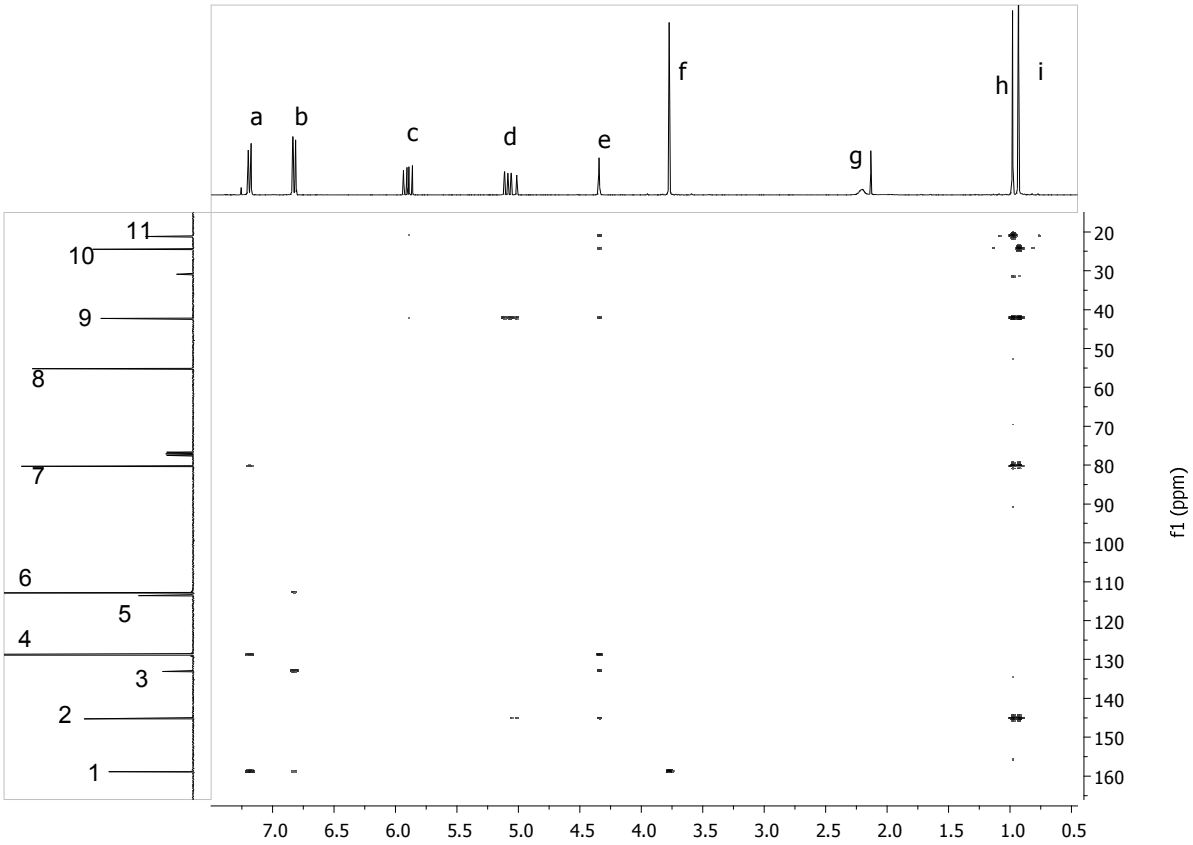

a
b
c
d
e
f
g
h
i
7.4 7.0 6.6 6.2 5.8 5.4 5.0 4.6 4.2 3.8 3.4 .6 2.2 1.8 1.4 1.0


1
2
3
4
5
6
7
8
9
10
11
155 145 135 125 115 105 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20


160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20


a
b
c
d
e
f
g
h
i
f1 (ppm)


a
b
c
d
e
f
g
h
i
11
10
9
8
7
6
5
4
3
2
f1 (ppm)


a
b
c
d
e
f
g
h
i
11
10
9
8
7
6
5
4
3
2
1
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
f1 (ppm)
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5

U 29 $C_{15}H_{22}O_3$.

1. Welche Fragmente finden Sie auf Grund der Spektren?
   Hilfestellungen:
   Schauen Sie im COSY, welche Protonen miteinander koppeln.
   Schauen Sie im HSQC, welche Protonen zu welchen Cs gehören.
   Welche C-Atome gehören zum Aromaten. Warum ist eines dieser C-Atome so stark Hochfeld-verschoben? (siehe Inkrementtabelle)

2. Ordnen Sie die Signale so gut wie möglich zu, um Frage 3 beantworten zu können.

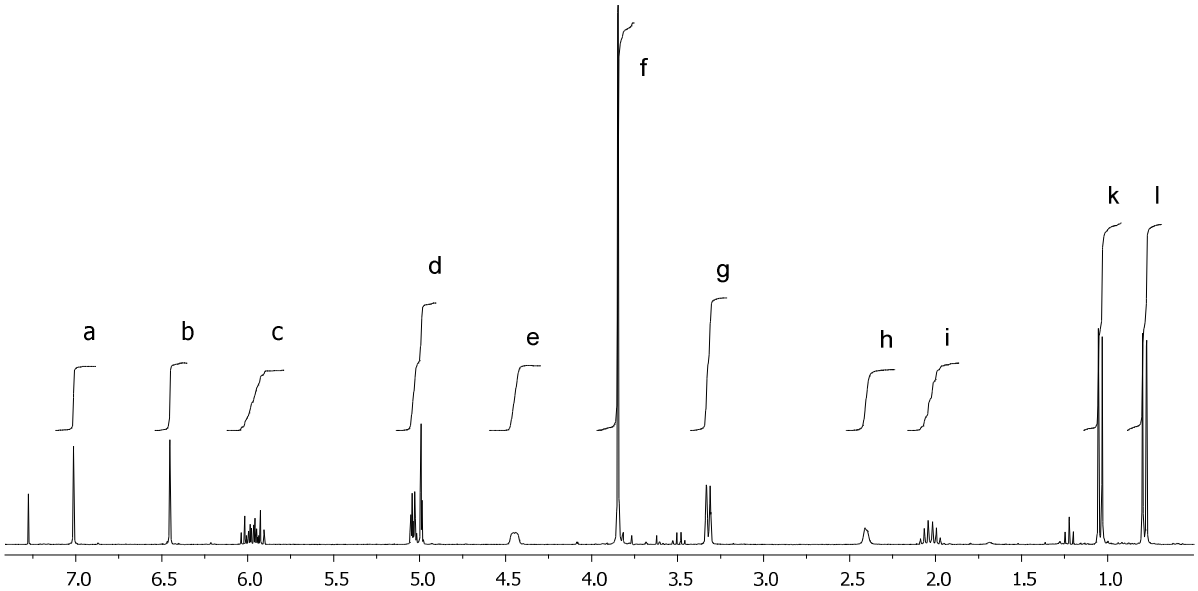
3. Geben Sie eine sinnvolle Struktur an.

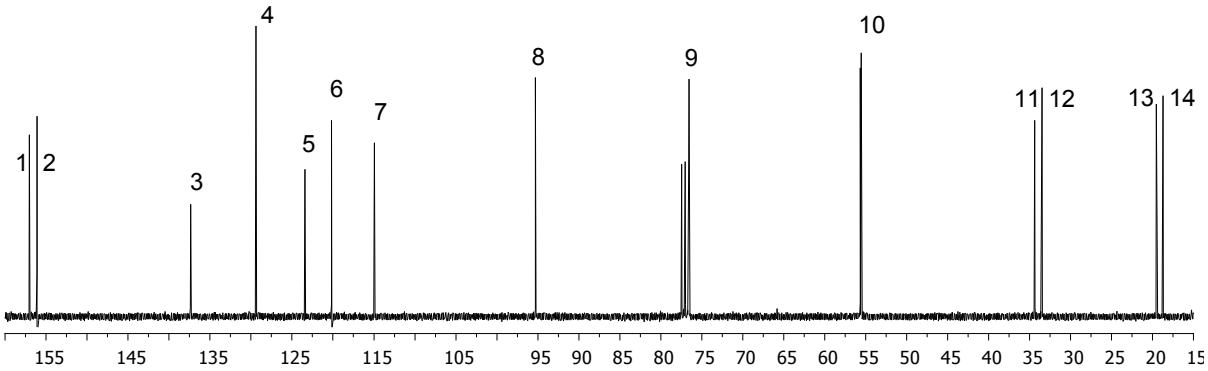
4. Ordnen Sie alle Signale zu.

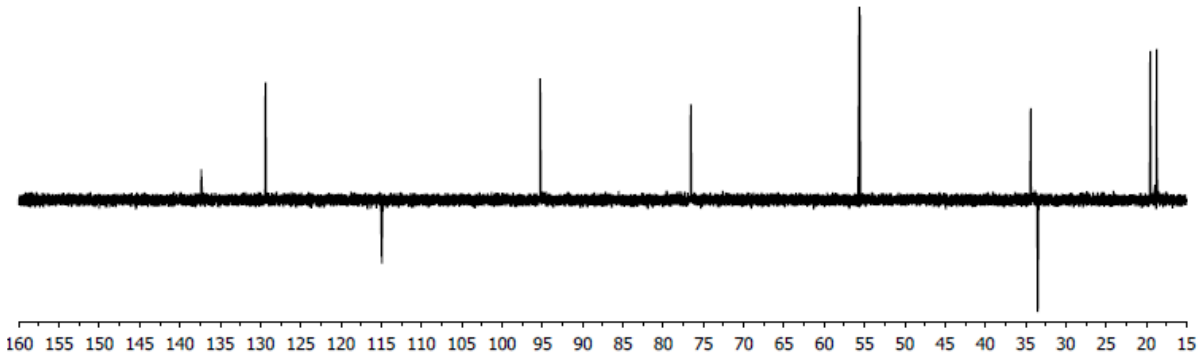
5. Zeichnen Sie die im HMBC sichtbare Kopplung der C-Atome 1, 2, 5und 6 in Ihr gefundenes Molekül ein. Verwenden Sie Farbstifte. Füllen Sie nachstehende Tabelle aus.

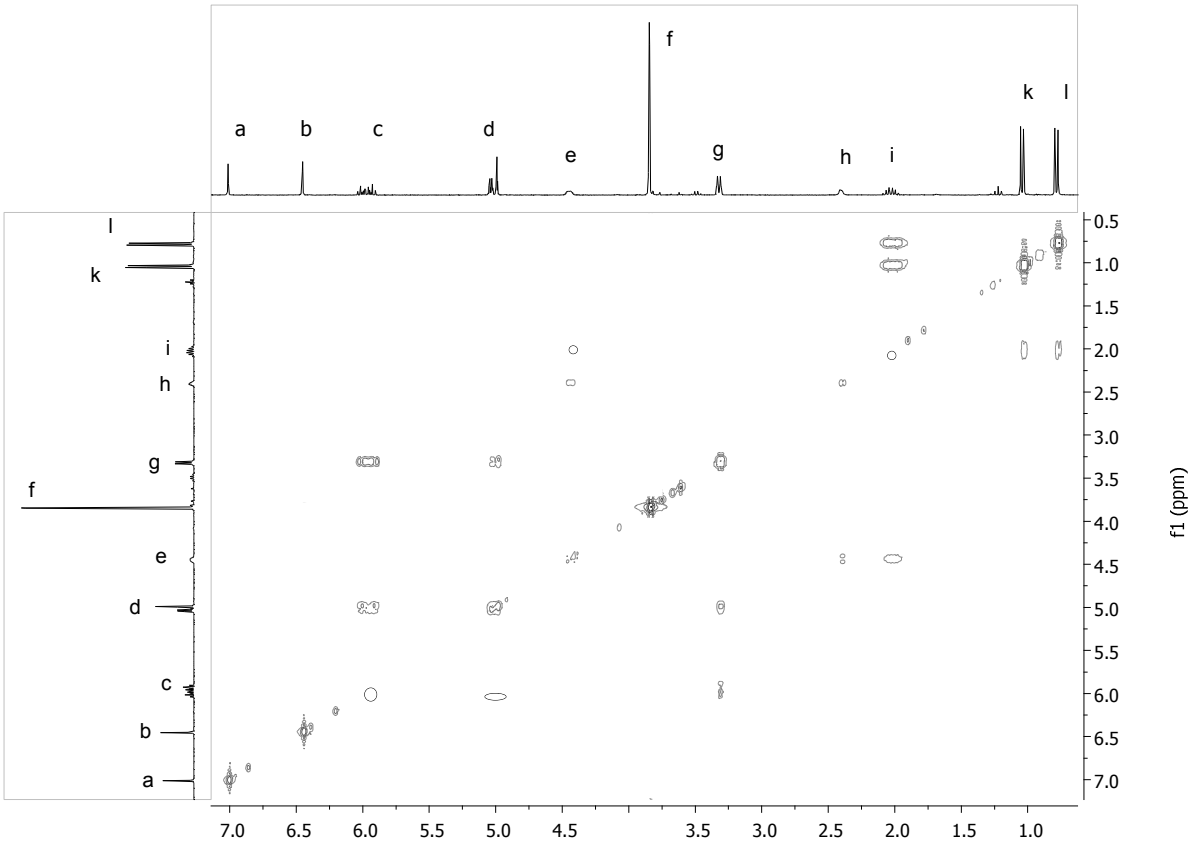
13C	**1H**	**J(C,H)**
1		**3 J**

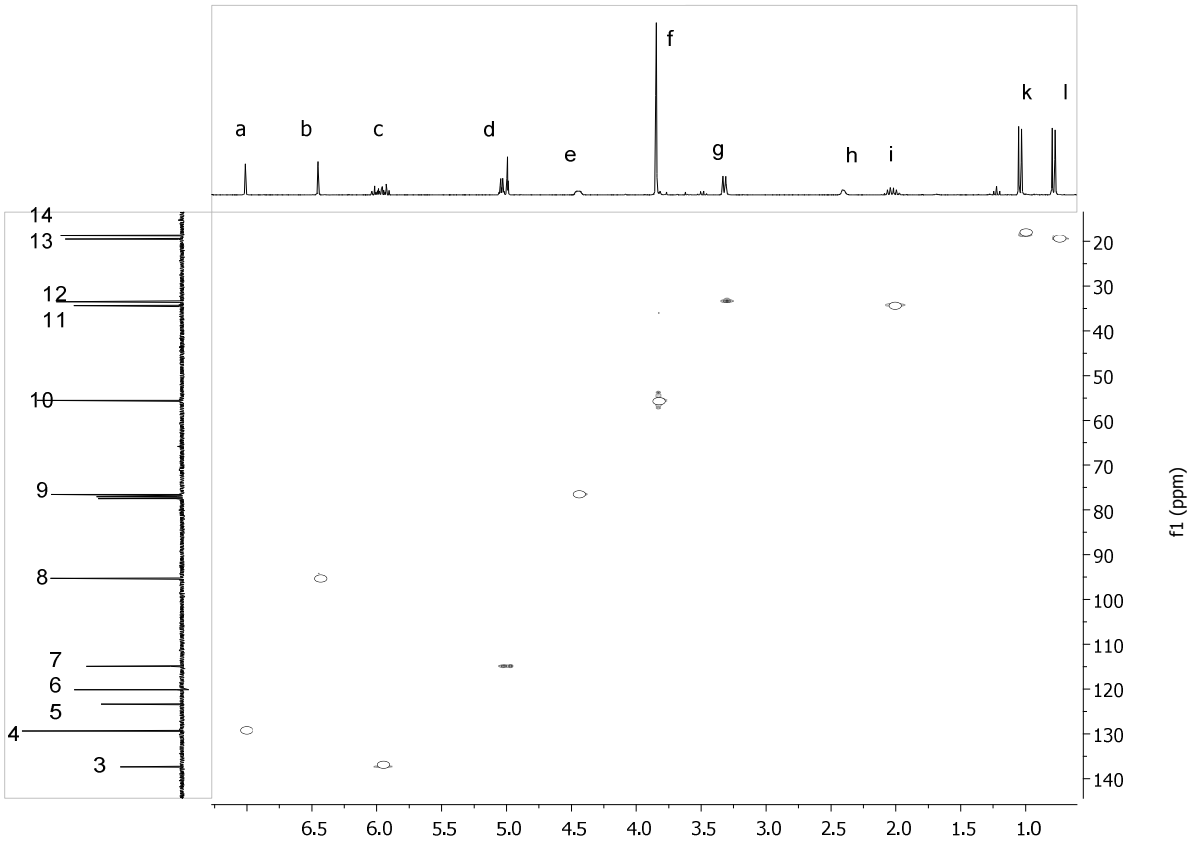
usw.

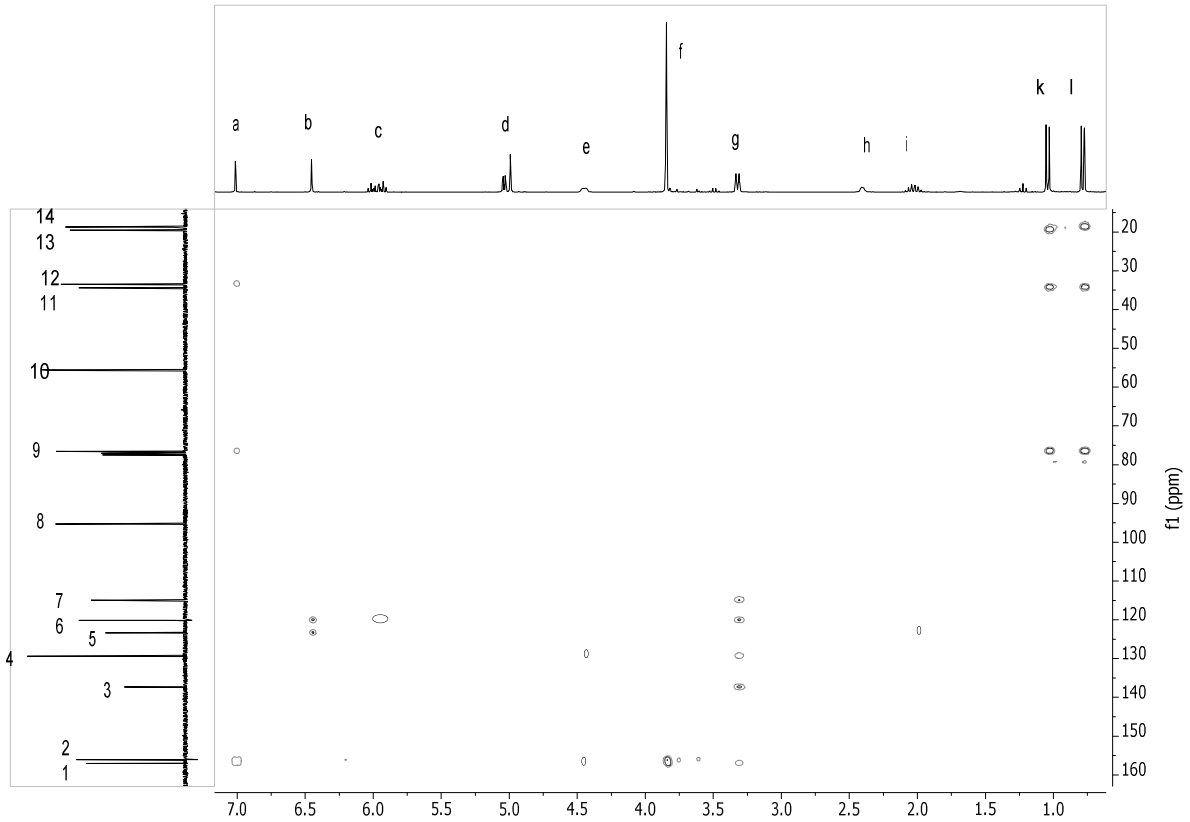

a
b
c
d
e
f
g
h
i
k
l
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0

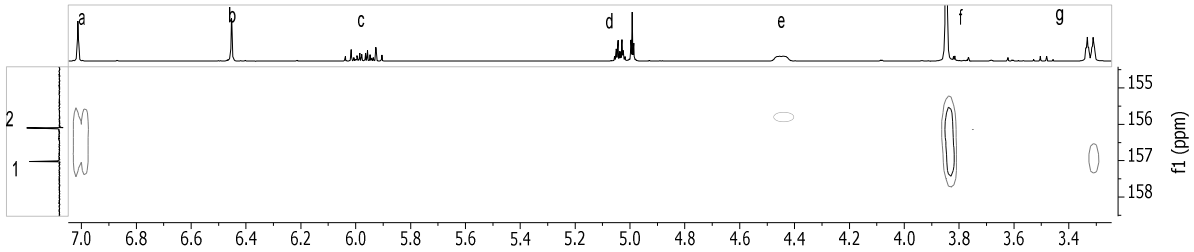

1
2
3
4
5
6
7
8
9
10
11
12
13
14
155
145
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15


160
155
150
145
140
135
130
125
120
115
110
105
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15

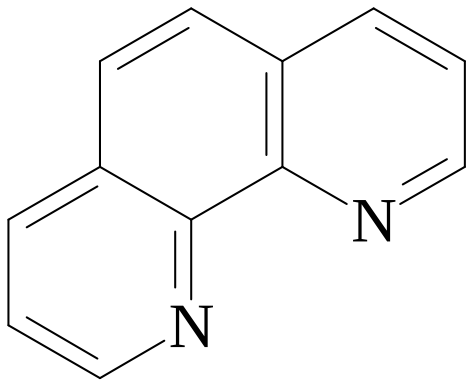

a
b
c
d
e
f
g
h
i
k
l
f1 (ppm)
7.0
6.5
6.0
5.5
5.0
4.5
3.5
3.0
2.5
2.0
1.5
1.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0
6.5
7.0


a
b
c
d
e
f
g
h
i
k
l
14
13
12
11
10
9
8
7
6
5
4
3
f1 (ppm)
20
30
40
50
60
70
80
90
100
110
120
130
140
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0


a
b
c
d
e
f
g
h
i
k
l
14
13
12
11
10
9
8
7
6
5
4
3
2
1
f1 (ppm)
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0


a
b
c
d
e
f
g
2
1
f1 (ppm)
7.0
6.8
6.6
6.4
6.2
6.0
5.8
5.6
5.4
5.2
5.0
4.8
4.6
4.4
4.2
4.0
3.8
3.6
3.4

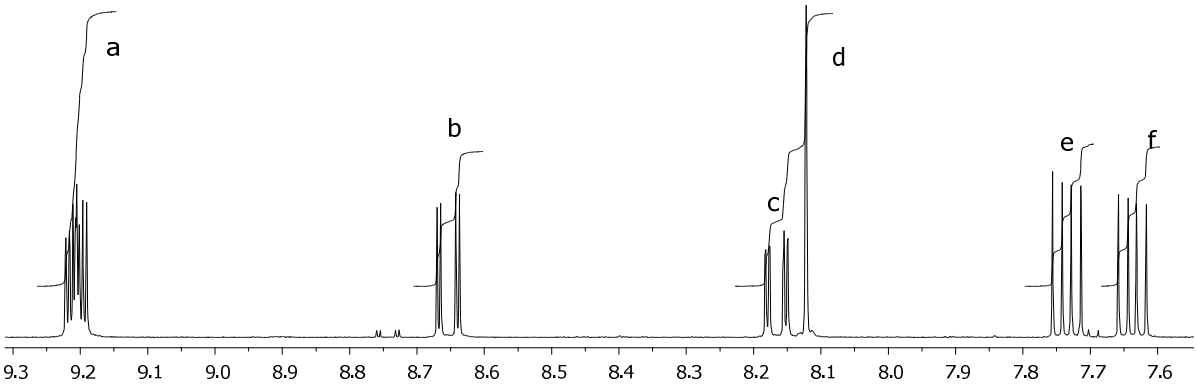
U30 $C_{12}H_7BrN_2$

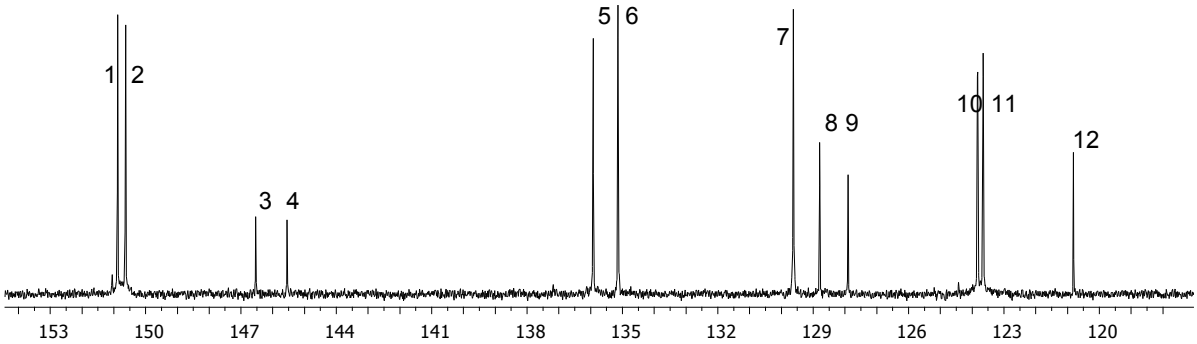


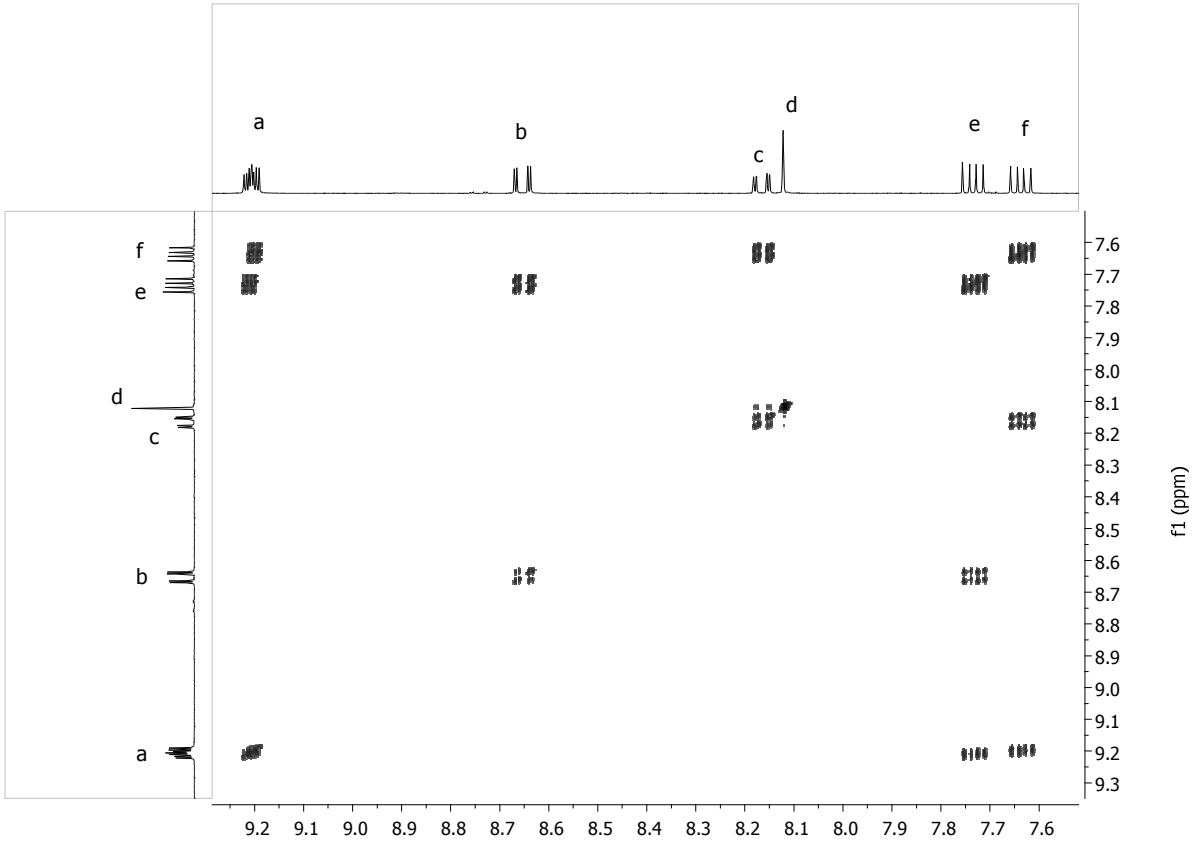
1. Bestimmen Sie, an welcher Stelle Br sitzt. (mit Begründung)

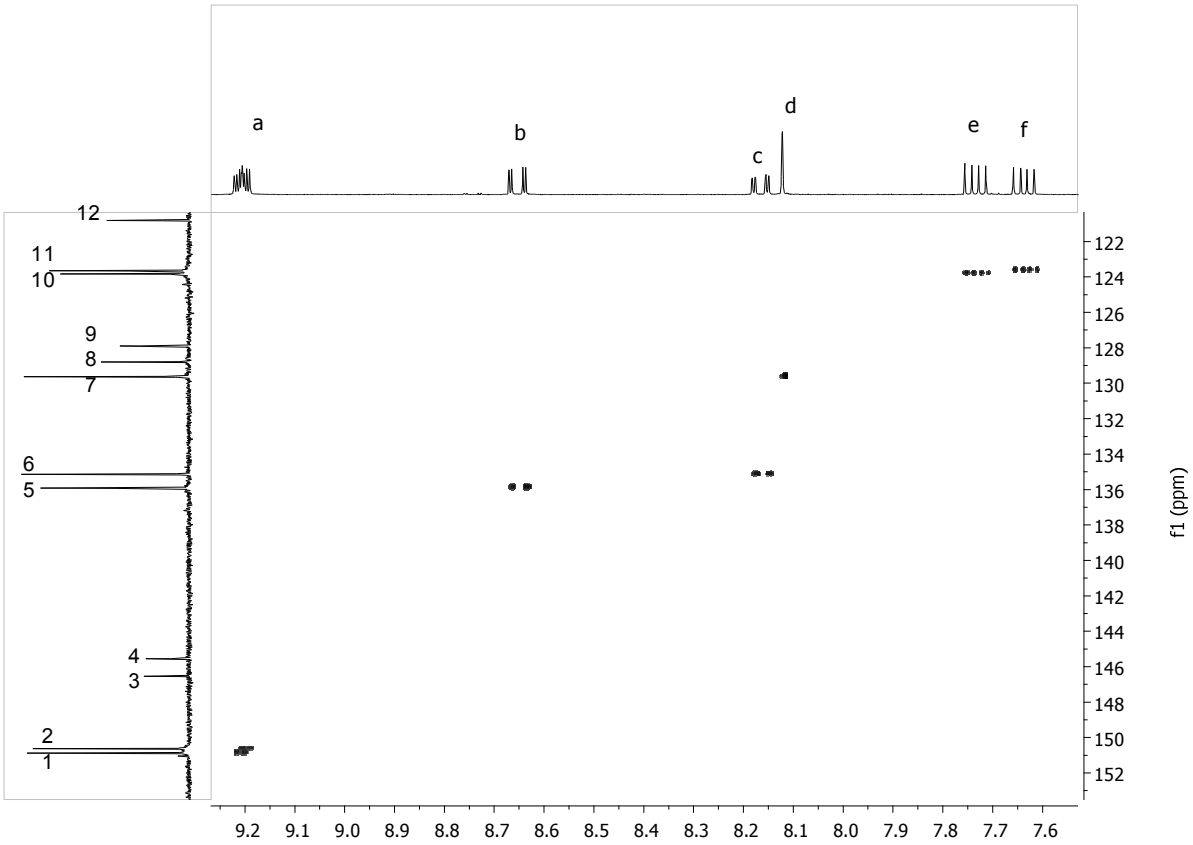
2. Ordnen Sie alle Signale zu.

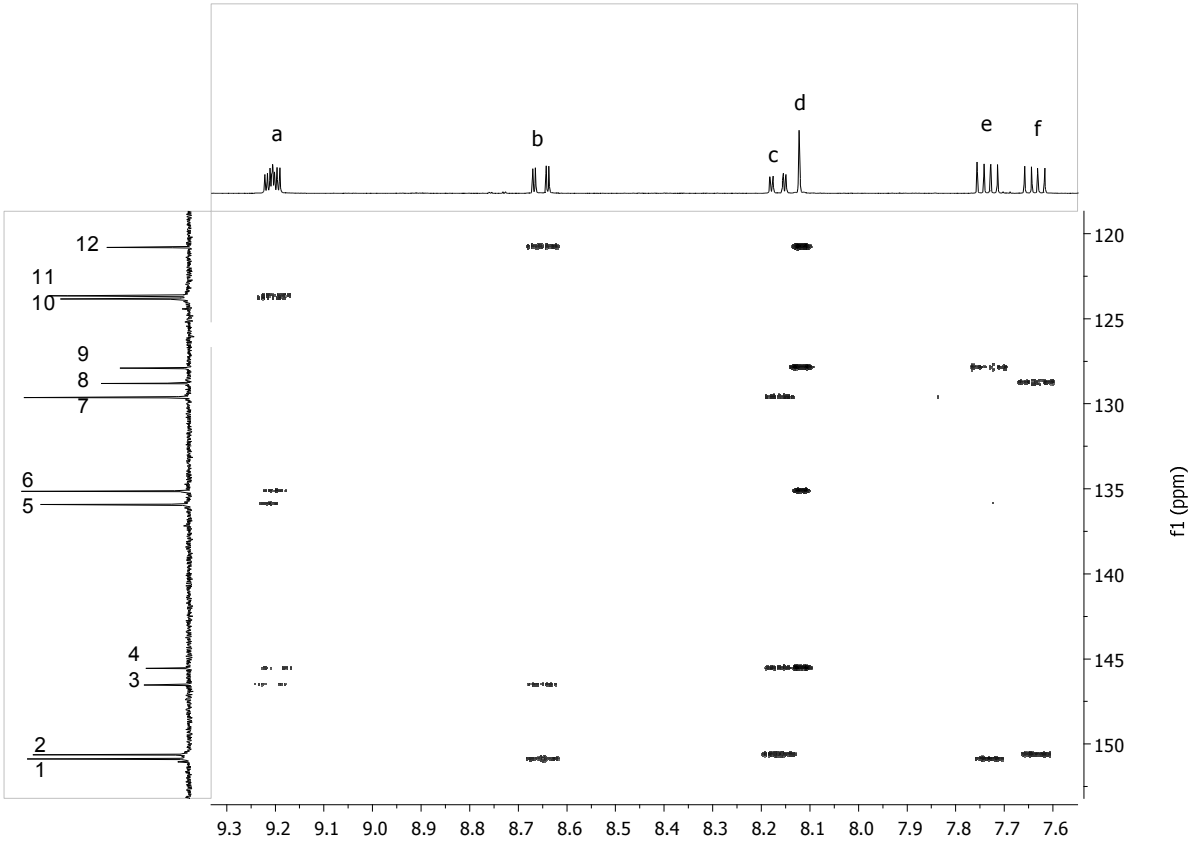
3. Begründen Sie Ihre Zuordnung, indem Sie für C-Atom 3, 4, 7, 8, 9 und 12 die im HMBC sichtbaren Kopplungen einzeichnen. Verwenden Sie Farbstifte.


a
b
c
d
e
f
9.3 9.2 9.1 9.0 8.9 8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6

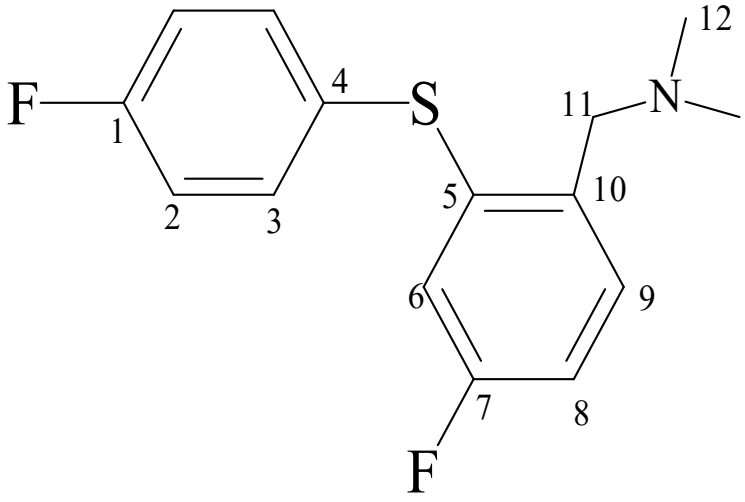

1 2
3 4
5 6
7
8 9
10 11
12
153 150 147 144 141 138 135 132 129 126 123 120

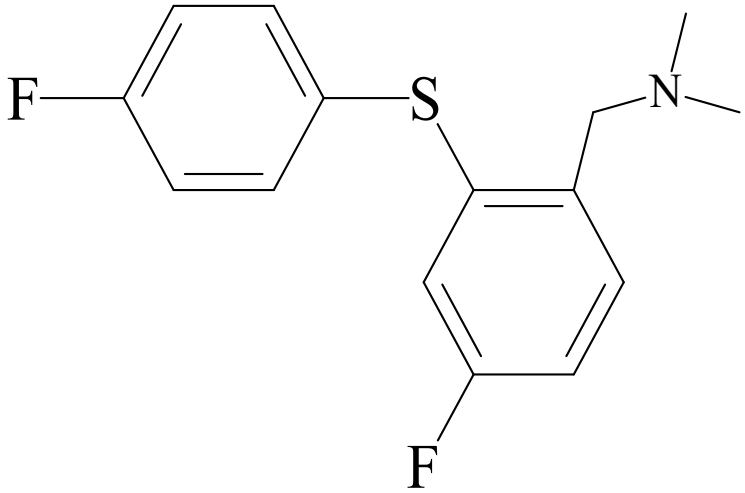

a
b
c
d
e
f
f1 (ppm)
9.2 9.1 9.0 8.9 8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6


a
b
c
d
e
f
12
11
10
9
8
7
6
5
4
3
2
1
f1 (ppm)


a
b
c
d
e
f
12
11
10
9
8
7
6
5
4
3
2
1
f1 (ppm)

U31

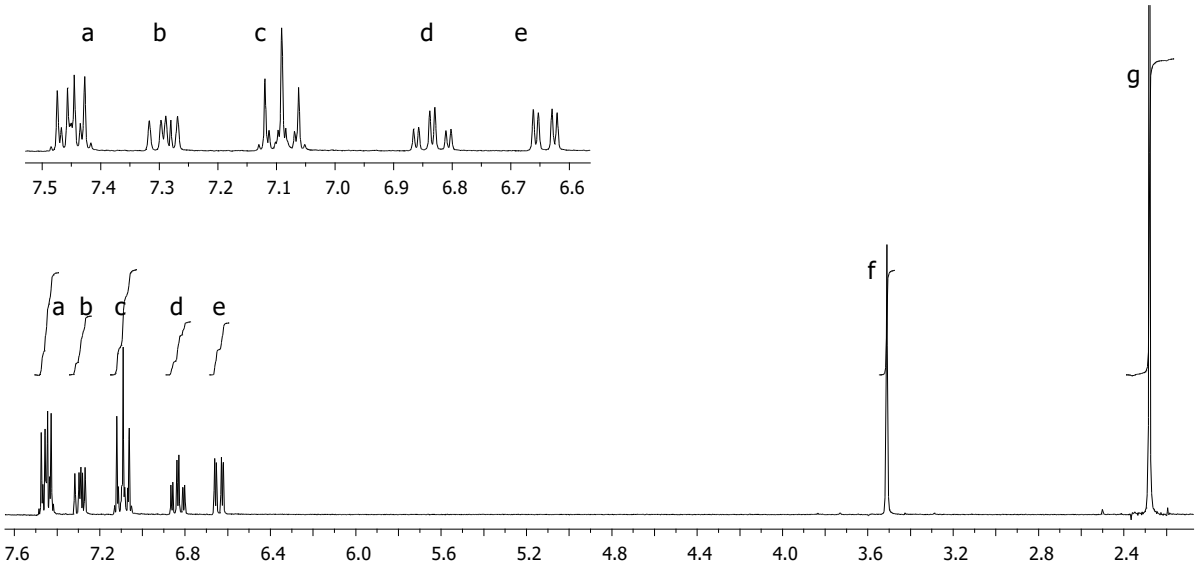


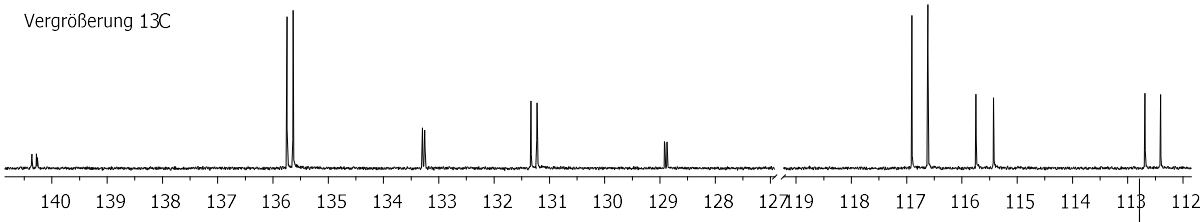


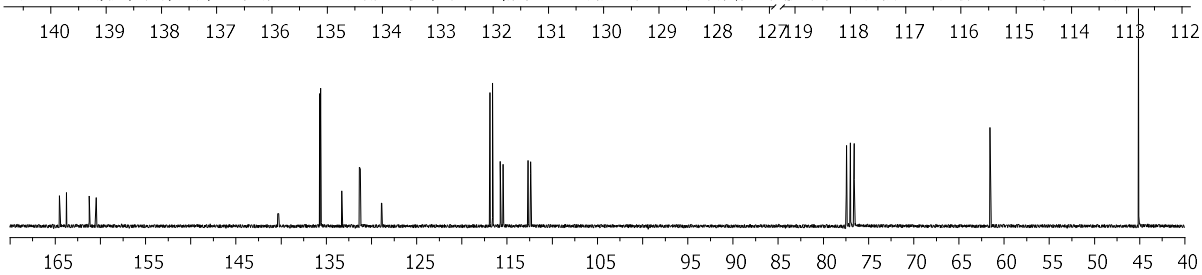
1. Ordnen Sie alle Signale zu.
   Für die ^{13}C-Signale tragen Sie obige Zahlen in das ^{13}C-Spektrum ein.
   Für die 1H-Signale tragen Sie wie üblich die Buchstaben in obiger Struktur ein. (6 P)

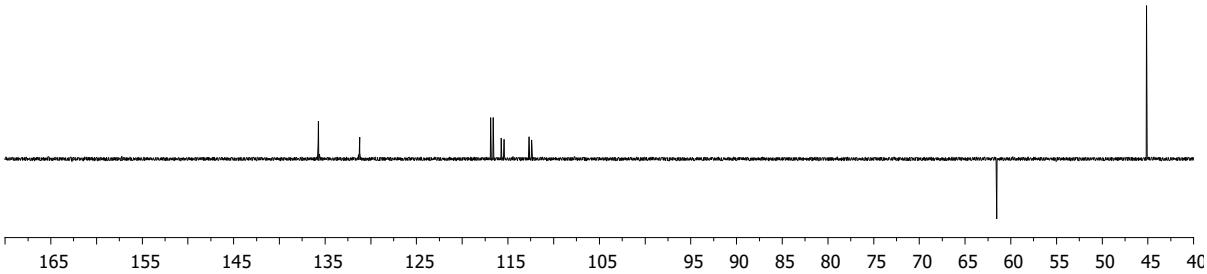
2. Zeichnen Sie einen Splittingschlüssel für die drei Protonen des rechten Aromaten.
   (letzte Seite)

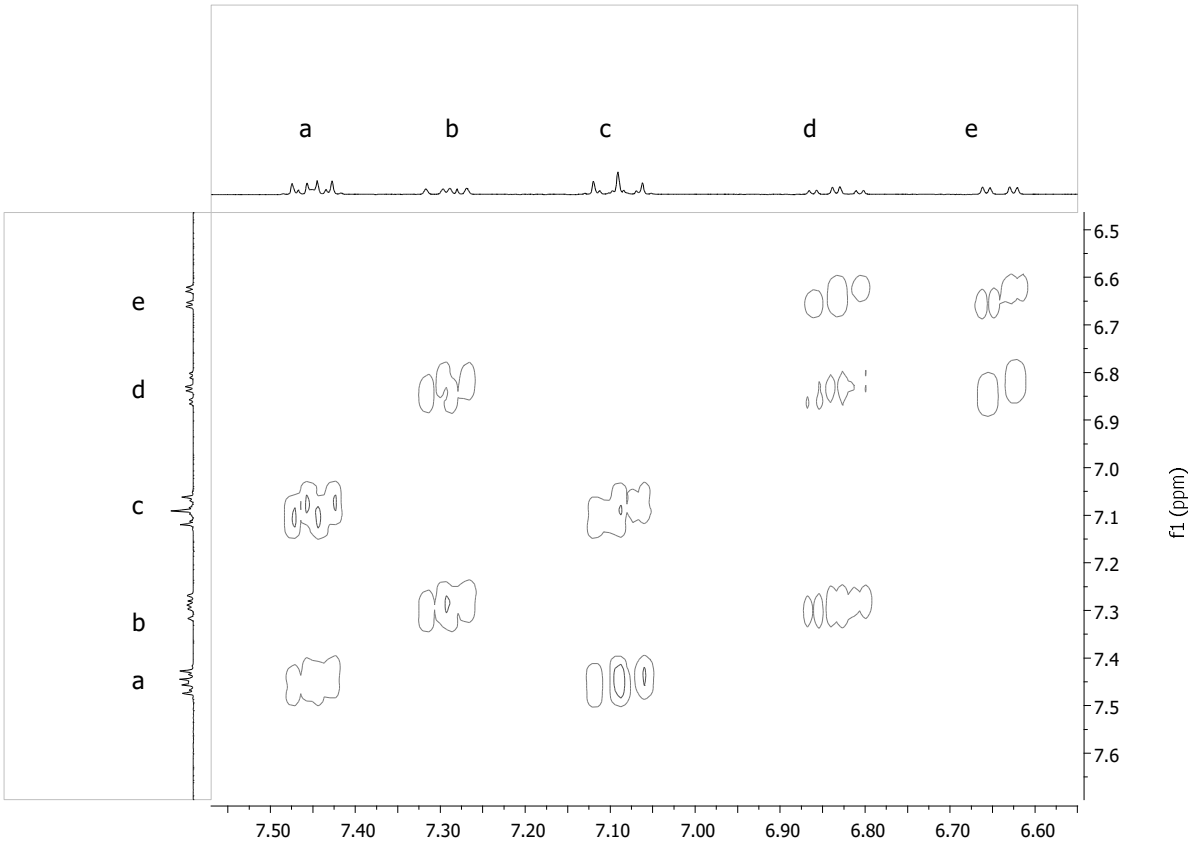
a
b
c
d
e
7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6

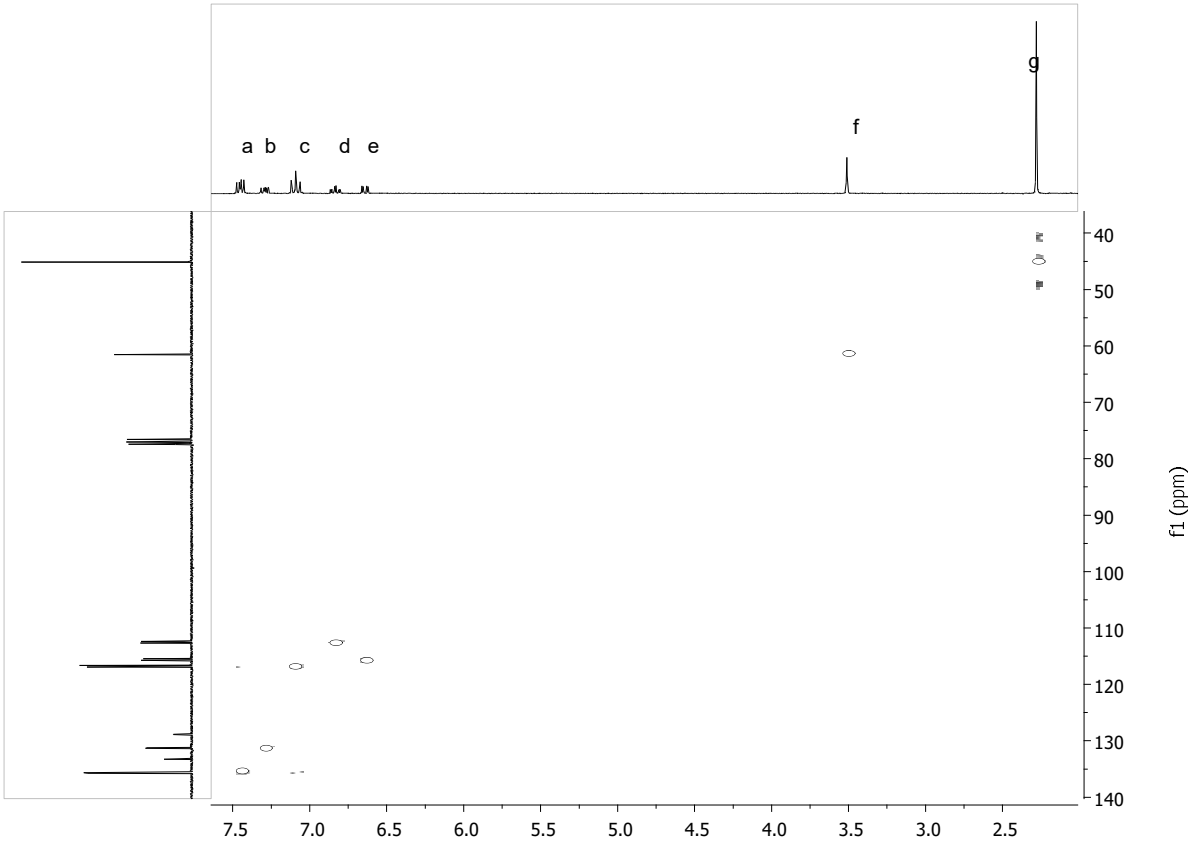

a b c d e
f
g
7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4

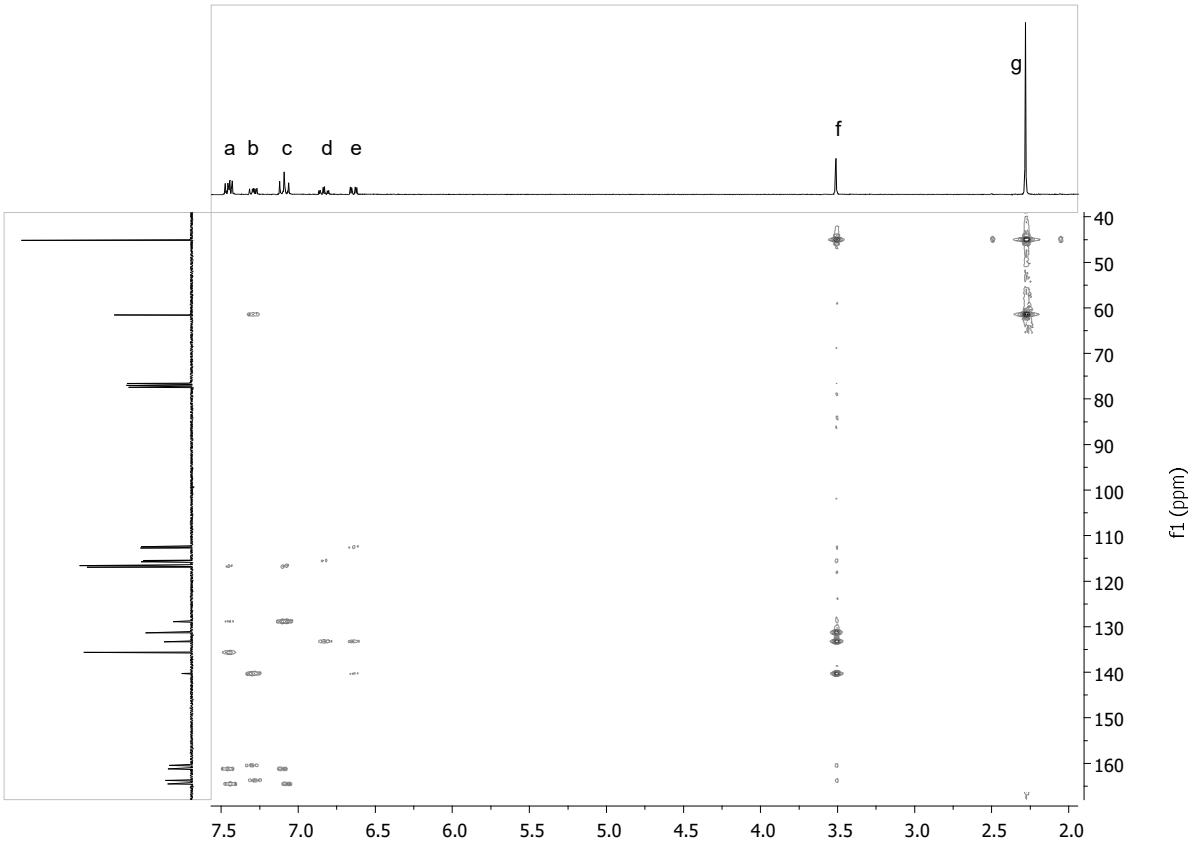

Vergrößerung 13C
140 139 138 137 136 135 134 133 132 131 130 129 128 127 119 118 117 116 115 114 113 112

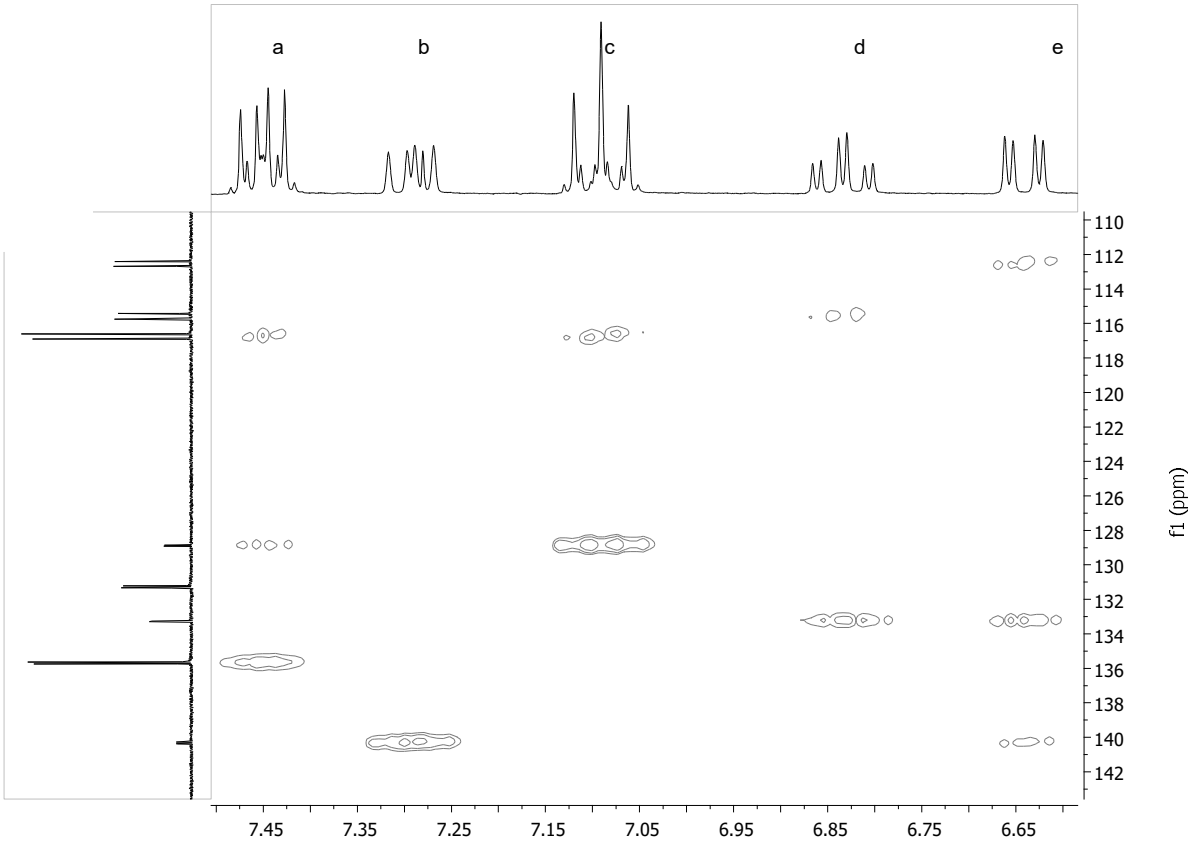

165 155 145 135 125 115 105 95 90 85 80 75 70 65 60 55 50 45 40

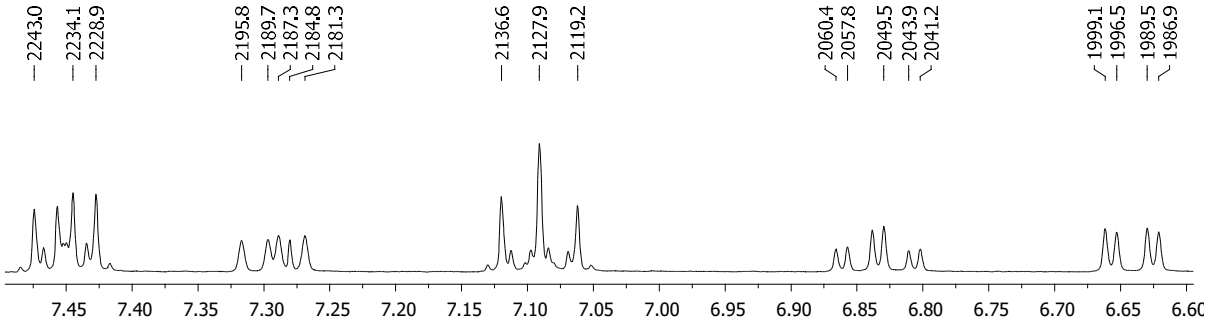

165 155 145 135 125 115 105 95 90 85 80 75 70 65 60 55 50 45 40


a
b
c
d
e
f1 (ppm)
7.50
7.40
7.30
7.20
7.10
7.00
6.90
6.80
6.70
6.60

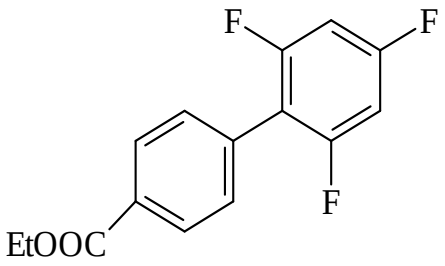

a b c d e
f
g
f1 (ppm)
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5


a b c d e
f
g
f1 (ppm)
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0
40 50 60 70 80 90 100 110 120 130 140 150 160


a
b
c
d
e
f1 (ppm)
7.45 7.35 7.25 7.15 7.05 6.95 6.85 6.75 6.65
110 112 114 116 118 120 122 124 126 128 130 132 134 136 138 140 142

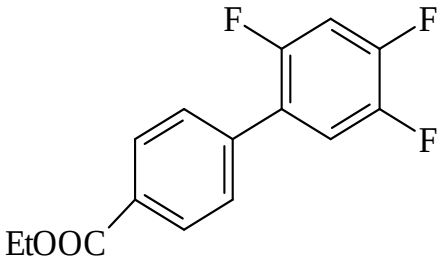

2243.0
2234.1
2228.9
2195.8
2189.7
2187.3
2184.8
2181.3
2136.6
2127.9
2119.2
2060.4
2057.8
2049.5
2043.9
2041.2
1999.1
1996.5
1989.5
1986.9
7.45
7.40
7.35
7.30
7.25
7.20
7.15
7.10
7.05
7.00
6.95
6.90
6.85
6.80
6.75
6.70
6.65
6.60

U32



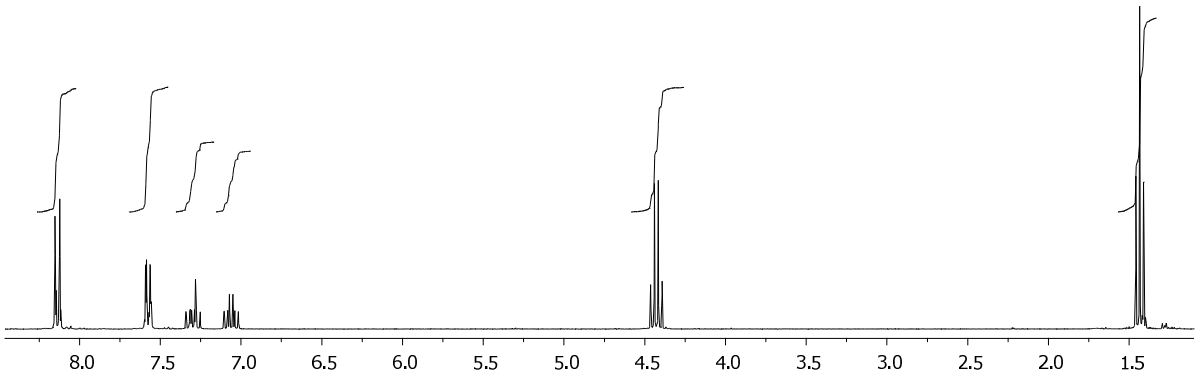
Struktur 1

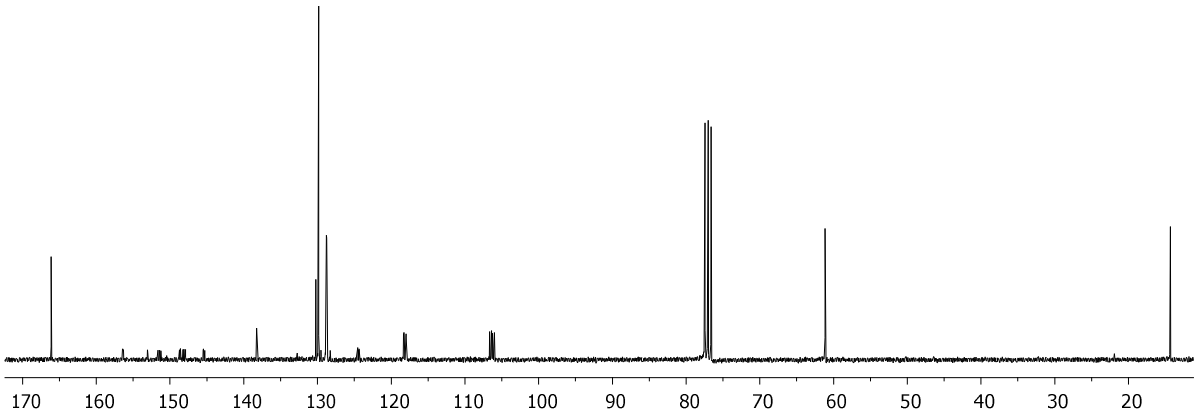
oder

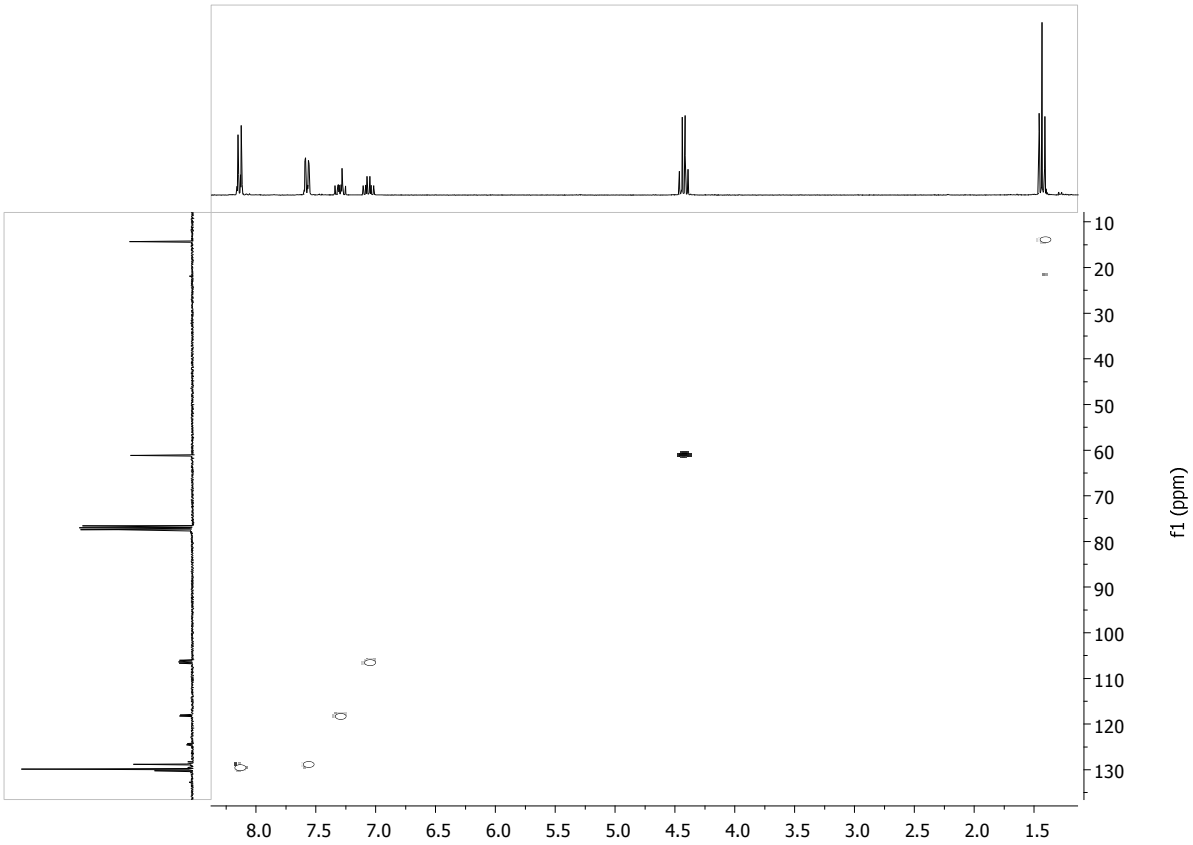


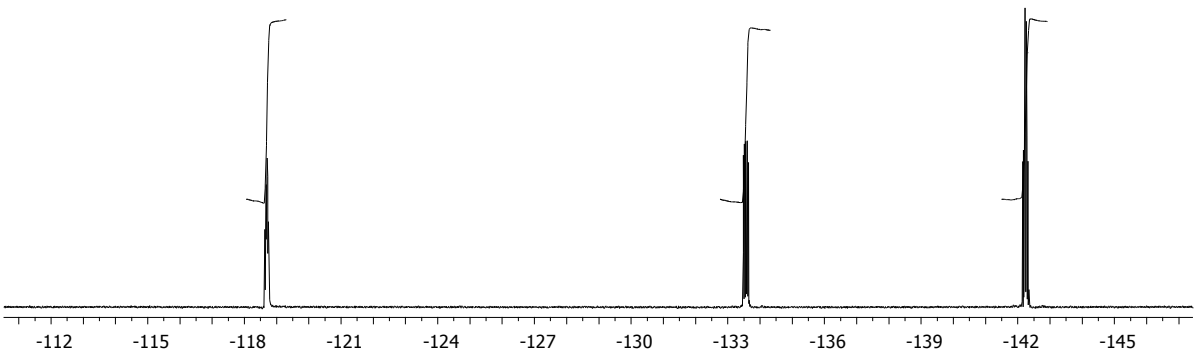
Struktur 2

1. Um welche Substanz handelt es sich? Geben Sie mind. 3 Gründe an, warum sich sich für Struktur 1 oder 2 entschieden haben.









^{19}F-Spektrum