

# Anhang

DBÄ=Doppelbindungs-Äquivalente

$$\text{DBÄ} = 1 + \frac{1}{2} [ \sum n_i ( v_i - 2) ]$$

$n_i$  = Anzahl der Atome

$v_i$  = Anzahl der Bindungen dieses Atoms

### Beispiele:

$$\text{C}_5\text{H}_9\text{Br: DBÄ} = 1 + \frac{1}{2} ( 5 \times 2 + 9 \times (-1) + 1 \times (-1) ) = 1$$

$$\text{C}_8\text{H}_8\text{O}_2: \text{DBÄ} = 1 + \frac{1}{2} ( 8 \times 2 + 8 \times (-1) + 1 \times (0) ) = 5$$

S: R-S-R  $\rightarrow 0$

R-SO-R (4wertiger S)  $\rightarrow + n(\text{S}) \times 2$  (wie C)

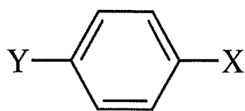
R-SO<sub>2</sub>-R (6wertiger S)  $\rightarrow + n(\text{S}) \times 4$

Strukturelemente:

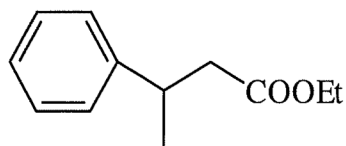
Doppelbindung: 1 DBÄ

Dreifachbindung: 2 DBÄ

Ring 1 DBÄ



4 DBÄ (1 x Ring, 3 x Doppelbindung)

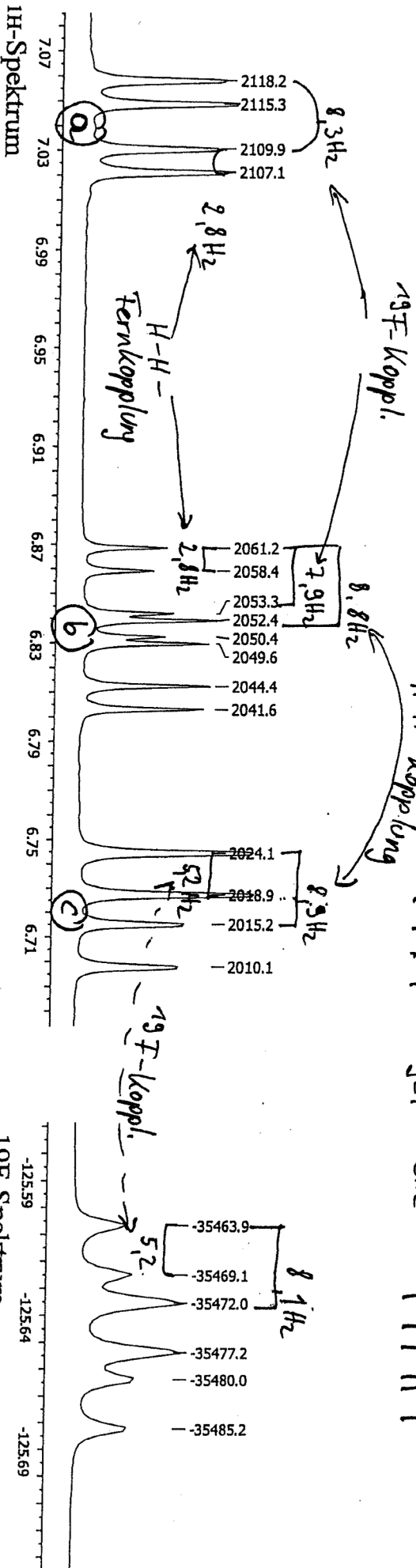
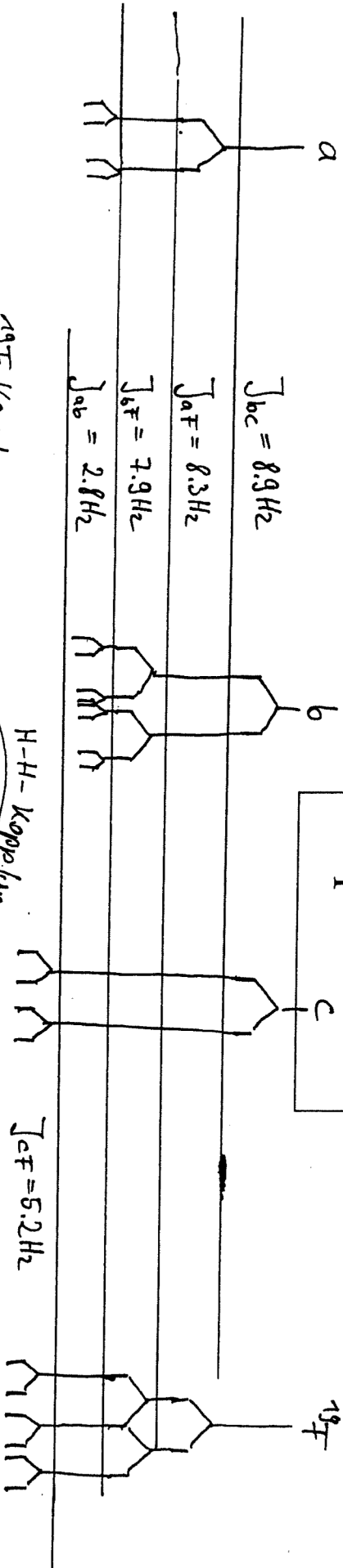
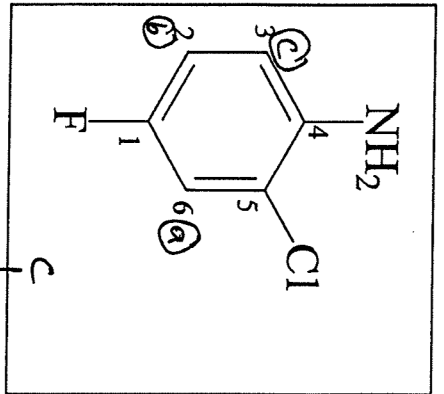


5 DBÄ (1 x Aromat, 1 x Ester-Doppelbindung)

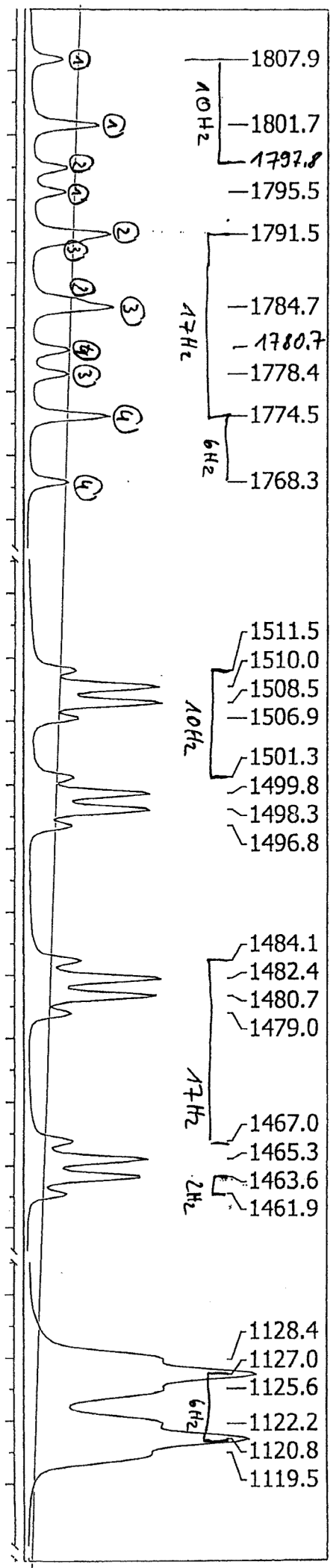
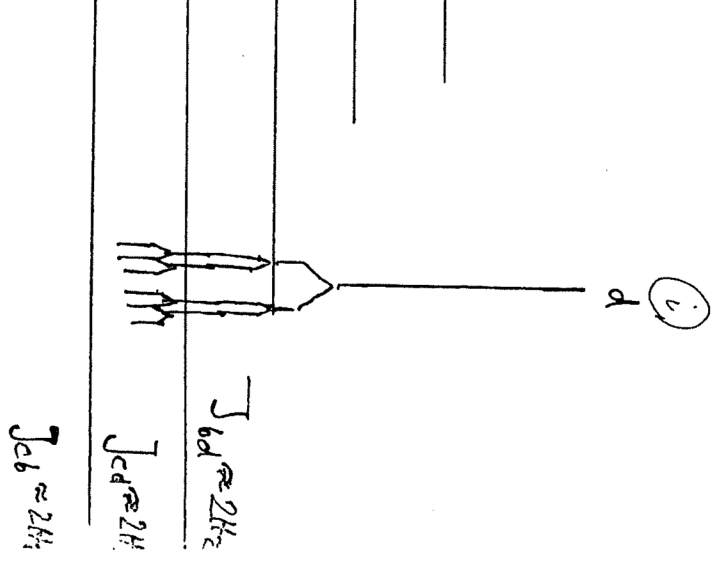
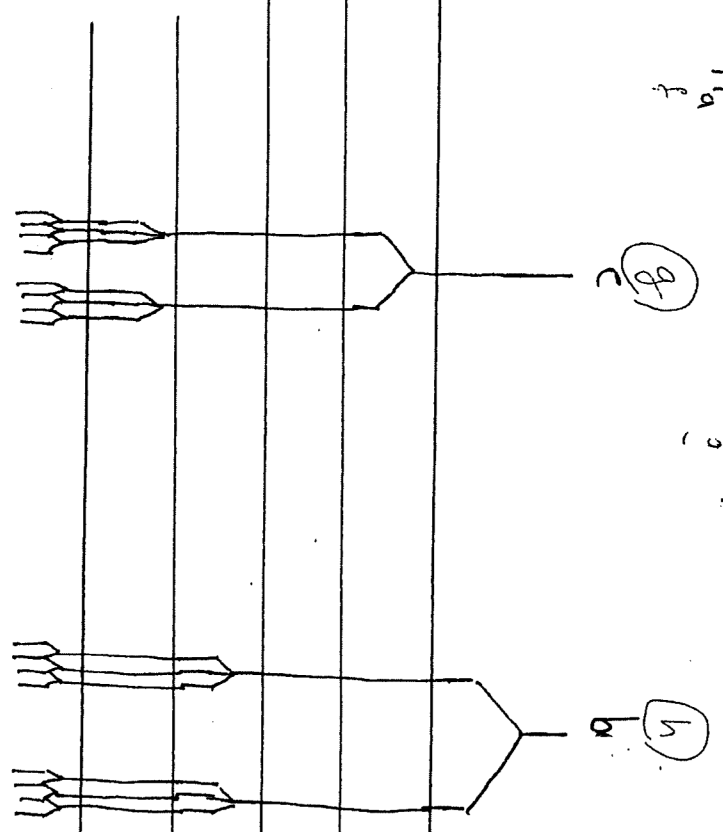
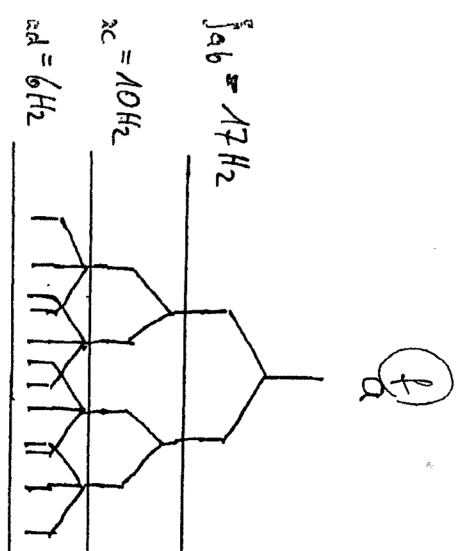
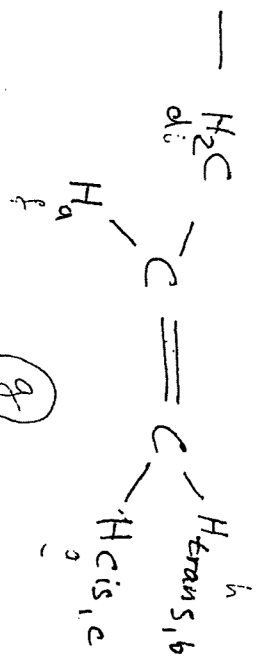
# 17 U17 - Lösung

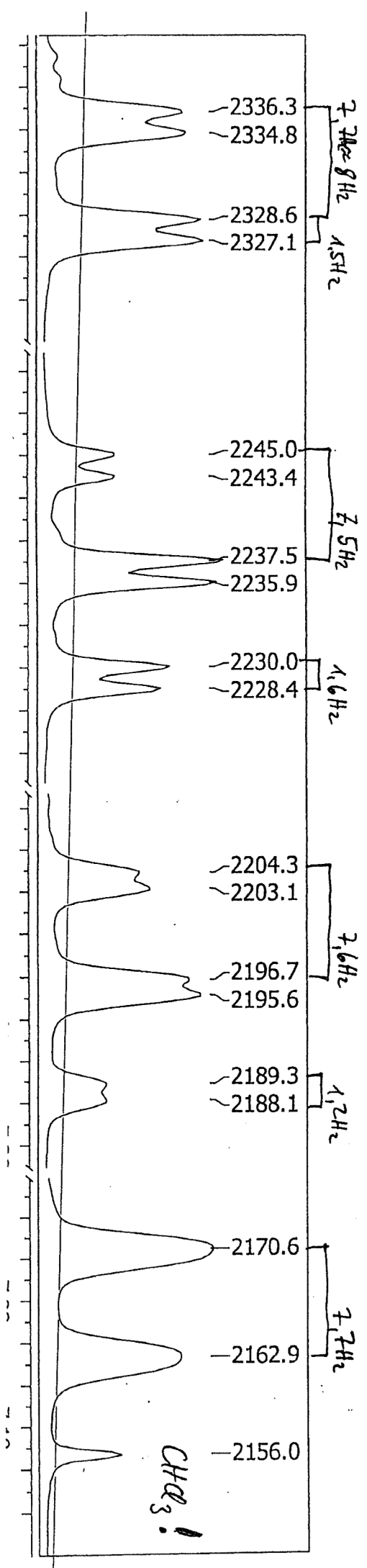
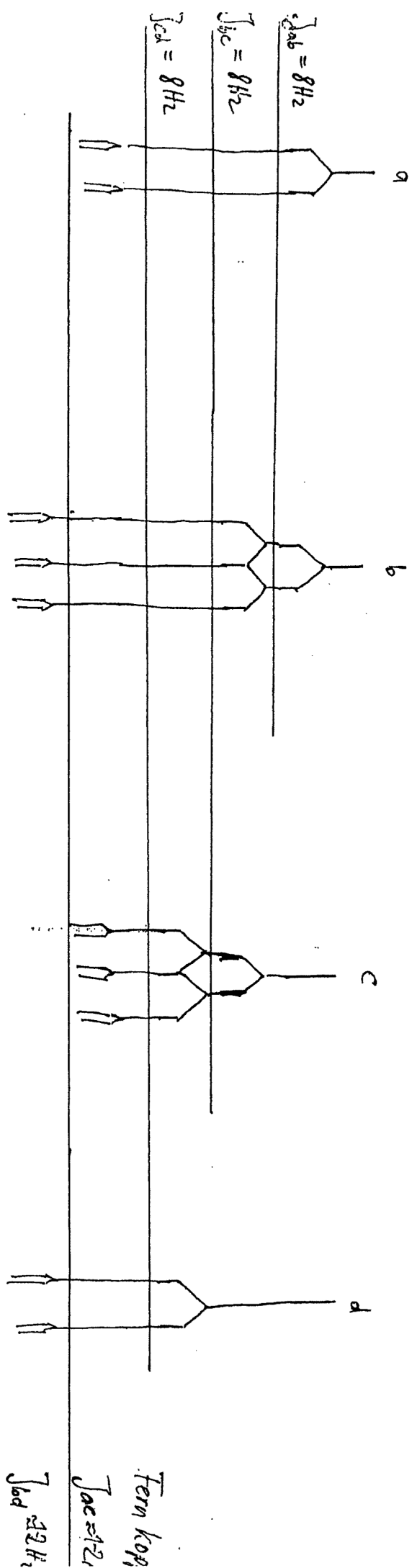
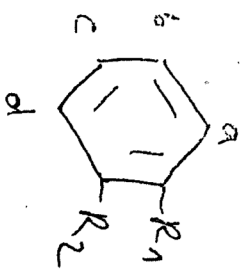
Zusatzfrage:

Auf welchem Gerät wurden diese Spektren gemessen?  
Bei welcher Grundfrequenz wurden das  $^1\text{H}$ ,  $^{13}\text{C}$  und  $^{19}\text{F}$ -Spektrum aufgenommen?



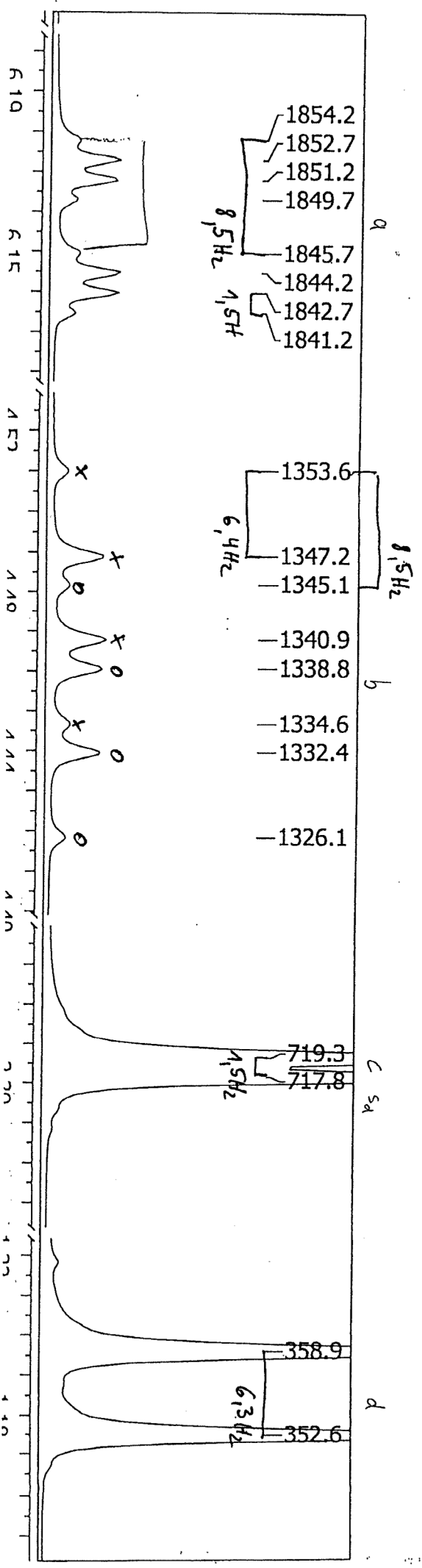
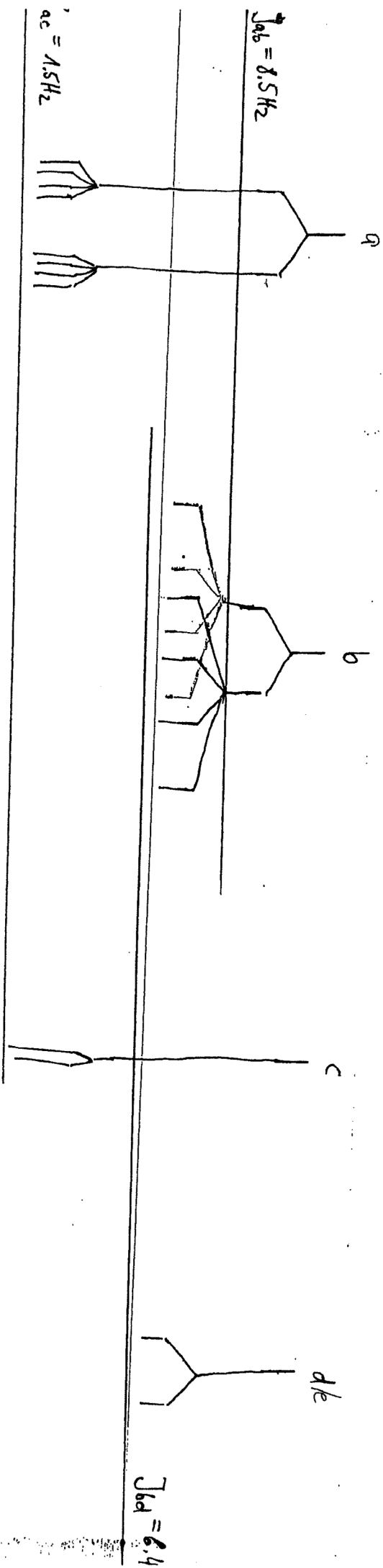
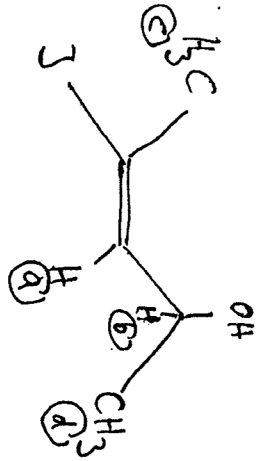
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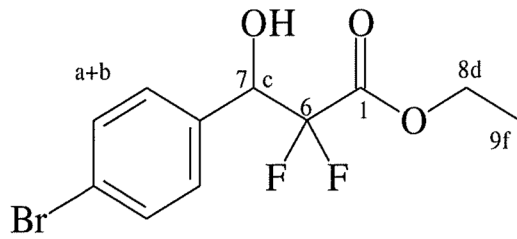




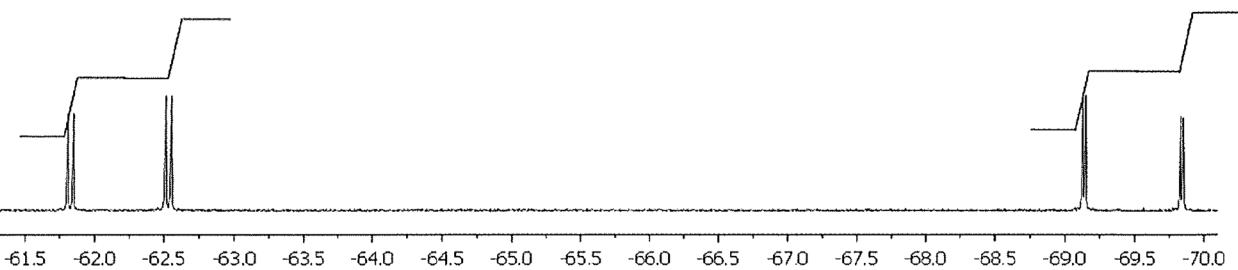
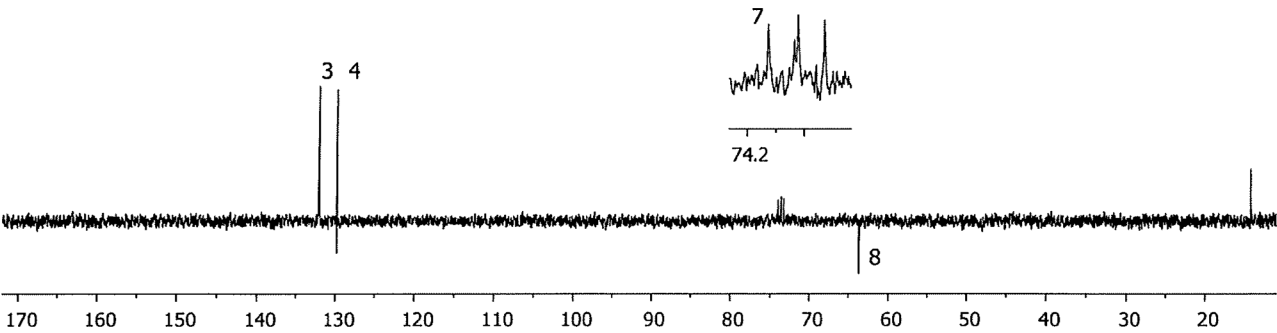
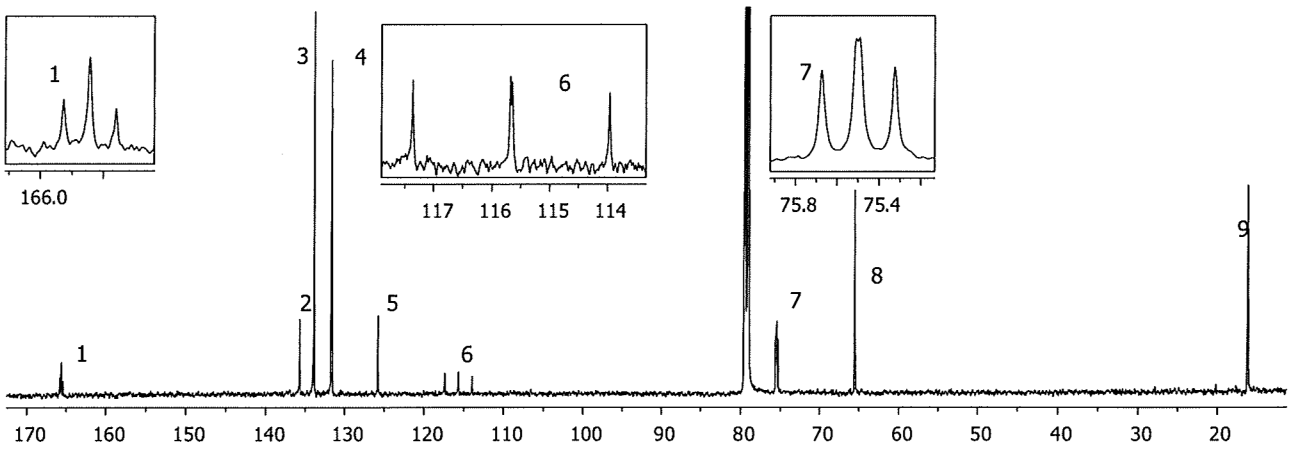
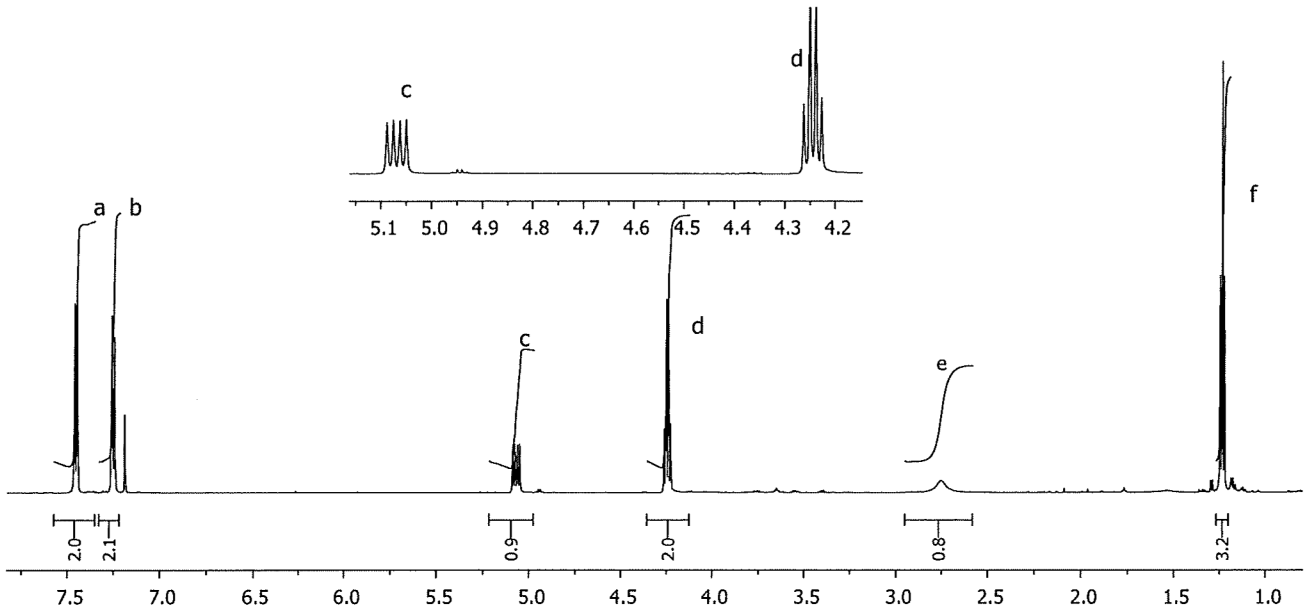
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Fern kop,  
 $J_{ac} = 12$   
 $J_{bd} = 22 \text{ Hz}$





Einführung Heteroatome  
am Beispiel  $^{19}\text{F}$  und Deuterium



## Deuterierte Lösungsmittel: $I(^2\text{H}) = 1$

	$^1\text{H}$	$^{13}\text{C}$
$\text{CDCl}_3$	7,24	77,00
Aceton	2,04	29,8/206,3
DMSO	2,49	39,70
MeOD	3,35	49,30
TFA	11,50	116,5/164,4
D <sub>2</sub> O	4,65	
$\text{CD}_3\text{CN}$	1,93	1,3/117,7
Pyridin	7,19/7,55/8,71	123,5/135,5/149,5
$\text{CD}_2\text{Cl}_2$	5,32	53,50
$\text{C}_6\text{D}_6$	7,20	128,00

### Größenverhältnisse der Peaks ( $I = 1$ )

n =									
0				1					
1			1	1	1				
2		1	2	3	2	1			
3	1	3	6	7	6	3	1		
4	1	4	10	16	19	16	10	4	1

n = Anzahl koppelnder Nachbarn

Spinquantenzahl I (wichtig, um Aufspaltungsmuster zu bestimmen!)

$I = 0$  :  $^{12}\text{C}$

$I = \frac{1}{2}$  :  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{19}\text{F}$ ,  $^{31}\text{P}$

$I = 1$  : D

Hinweis:

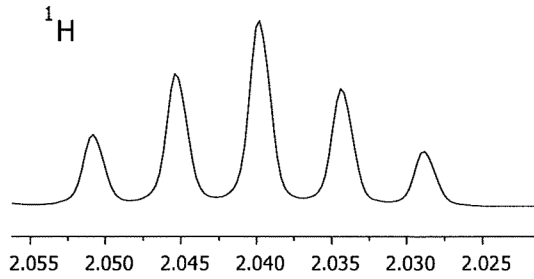
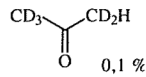
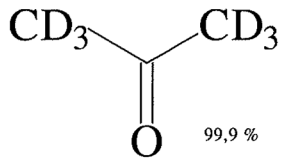
$I=1, n=1 \rightarrow$  Triplett im Verhältnis 1:1:1

$I= \frac{1}{2}, n=2 \rightarrow$  Triplett im Verhältnis 1:2:1

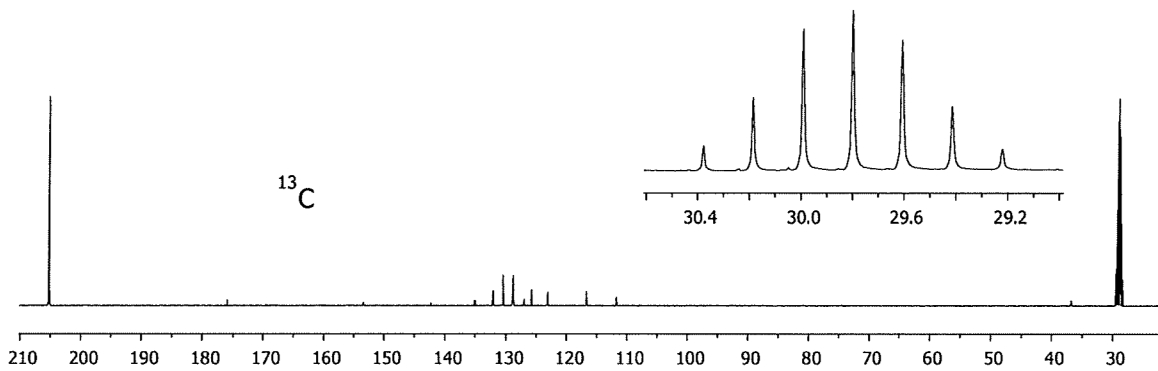


# Kopplungsmuster von Aceton-d6

$$\text{Aufspaltung} = n * 2I + 1$$



$$\text{Aufspaltung} = 2 * 2 * 1 + 1 = 5$$

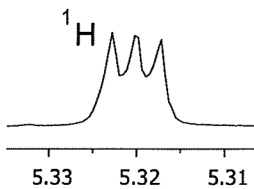


$$\text{Aufspaltung} = 3 * 2 * 1 + 1 = 7$$

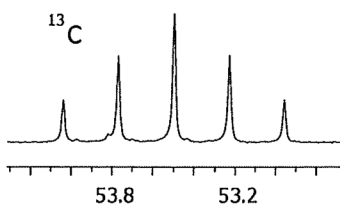
# Kopplungsmuster von CD<sub>2</sub>Cl<sub>2</sub>

$$\text{Aufspaltung} = n * 2I + 1$$

99,5 % CD<sub>2</sub>Cl<sub>2</sub>    0,5 % CDHCl<sub>2</sub>



$$\text{Aufspaltung} = 1 * 2 * 1 + 1 = 3$$



$$\text{Aufspaltung} = 2 * 2 * 1 + 1 = 5$$