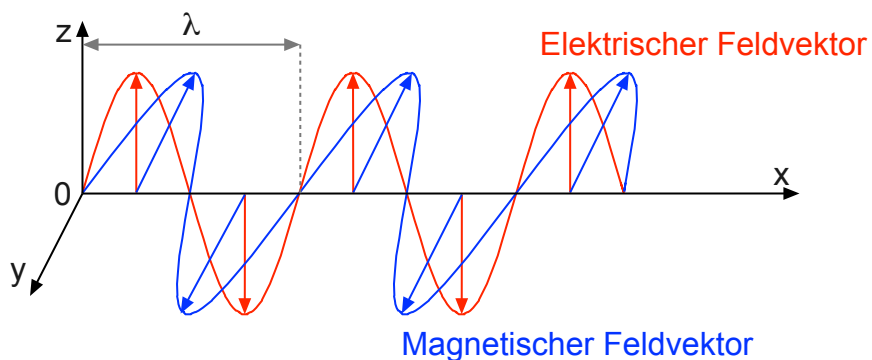
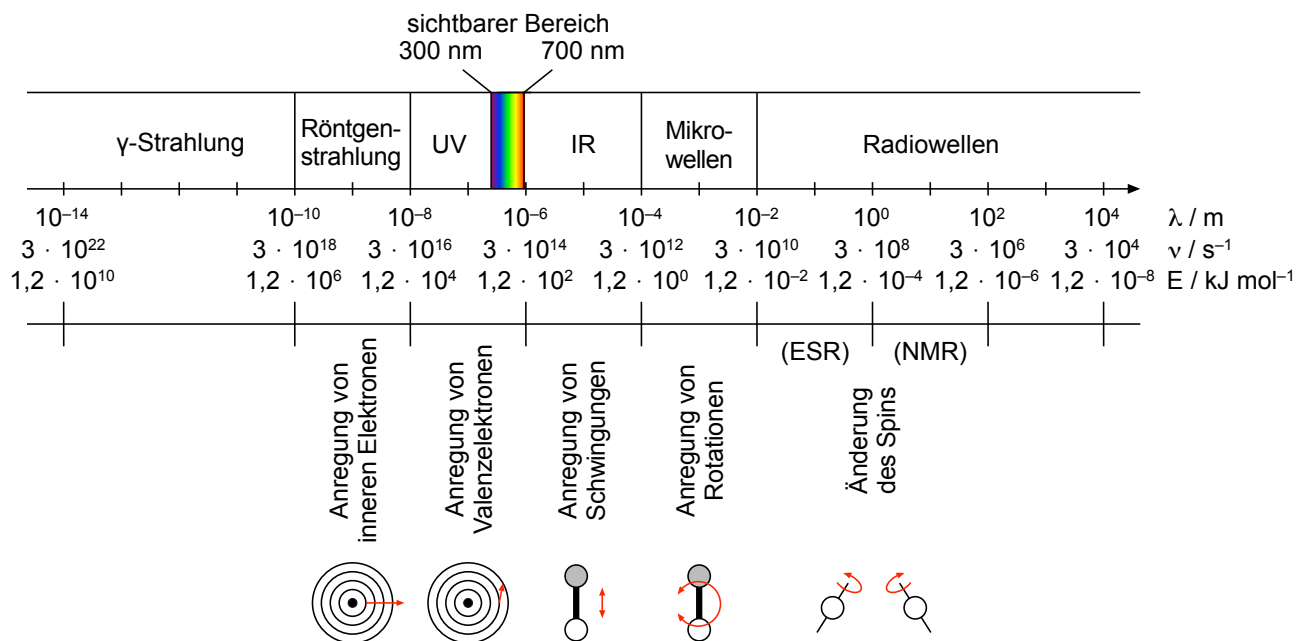


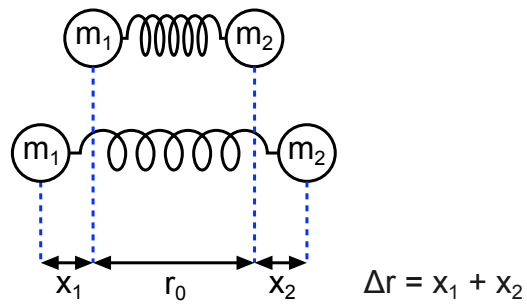
### Elektromagnetische Strahlung



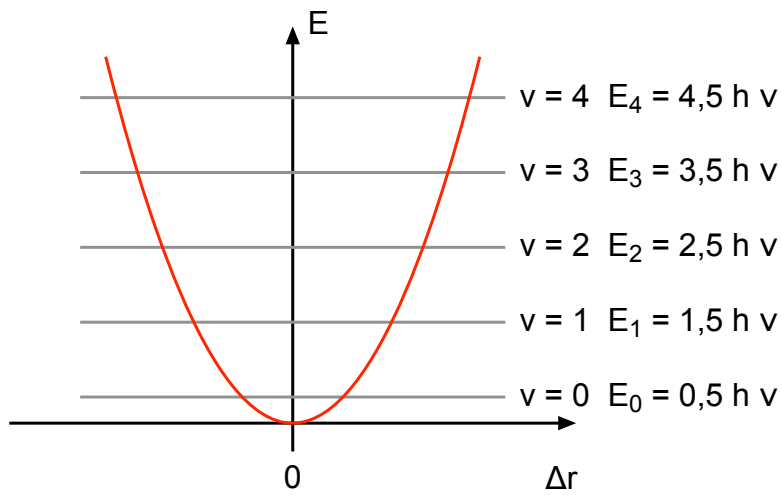
### Elektromagnetisches Spektrum



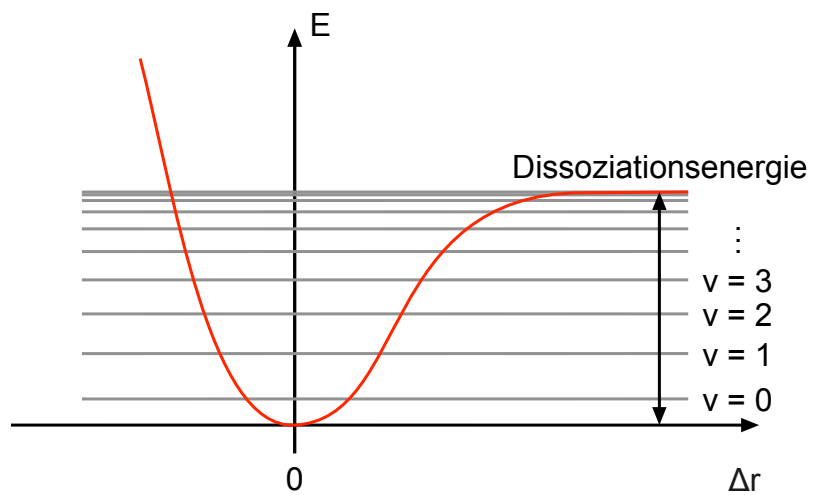
### Hookssches Gesetz



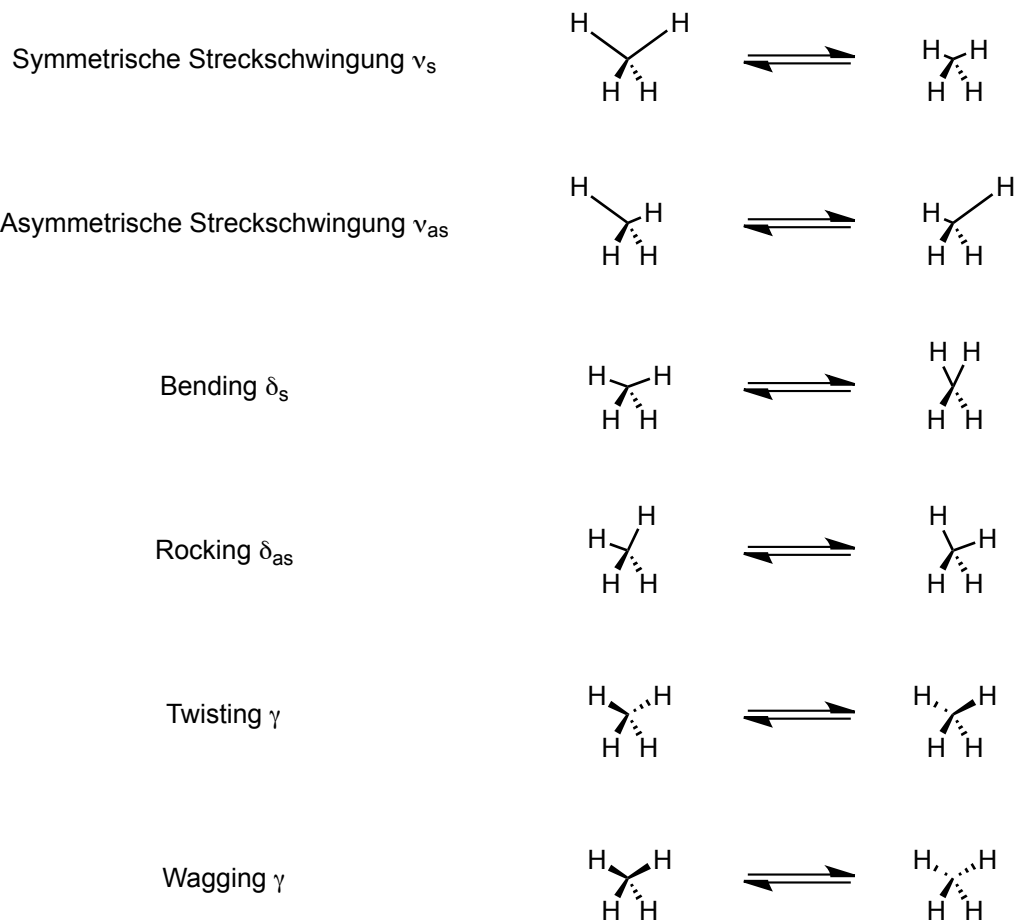
### Harmonischer Oszillator



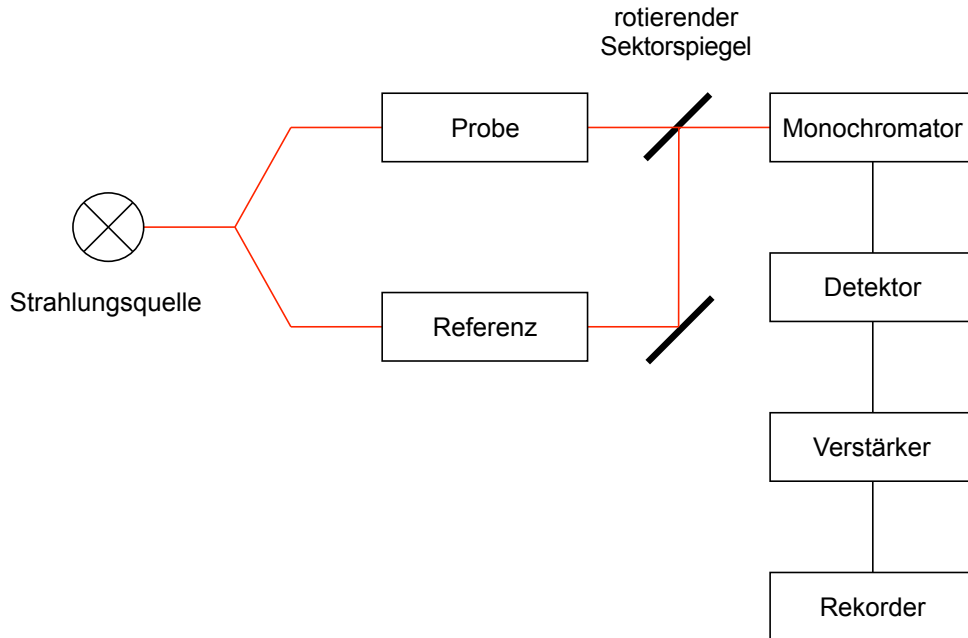
### Anharmonischer Oszillator



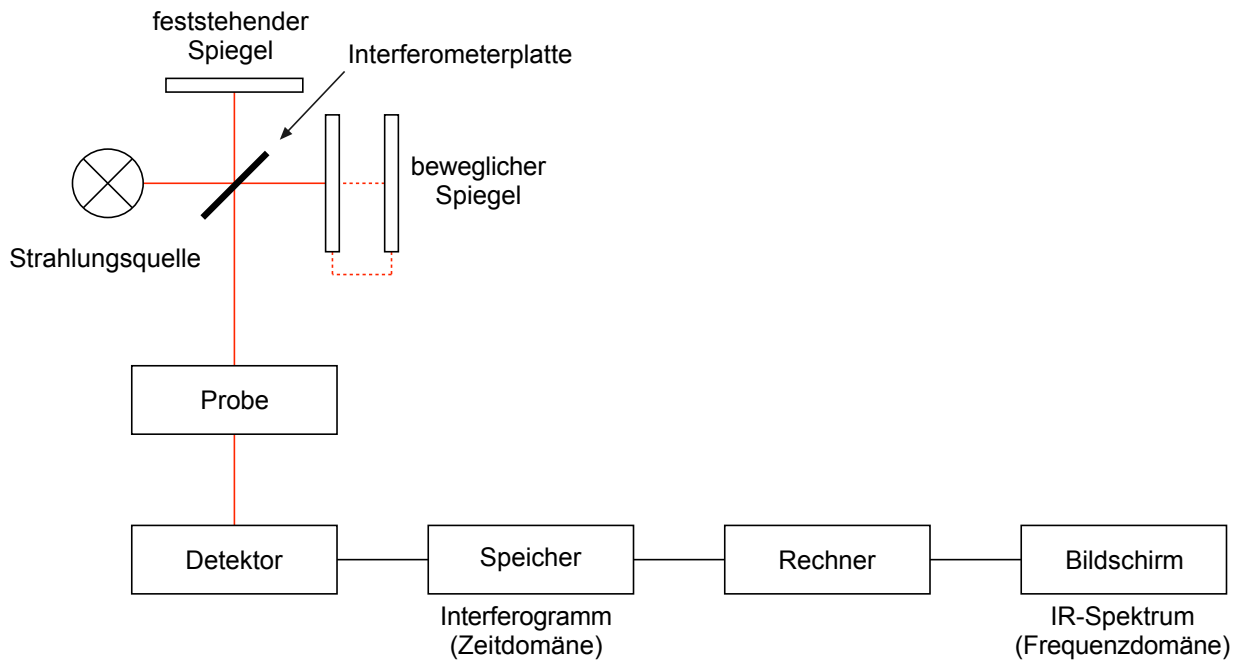
### Schwingungsmoden von Methan



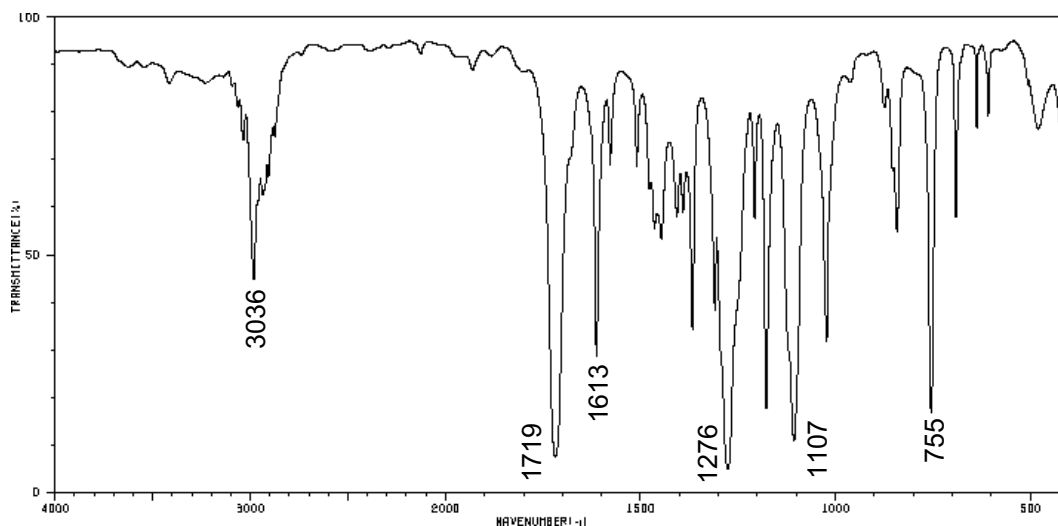
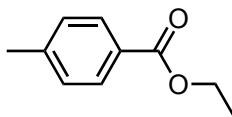
### Schematischer Aufbau eines Scanning IR-Spektrometers



### Schematischer Aufbau eines FT-IR Spektrometers



## IR Spektrum von 4-Methylbenzoesäureethylester

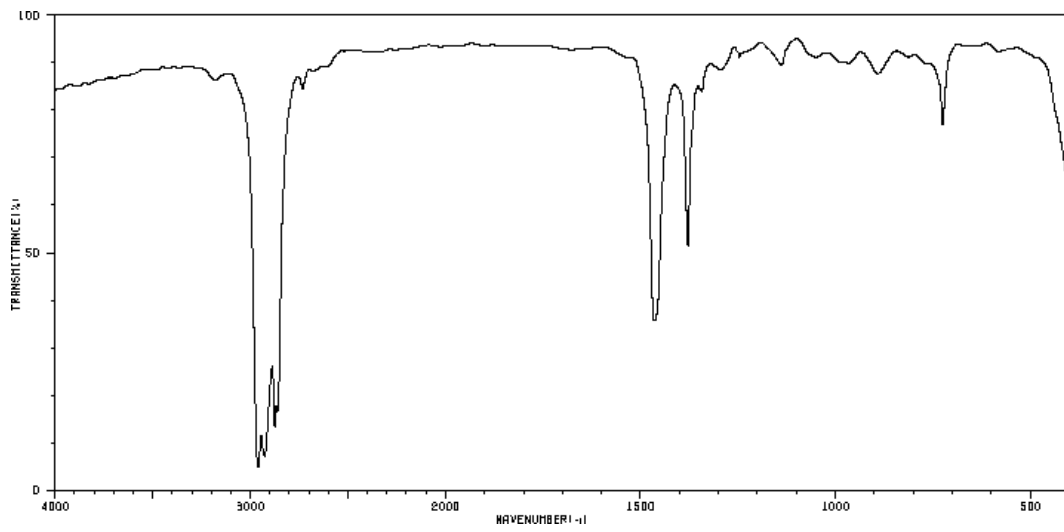


$1/\lambda / \text{cm}^{-1}$	Zuordnung
3036	$\nu(\text{C-H})$ Aryl (darunter $\nu(\text{C-H})$ Alkyl)
1719	$\nu(\text{C=O})$ Ester
1613	$\nu(\text{C=C})$
1276	$\nu(\text{C-O-C})$
1107	$\nu(\text{C-O-C})$
755	$\delta(\text{C-H})$ des <i>para</i> -substituierten Aromaten

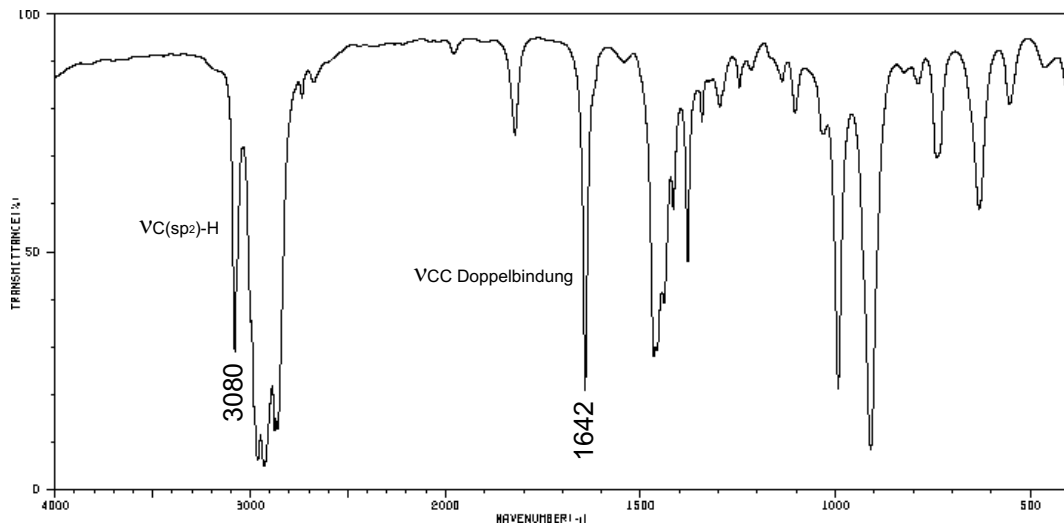
## Bereiche im IR Spektrum

$1/\lambda$ -Bereich / $\text{cm}^{-1}$	Absorptionen
3700 - 2500	O-H, N-H, C-H Einfachbindungen
2500 - 1900	Dreifachbindungen und kumulierte Doppelbindungen
1900 - 1500	C=O, C=C, C=N, N=O Doppelbindungen
unterhalb 1500	fingerprint Bereich (Deformationsschwingungen, Valenzschwingungen von Gruppen mit schweren Atomen, Gerüstschwingungen)

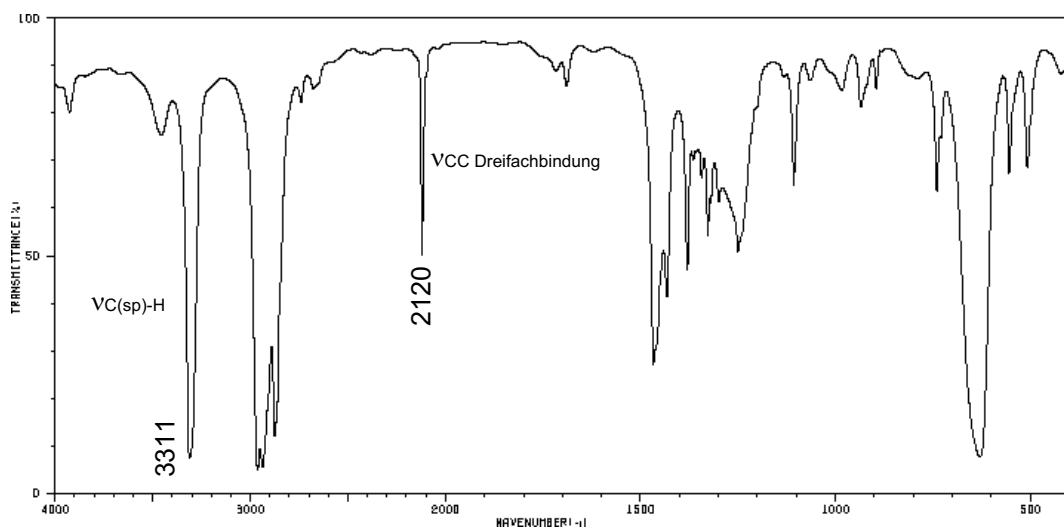
### Hexan



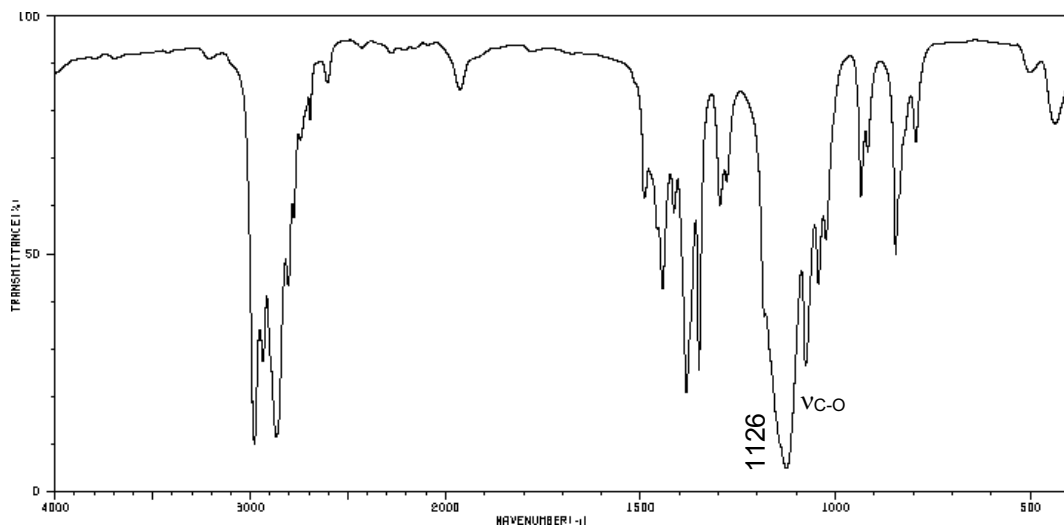
### 1-Hexen



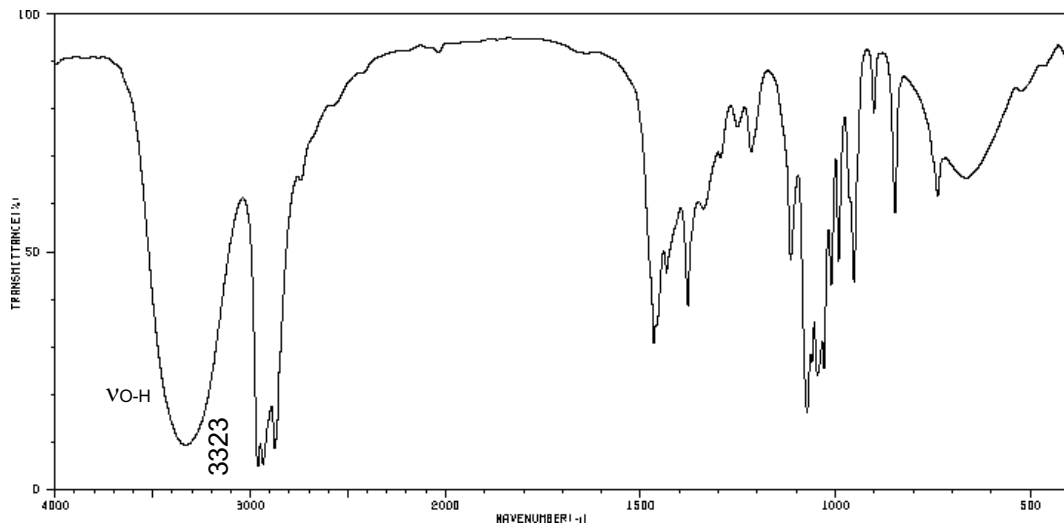
### 1-Hexin



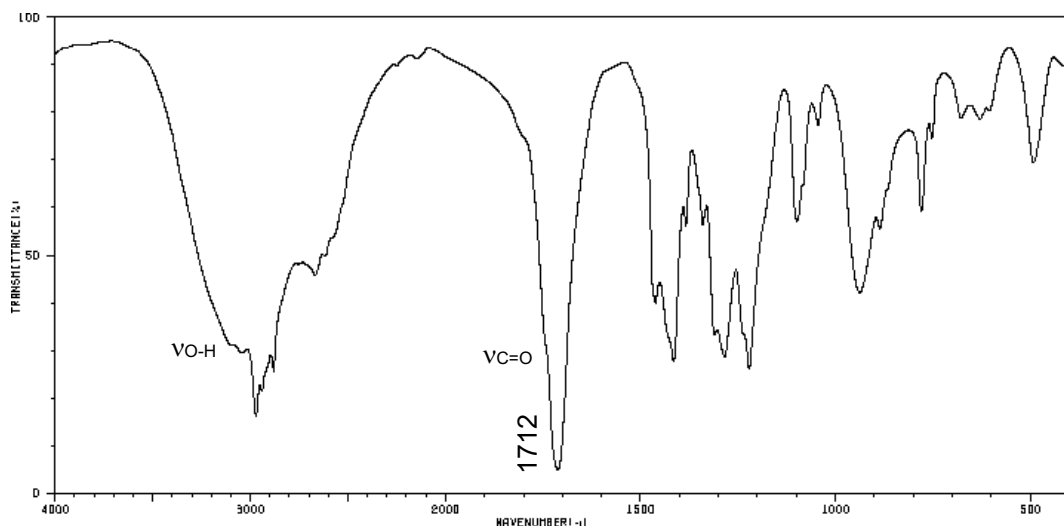
### Diethylether



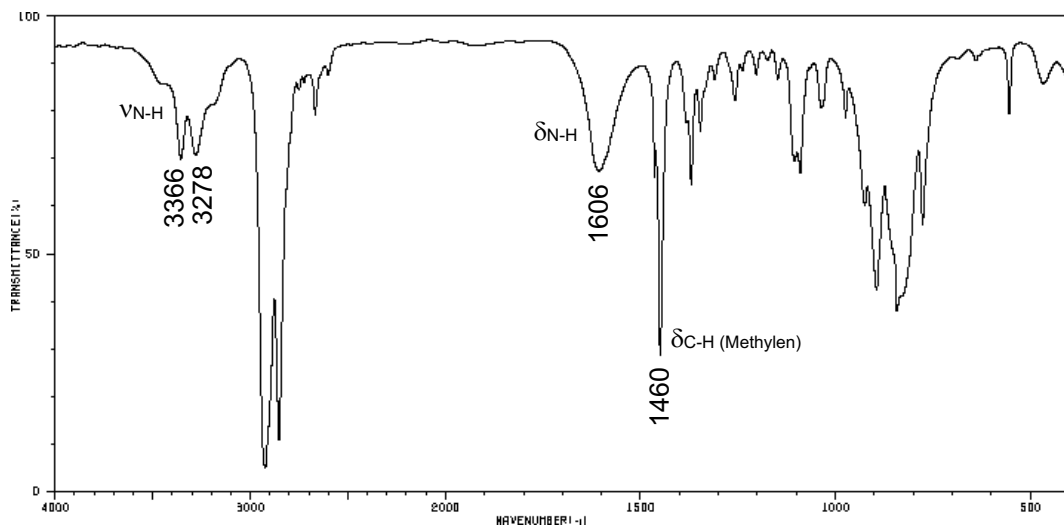
### 1-Butanol



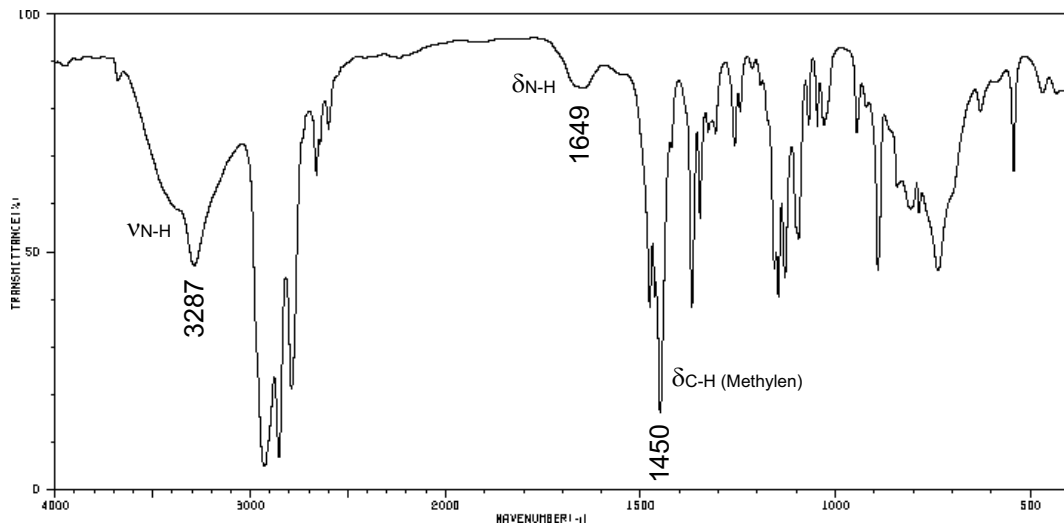
### Buttersäure



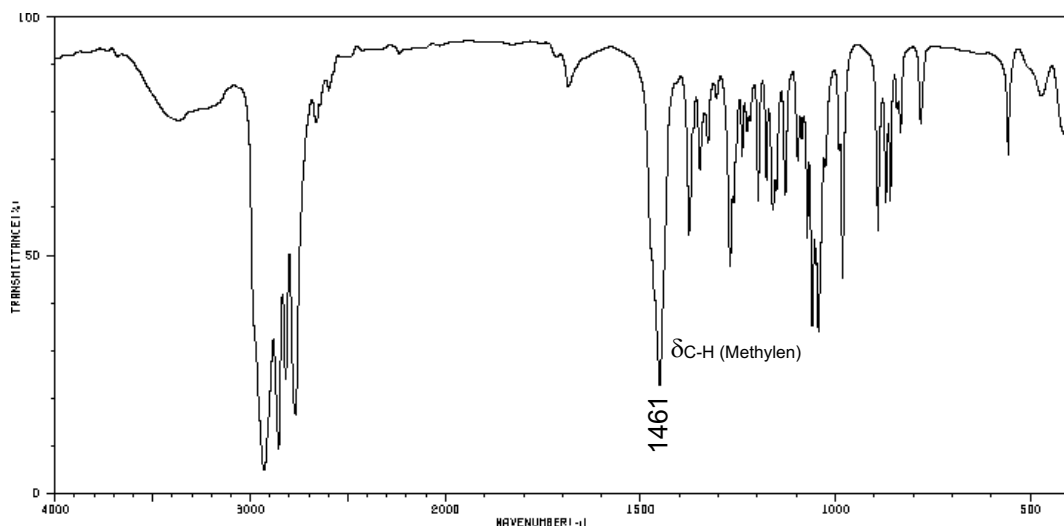
### Cyclohexylamin



### N-Methylcyclohexylamin



### N,N-Dimethylcyclohexylamin





### Absorptionsfrequenzen der C=O Valenzschwingung verschiedener Substanzklassen



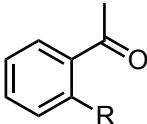
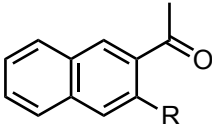
Ist R = Aryl, verringert sich die Wellenzahl im Vergleich zu R = Alkyl um ca. 25 cm<sup>-1</sup>

X	Substanzklasse	Wellenzahlbereich in cm <sup>-1</sup>
Cl	Carbonsäurechlorid	1815 - 1790
OC(O)R	Carbonsäureanhydrid	1850 - 1800
OR	Carbonsäureester	1750 - 1735
H	Aldehyd	1740 - 1720
R	Keton	1725 - 1705
OH	Carbonsäure	1725 - 1700
NR <sub>2</sub>	Carbonsäureamid	1670 - 1630
COO <sup>-</sup>	Carboxylat	1610 - 1550

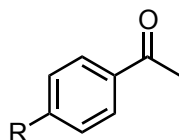
### Abhängigkeit der Absorptionsfrequenz der C=O Valenzschwingung cyclischer Ketone, Ester (Lactone) und Amide (Lactame) von der Ringgröße

	Wellenzahl der C=O Valenzschwingung in cm <sup>-1</sup> für n =			
	1	2	3	4
	1775	1751	1718	1706
	1840	1775	1750	1730
	1750	1717	1670	1669

### Einfluss von intramolekularen Wasserstoffbrücken auf die Absorptionsfrequenz der C=O Valenzschwingung

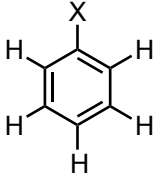
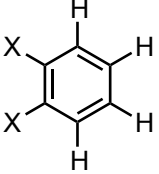
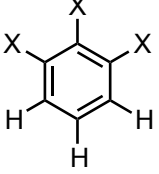
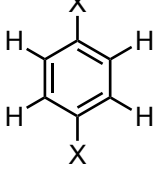
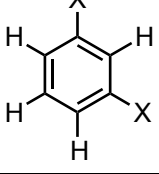
	Wellenzahl der C=O Valenzschwingung in $\text{cm}^{-1}$ (Messung im Film)	
	R = H	1686
	R = OH	1643
	R = H	1673
	R = OH	1659

### Einfluss von Kernsubstituenten auf die Absorptionsfrequenz der C=O Valenzschwingung von Acetophenonen

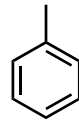
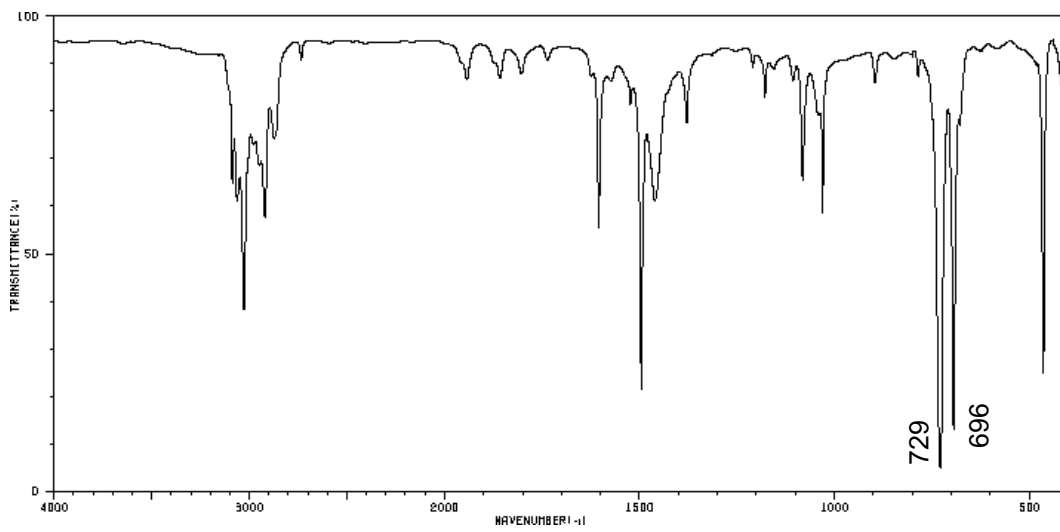


R	Wellenzahl der C=O Valenzschwingung in $\text{cm}^{-1}$ (Messung in $\text{CCl}_4$ )
OCH <sub>3</sub>	1682
CH <sub>3</sub>	1687
H	1691
Cl	1693
NO <sub>2</sub>	1701

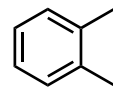
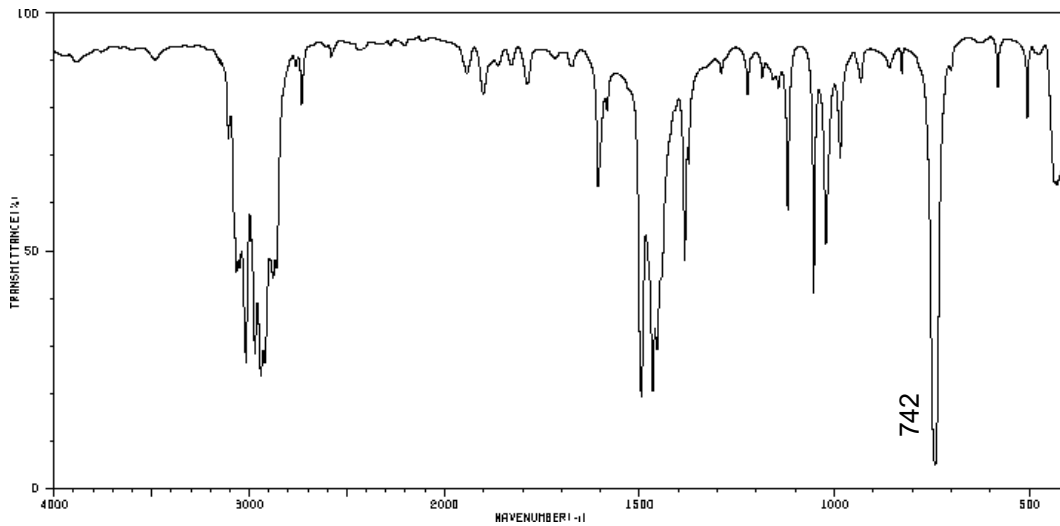
### Absorptionsfrequenzen der C-H Deformationsschwingungen (*out of plane*) von Aromaten in Abhängigkeit des Substitutionsmusters

	Wellenzahl der C-H Deformationsschwingung in $\text{cm}^{-1}$	
	770 - 735 (s) 710 - 685 (s)	gewöhnlich zwei Banden
	760 - 740 (s)	
	800 - 770 (s)	
	840 - 800 (s)	
	900 - 800 (w)	Bande des isolierten H gewöhnlich sehr schwach

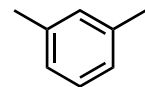
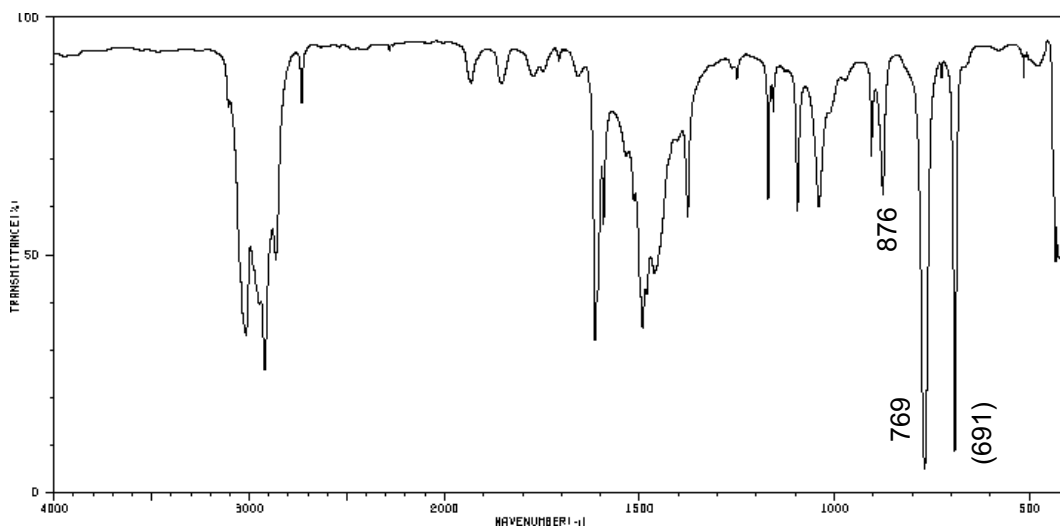
### Toluol



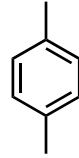
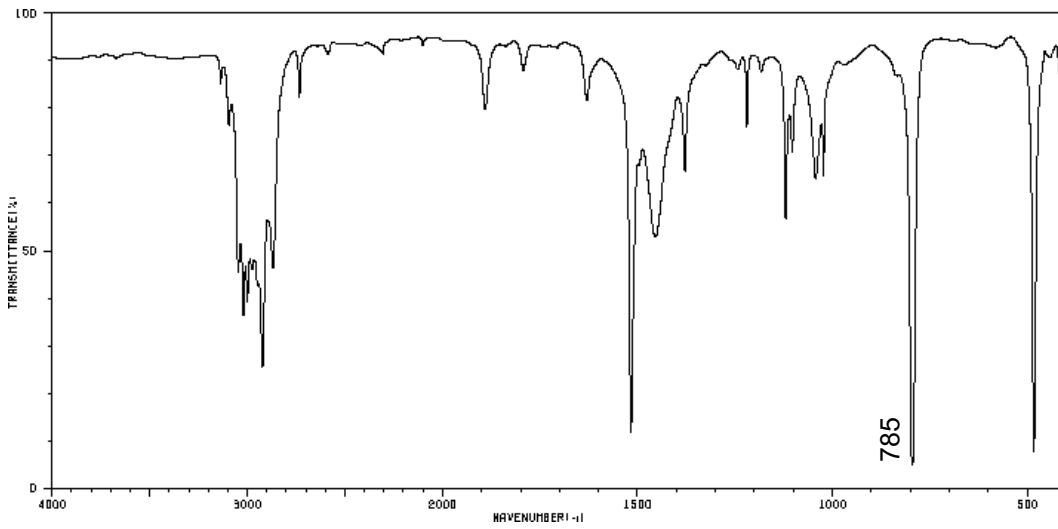
### 1,2-Dimethylbenzol (o-Xylol)



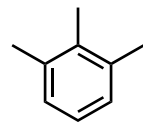
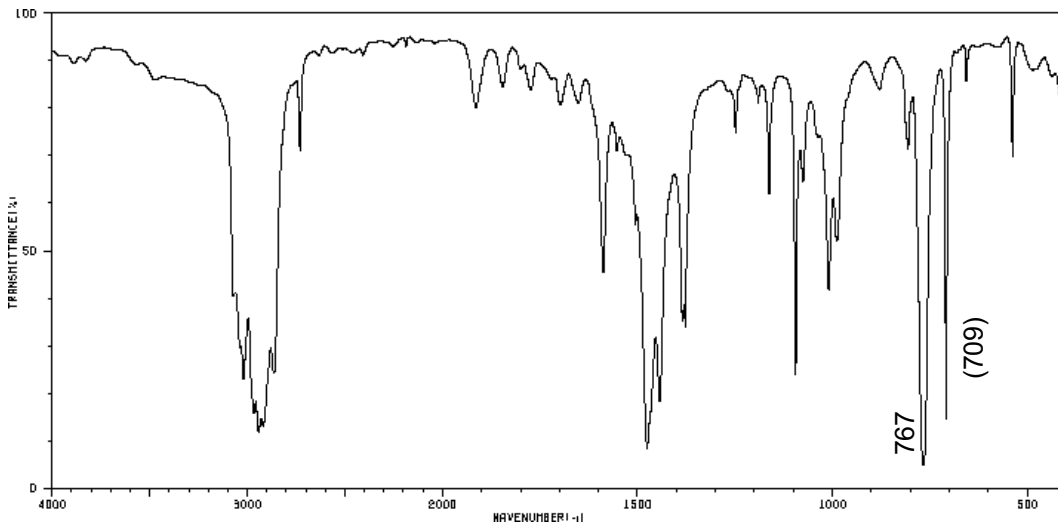
### 1,3-Dimethylbenzol (m-Xylol)



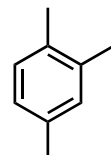
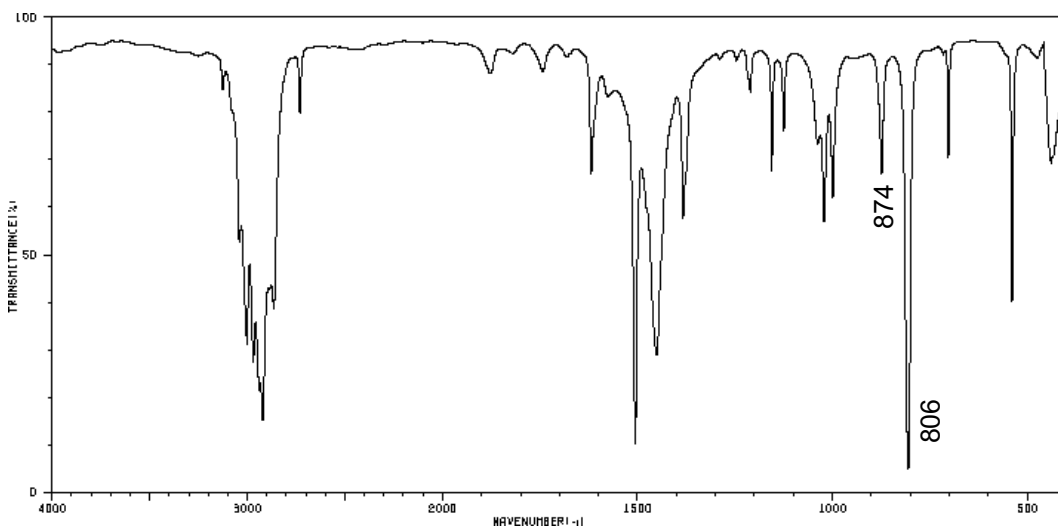
### 1,4-Dimethylbenzol (p-Xylol)



### 1,2,3-Trimethylbenzol



### 1,2,4-Trimethylbenzol



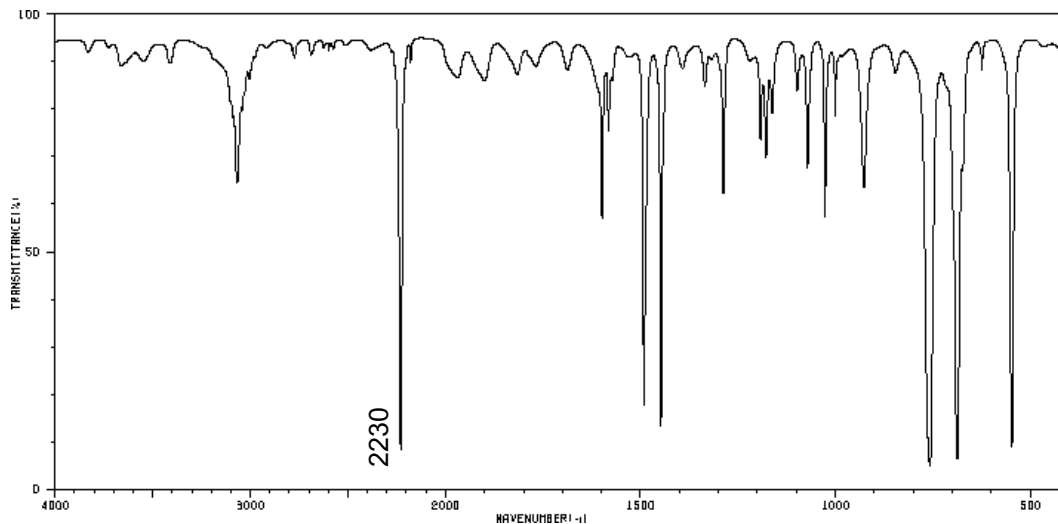
**Absorptionsfrequenzen von Dreifachbindungen**

	Wellenzahl in $\text{cm}^{-1}$	
$-\text{C}\equiv\text{C}-\text{H}$	3300 (s)	C–H Valenzschwingung
	2140 - 2100 (s)	C–C Valenzschwingung
$-\text{C}\equiv\text{C}-$	2260 - 2150 (s)	C–C Valenzschwingung
$-\text{C}\equiv\text{N}$	2260 - 2200 (v)	C–N Valenzschwingung

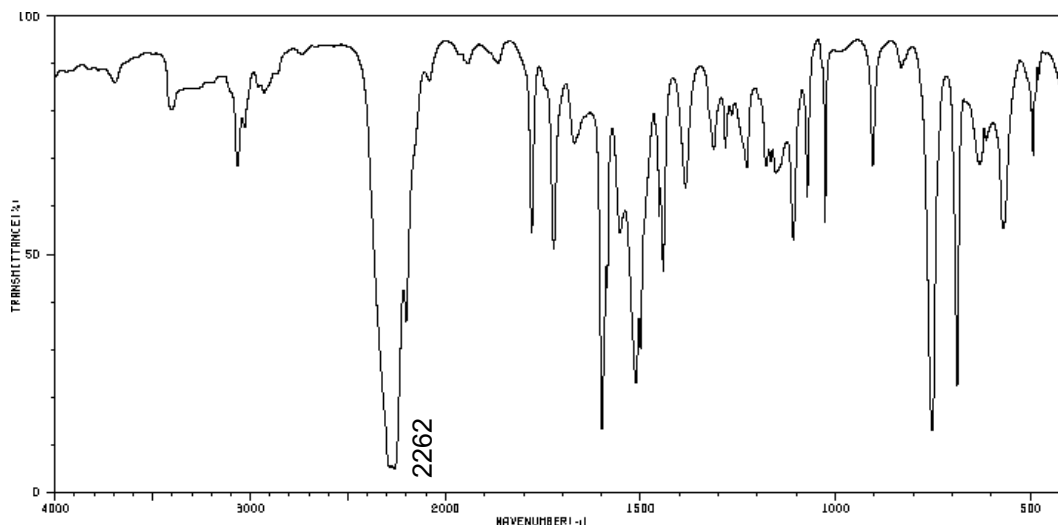
**Absorptionsfrequenzen von kumulierten Doppelbindungen**

	Wellenzahl in $\text{cm}^{-1}$	
$\text{O}=\text{C}=\text{O}$	2349 (s)	
$-\text{N}=\text{N}=\text{N}^{\oplus}$ $\ominus$	2160 - 2120 (s)	
$-\text{N}=\text{C}=\text{O}$	2275 - 2250 (s)	sehr hohe Intensität
$-\text{N}=\text{C}=\text{N}-$	2155 - 2130 (s)	sehr hohe Intensität
$\diagdown \text{C}=\text{C}=\text{C} \diagup$	~ 1950 (s)	
$\diagdown \text{C}=\text{C}=\text{O}$	~ 2150 (s)	

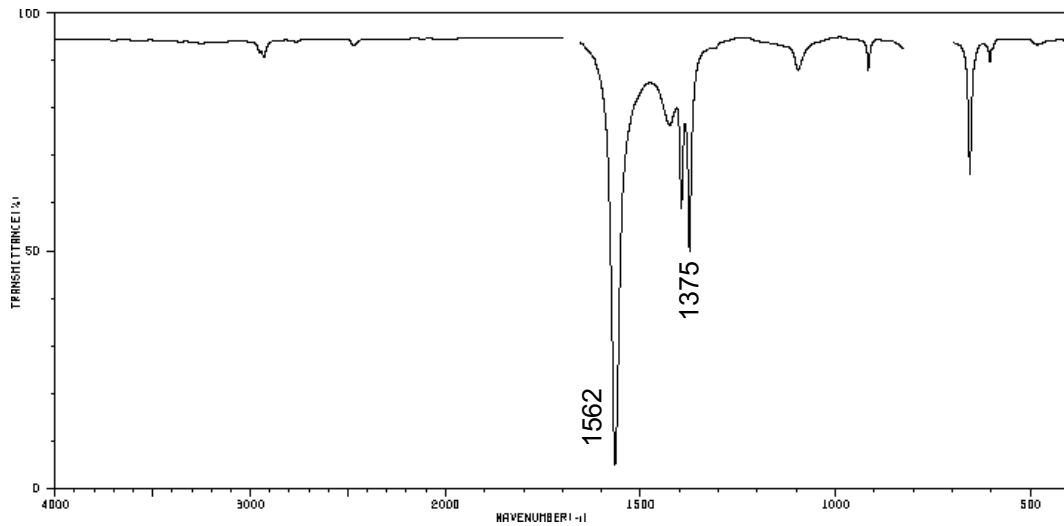
### Benzonitril



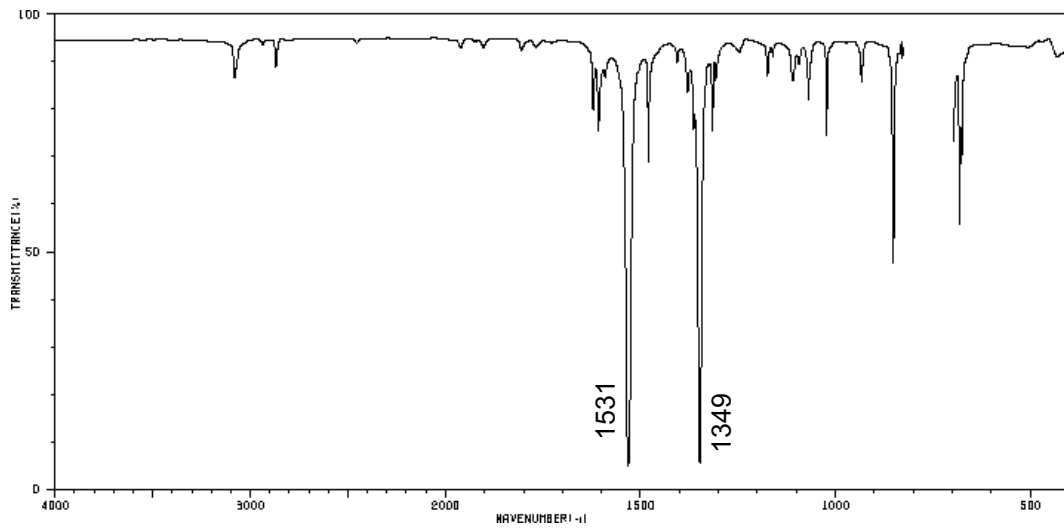
### Phenylisocyanat



### Nitromethan

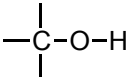
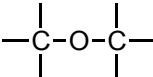
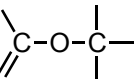
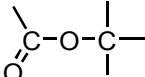


### Nitrobenzol





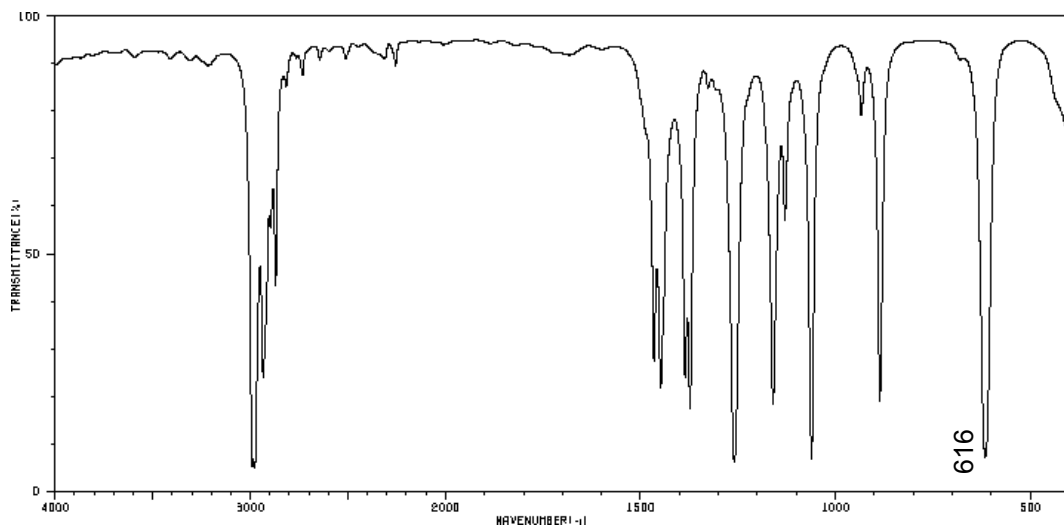
**Absorptionsfrequenzen von C–O Valenzschwingungen**

		Wellenzahlbereich der C–O Valenzschwingung in $\text{cm}^{-1}$
Alkohol		1250 - 1000 (s)
Ether		1150 - 1070 (s)
		1275 - 1200 (s) 1075 - 1020 (s)
Ester		1330 - 1050 (s) (zwei Banden)

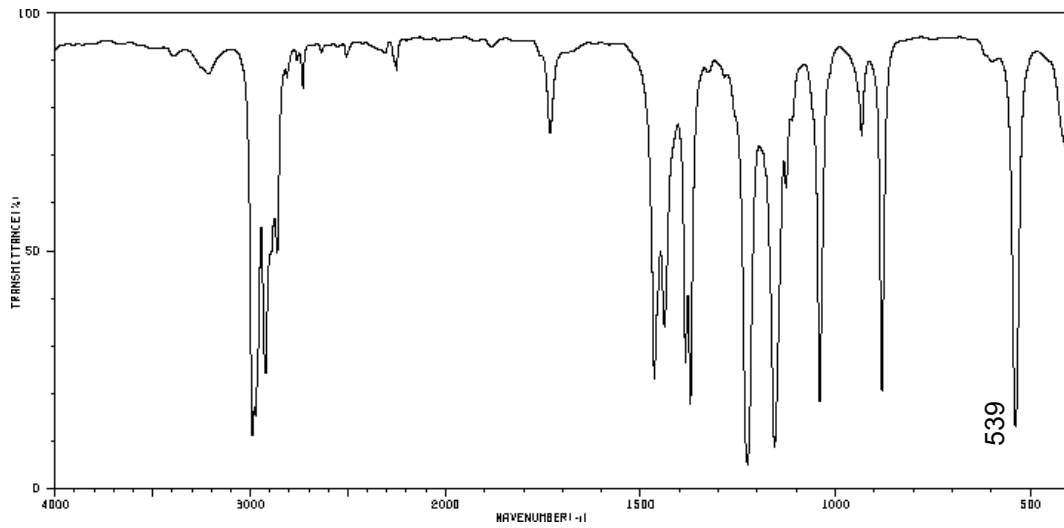
**Absorptionsfrequenzen von C–Hal Valenzschwingungen**

	Wellenzahlbereich der Alkyl–Hal Valenzschwingung in $\text{cm}^{-1}$	Wellenzahlbereich der Aryl–Hal Valenzschwingung in $\text{cm}^{-1}$
C–F	1365 - 1120 (s)	1270 - 1100
C–Cl	830 - 560 (s)	1100 - 1030
C–Br	680 - 515 (s)	1075 - 1030
C–I	~ 500 (s)	~ 1060

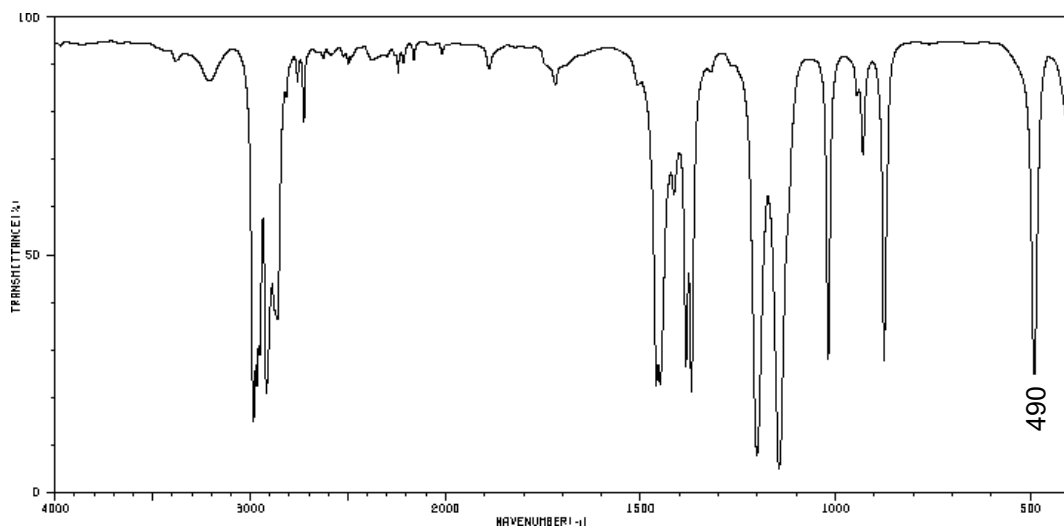
### 2-Chlorpropan



### 2-Bromopropan



### 2-Iodopropan

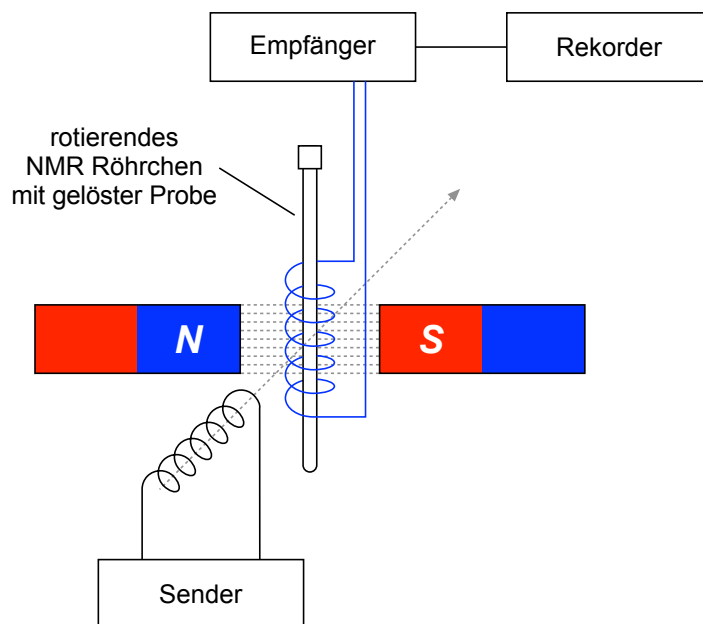


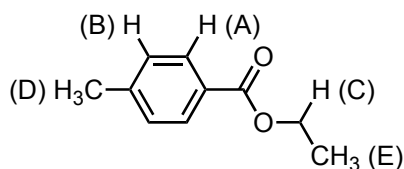
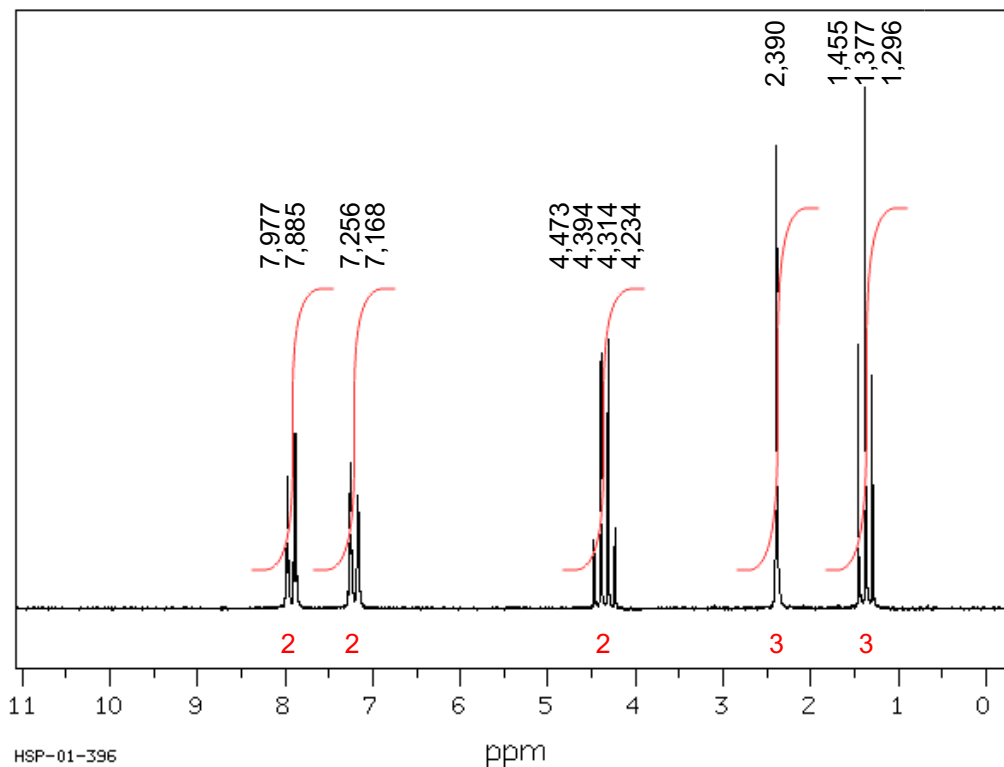
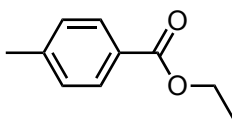
**NMR-aktive Kerne**

Isotop	I	$\gamma \cdot 10^{-7}$ $T^{-1} s^{-1}$	Häufigkeit %	Resonanzfrequenz MHz*
$^1H$	1/2	26,752	99,985	100,0
$^2H$	1	4,107	0,015	15,351
$^{13}C$	1/2	6,728	1,10	25,144
$^{14}N$	1	1,934	99,634	7,224
$^{17}O$	5/2	-3,628	0,038	13,557
$^{19}F$	1/2	25,181	100,0	94,077
$^{31}P$	1/2	10,841	100,0	40,481
$^{33}S$	3/2	2,053	0,76	7,670

\* Bei einem magnetischen Feld der Feldstärke 2,3488 T

### Schematischer Aufbau eines CW-NMR Spektrometers

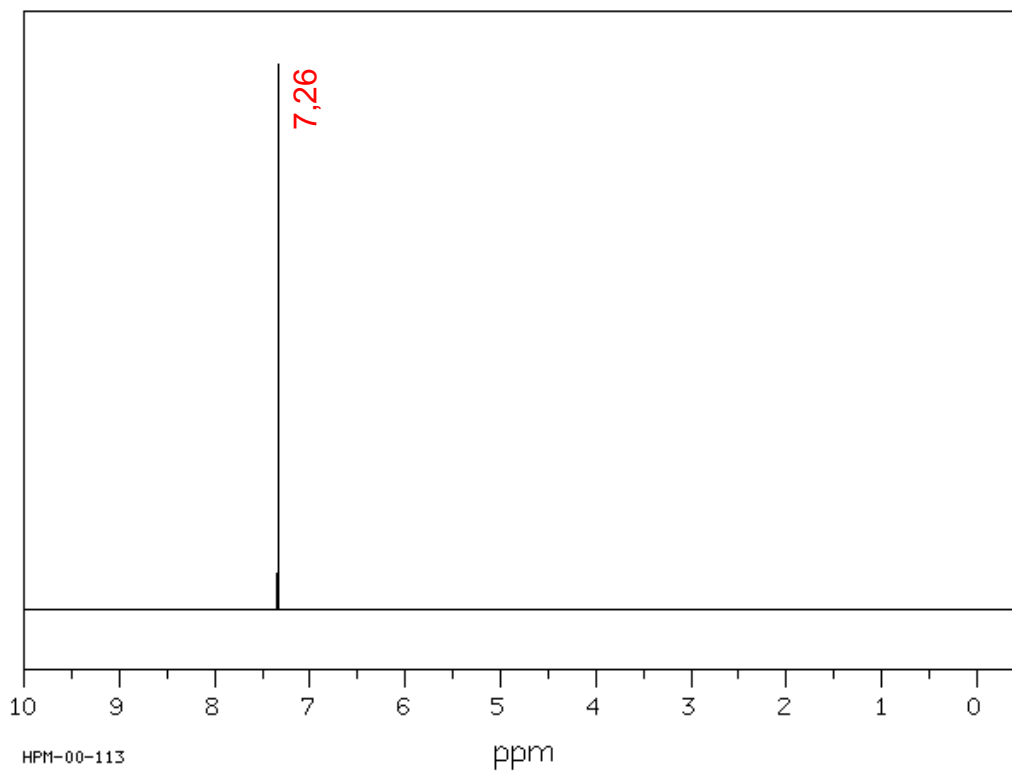


**<sup>1</sup>H-NMR Spektrum von 4-Methylbenzoesäureethylester**(CDCl<sub>3</sub>, 90 MHz)

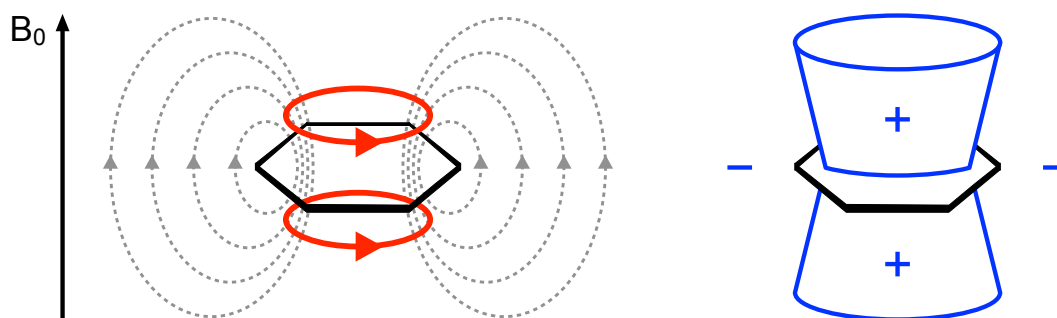
Hz	ppm	Int.	Zuordn.	$\delta$	$J$
714,38	7,977	243			
706,13	7,885	321	A	7,93	$^3J = 8,3$ Hz
650,15	7,260	267			
641,94	7,168	206	B	7,21	$^3J = 8,2$ Hz
400,56	4,473	127			
393,44	4,394	468			
386,31	4,314	494	C	4,35	$^3J = 7,1$ Hz
379,19	4,234	148			
214,00	2,390	848	D	2,39	
130,25	1,455	485			
123,25	1,377	1000	E	1,38	$^3J = 7,1$ Hz
116,06	1,296	427			

### <sup>1</sup>H-NMR Spektrum von Benzol

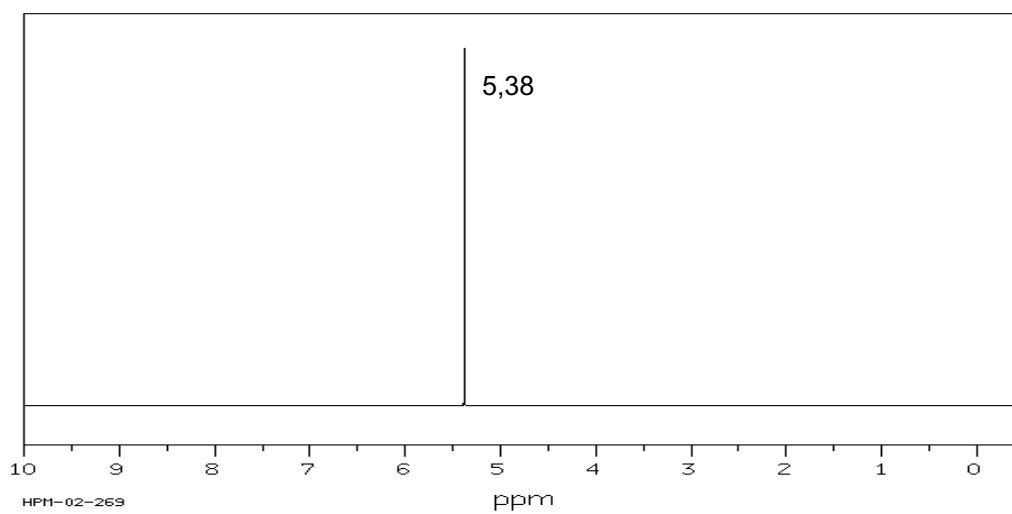
(300 MHz, CDCl<sub>3</sub>)



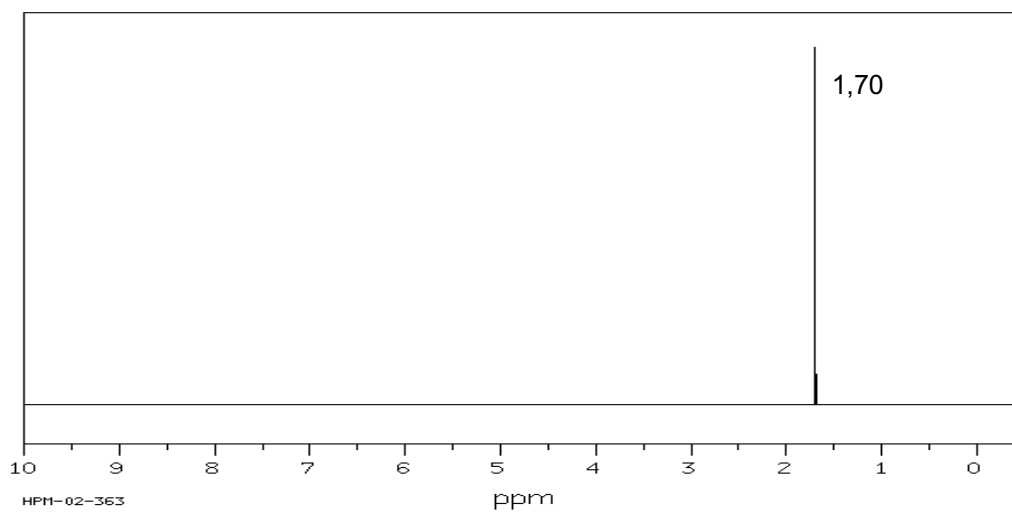
### Ringstrommodell



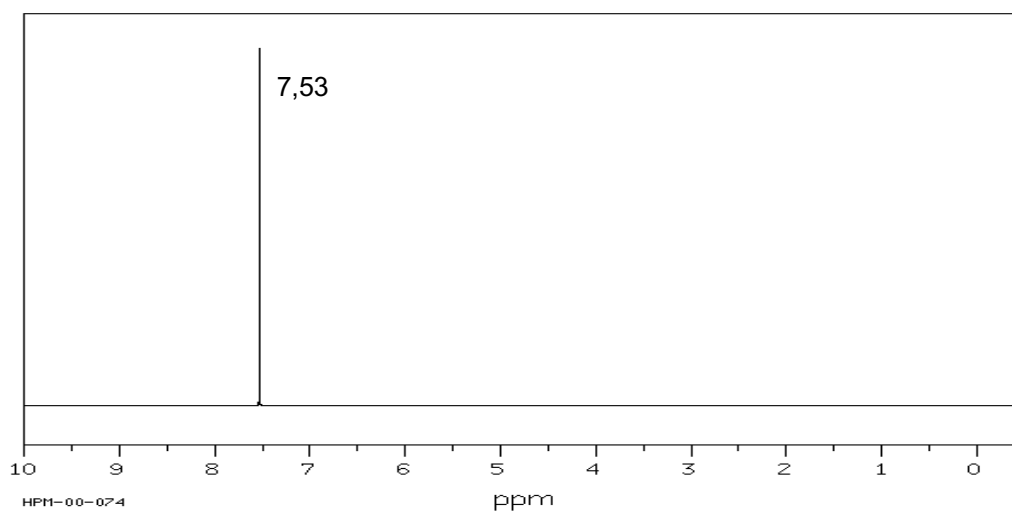
### 1,1-Dichlorethen



### Chloracetylen



### Pentachlorbenzol

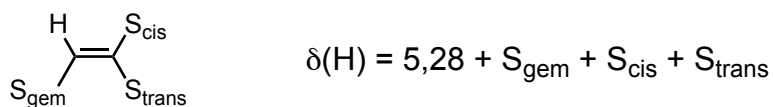


(1,1,1-Trichlorethan  $\delta = 2,80$ )

**Inkrementen zur Abschätzung der Resonanz von Methylenprotonen**  
(Regel von Shoolery)

X-CH <sub>2</sub> -Y	$\delta(\text{CH}_2) = 0,23 + S_x + S_y$		
Substituent	S	Substituent	S
CH <sub>3</sub>	0,47	NR'R''	1,57
CF <sub>3</sub>	1,14	SR	1,64
CR=CR'R''	1,32	I	1,82
C≡CH	1,44	Br	2,33
COOR	1,55	OR	2,36
CONH <sub>2</sub>	1,59	Cl	2,53
COR	1,70	OH	2,56
CN	1,70	OCOR	3,13
C <sub>6</sub> H <sub>5</sub>	1,83	OC <sub>6</sub> H <sub>5</sub>	3,23

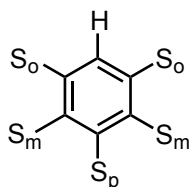
**Inkrementen zur Abschätzung der Resonanz von olefinischen Protonen**  
(Regel von Pascual, Meier und Simon)



Substituent	S <sub>gem</sub>	S <sub>cis</sub>	S <sub>trans</sub>
H	0,00	0,00	0,00
CH <sub>3</sub>	0,44	-0,26	-0,29
Cl	1,00	0,19	0,03
NR <sub>2</sub> (aliph.)	0,69	-1,19	-1,31
OAlkyl	1,18	-1,06	-1,28
OCOCH <sub>3</sub>	2,09	-0,40	-0,67
C <sub>6</sub> H <sub>5</sub>	1,35	0,37	-0,10
CH=CH <sub>2</sub> (konj.)	1,26	0,08	-0,01
COOH (konj.)	0,69	0,97	0,39
NO <sub>2</sub>	1,84	1,29	0,59



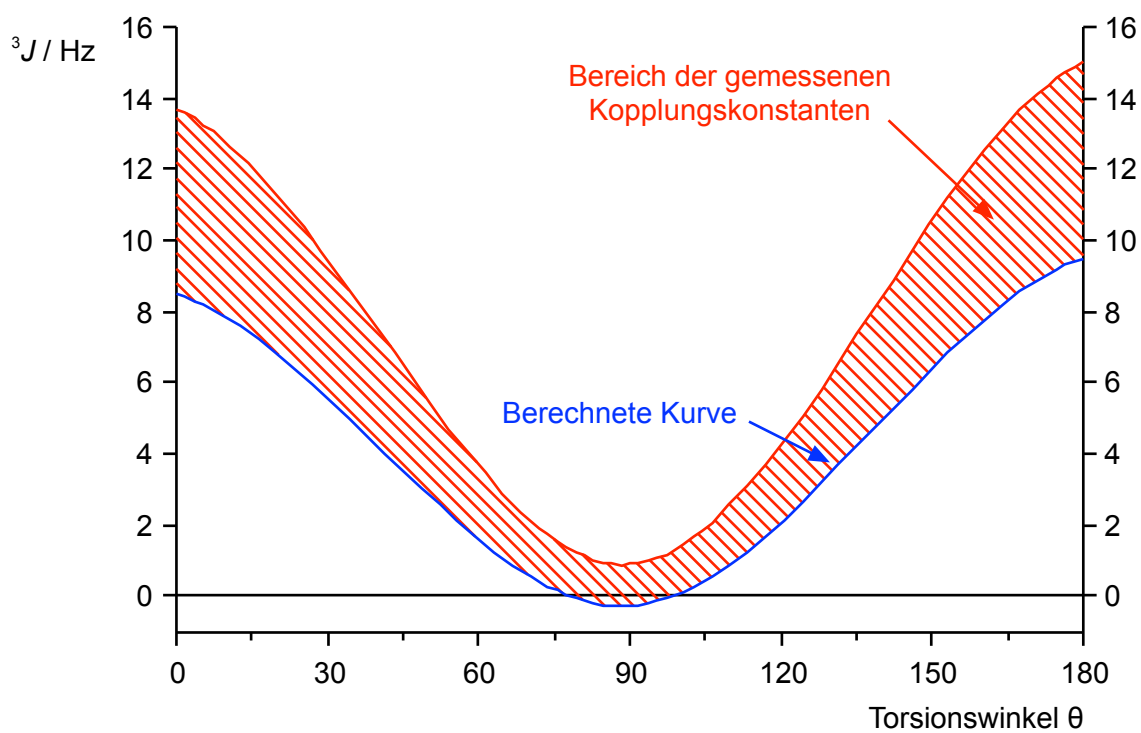
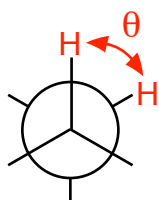
### Inkrementen zur Abschätzung der Resonanz von aromatischen Protonen



$$\delta(\text{H}) = 7,27 + \Sigma(\text{S}_o, \text{S}_m, \text{S}_p)$$

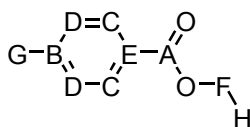
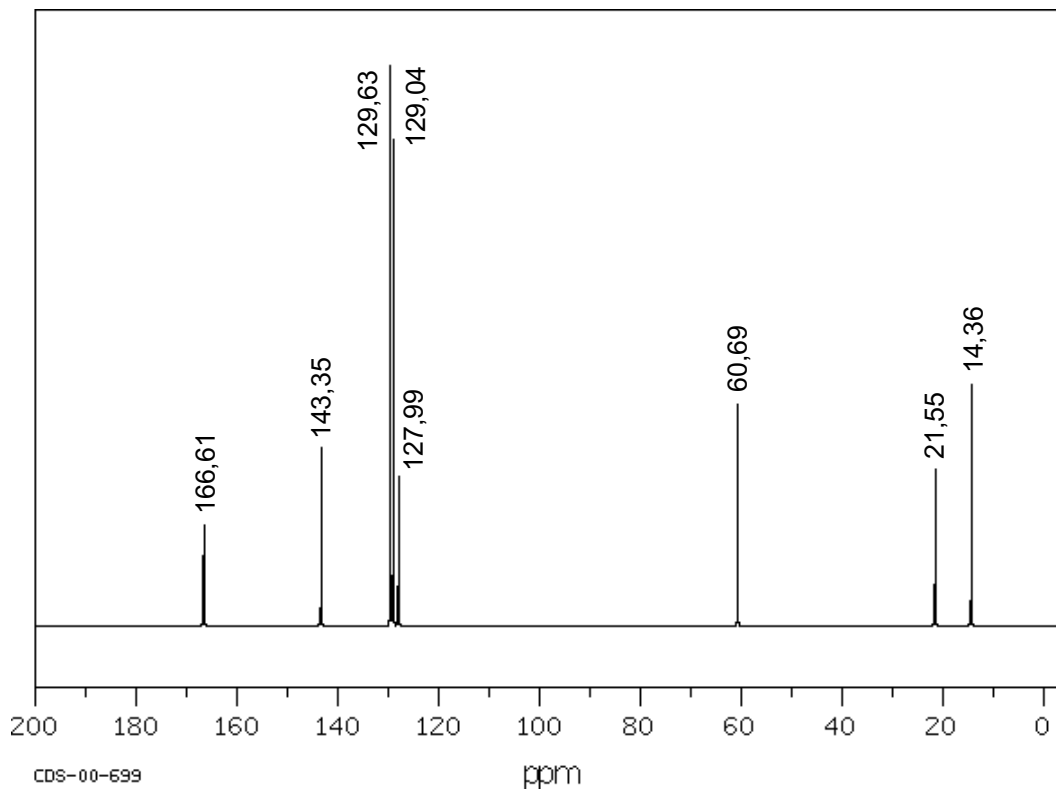
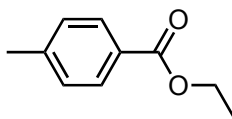
Substituent	S <sub>o</sub>	S <sub>m</sub>	S <sub>p</sub>
CH <sub>3</sub>	-0,17	-0,09	-0,18
Cl	0,02	-0,06	-0,04
OH	-0,50	-0,14	-0,40
OCH <sub>3</sub>	-0,43	-0,09	-0,37
OCOCH <sub>3</sub>	-0,21	-0,02	0,00
NH <sub>2</sub>	-0,75	-0,24	-0,63
C <sub>6</sub> H <sub>5</sub>	0,18	0,00	0,08
CHO	0,58	0,21	0,27
COCH <sub>3</sub>	0,64	0,09	0,30
COOCH <sub>3</sub>	0,74	0,07	0,20
NO <sub>2</sub>	0,95	0,17	0,33

### Karplus Kurve



$$\begin{aligned}
 {}^3J &= 8,5 \cos^2 \theta - 0,28 & \text{für} & & 0^\circ \leq \theta \leq 90^\circ \\
 {}^3J &= 9,5 \cos^2 \theta - 0,28 & \text{für} & & 90^\circ \leq \theta \leq 180^\circ
 \end{aligned}$$

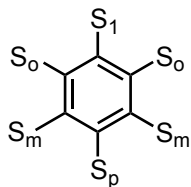
## Spektrum von 4-Methylbenzoesäureethylester

(CDCl<sub>3</sub>, 25 MHz)

ppm	Int.	Zuordn.
166,61	179	A
143,35	318	B
129,63	100	C
129,04	866	D
127,99	264	E
60,69	393	F
21,55	279	G
14,36	428	H

Anwendung des **Inkrement-Systems** zur Zuordnung der aromatischen C-Atome:

$$\begin{array}{lll}
 \text{C(B): } 128,5 + S_1(\text{CH}_3) + S_p(\text{COOEt}) & = 128,5 + 9,2 + 4,3 & = 142,0 \\
 \text{C(C): } 128,5 + S_o(\text{COOEt}) + S_m(\text{CH}_3) & = 128,5 + 1,2 - 0,1 & = 129,6 \\
 \text{C(D): } 128,5 + S_m(\text{COOEt}) + S_o(\text{CH}_3) & = 128,5 - 0,1 + 0,7 & = 129,1 \\
 \text{C(E): } 128,5 + S_1(\text{COOEt}) + S_p(\text{CH}_3) & = 128,5 + 2,0 - 3,1 & = 127,4
 \end{array}$$

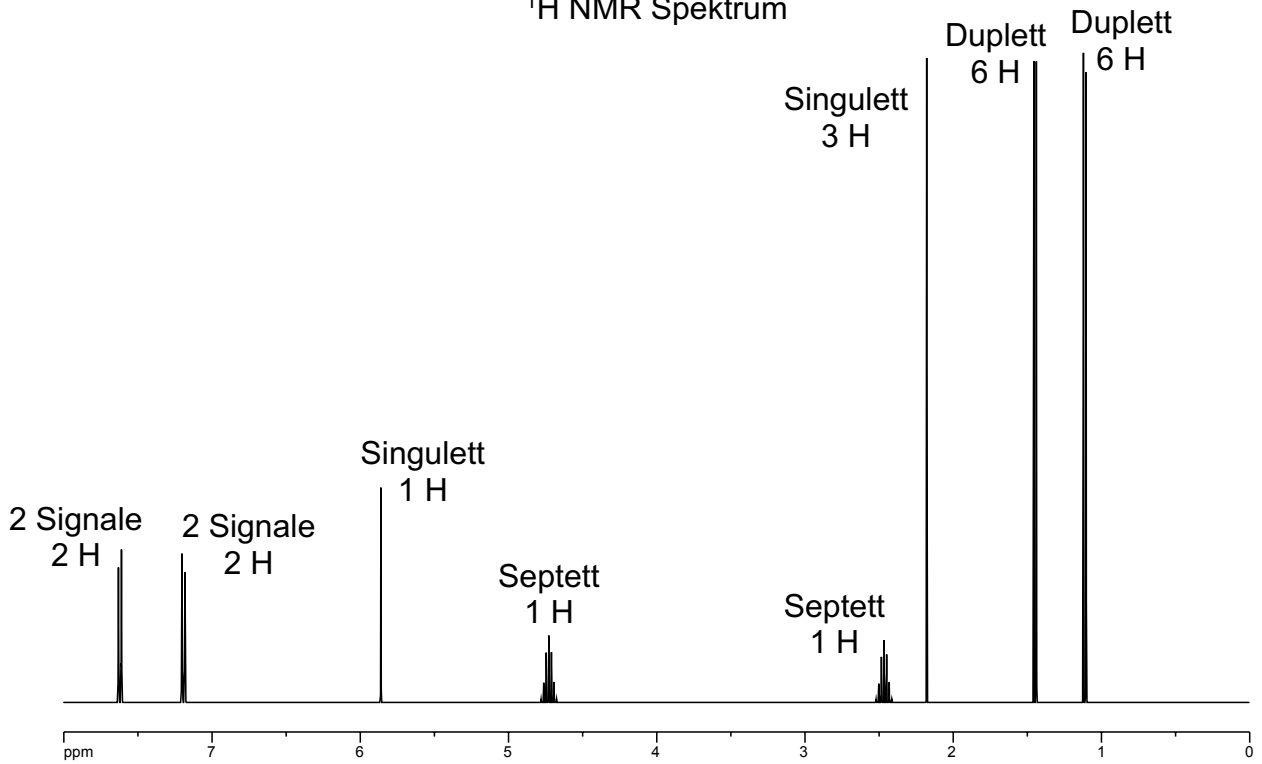
Inkrementen zur Abschätzung der Resonanz von aromatischen  $^{13}\text{C}$ -Kernen

$$\delta(^{13}\text{C}) = 128,5 + \Sigma(S_1, S_o, S_m, S_p)$$

Substituent	$S_1$	$S_o$	$S_m$	$S_p$
$\text{CH}_3$	9,2	0,7	-0,1	-3,1
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
OH	26,9	-12,8	1,4	-7,4
$\text{OCH}_3$	31,4	-14,4	1,0	-7,7
$\text{OCOCH}_3$	22,4	-7,1	0,4	-3,2
$\text{NH}_2$	18,2	-13,4	0,8	-10,0
$\text{C}_6\text{H}_5$	13,1	-1,1	0,4	-1,1
CHO	8,4	1,2	0,5	5,7
$\text{COCH}_3$	8,9	0,1	-0,1	4,4
$\text{COOCH}_3$	2,0	1,2	-0,1	4,3
$\text{NO}_2$	19,9	-4,9	0,9	6,1

## Zweidimensionale NMR Spektroskopie

$^1\text{H}$  NMR Spektrum



$^{13}\text{C}$  NMR Spektrum

