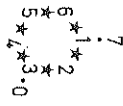
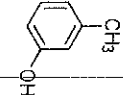


5. ¹H- und ¹³C-NMR-Daten exemplarischer Vertreter der wichtigsten Verbindungsklassen^a

C	δ
1	139,8
2	116,2
3	155,0
4	112,5
5	129,4
6	121,8
7	21,1



Strukturaufklärung mit instrumenteller Analytik, die computergestützte, sollte auf möglichst viele Messungen UV-, IR-, NMR- und MS-Daten mit Hilfe von Computerauswertung direkt zu Strukturvorschlägen zu führen. Das bedingt Programme, die nicht nur auf Daten zurückgreifen können, sondern auch die auf Loos und Empirie aufgebauten Kombinationsprozesse des Experten übernehmen. Die automatische Konvergenz von Programmen ist allerdings höchstens für relativ einfache Strukturprobleme zu erwarten, bei komplexeren Fällen der Dialog mit dem Analytiker, die halbautomatische Lösung anzustreben. Für die instrumentelle Analytik setzt sich hier eine neue, vielversprechende Perspektive.

Alkane

CH ₄	C ₂ H ₆	H ₃ C-CH ₂ -CH ₃	H ₃ C-CH ₂ -CH ₂ -CH ₃	H ₃ C-CH ₂ -CH ₂ -CH ₂ -CH ₃
-2,3	6,5	16,0	16,3	13,0
0,23	0,86	0,91	1,33	0,90

Methan Ethan Propan Butan 2-Methylpropan (isobutan)

H ₃ C-CH ₂ -CH ₂ -CH ₂ -CH ₂ -CH ₂ -CH ₃	H ₃ C-CH ₂ -CH ₂ -CH ₂ -CH ₂ -CH ₂ -CH ₂ -CH ₃	H ₃ C-CH ₂ -CH ₂ -CH ₂ -CH ₂ -CH ₂ -CH ₂ -CH ₂ -CH ₃
13,7	22,8	32,1
0,88	~1,27	~1,27

2,2-Dimethylpropan (Neopentan) n-Octan 2,2,4-Trimethylpentan (isooctan)

H ₃ C-C(CH ₃) ₃	H ₃ C-C(CH ₃) ₂ -CH ₂ -CH ₂ -CH ₂ -CH ₂ -CH ₂ -CH ₂ -CH ₃	H ₃ C-C(CH ₃) ₂ -CH ₂ -CH ₂ -CH(CH ₃) ₂ -CH ₃
131,6	13,7	30,2
0,93	~1,27	0,91

Alkene

H ₂ C=CH ₂	H ₂ C=CH-CH ₃	H ₃ C-CH=CH-CH ₃	H ₃ C-CH=CH-CH ₂ -CH ₃
123,3	135,3	135,3	124,2
5,28	4,95	27,4	13,4

Ethylen 1-Buten (Z)-2-Buten (E)-2-Buten

H ₂ C=CH ₂	H ₂ C=CH-CH ₂ -CH ₃	H ₃ C-CH=CH-CH ₃	H ₃ C-CH=CH-CH ₂ -CH ₃
113,3	133	133	125,4
4,80	141,8	118,6	5,43

2-Methylpropen 2-Methyl-2-buten 2,3-Dimethyl-2-buten

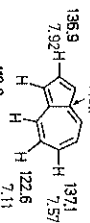
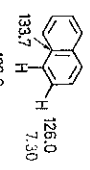
H ₂ C=C(CH ₃) ₂	H ₃ C-C(CH ₃)=CH-CH ₃	H ₃ C-C(CH ₃)=C(CH ₃) ₂
113,2	133	133
5,05	118,6	118,6

1-Octen 1,3-Butadien 2,3-Dimethyl-1,3-butadien

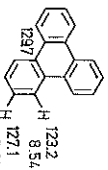
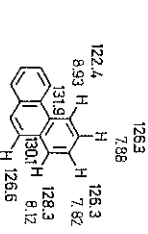
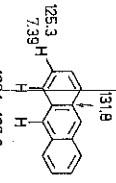
H ₂ C=CH-CH ₂ -CH ₂ -CH ₂ -CH ₂ -CH ₂ -CH ₂ -CH ₃	H ₂ C=CH-CH=CH ₂	H ₃ C-C(CH ₃)=CH-CH=CH ₂
113,2	113,2	113,0
5,05	4,85	4,95

^a Die schwarz gedruckten Zahlen geben die δ-Werte der ¹³C-Signale an, die grünen Zahlen die δ-Werte der ¹H-Resonanzen. Die meisten Angaben beziehen sich auf Messungen in CDCl₃ oder CCl₄ mit TMS als internem Standard. Anstelle des Dezimalkommata wird in dieser Übersicht der Punkt verwendet, der sich bei der Angabe von chemischen Verschiebungen allgemein durchgesetzt hat.

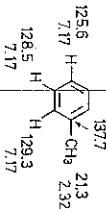
Aromatische Kohlenwasserstoffe



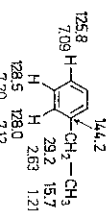
Benzol



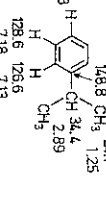
Anthracen



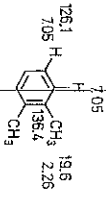
Phenanthren



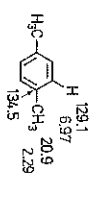
Triphenylen



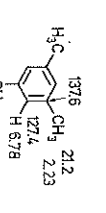
Toluol



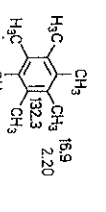
Ethylbenzol



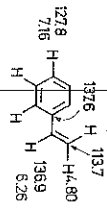
Isopropylbenzol



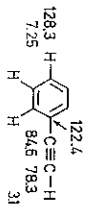
t-Butylbenzol



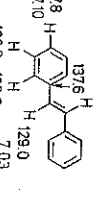
1,2-Dimethylbenzol (o-Xylol)



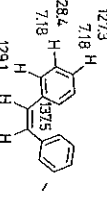
1,4-Dimethylbenzol (p-Xylol)



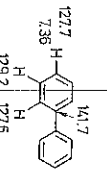
1,3,5-Trimethylbenzol (Mesitylen)



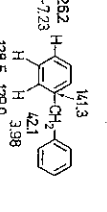
Hexamethylbenzol



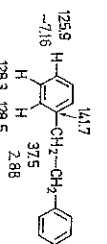
Styrol



Phenylacetylen



(E)-1,2-Diphenylethylen (E-Stilben)



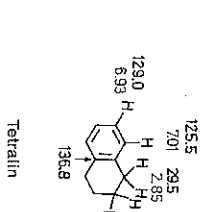
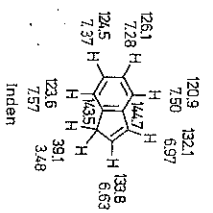
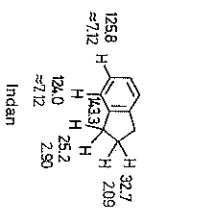
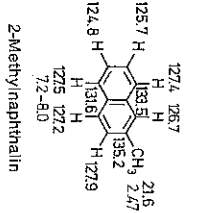
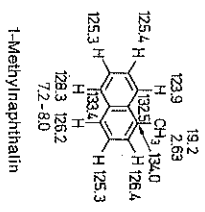
(Z)-1,2-Diphenylethylen (Z-Stilben)



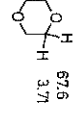
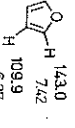
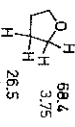
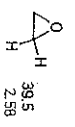
Diphenyl

Diphenylmethan

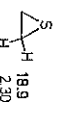
1,2-Diphenylethan



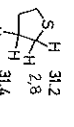
Heterocyclen



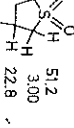
Oxiran (Ethylenoxid)



Tetrahydrofuran



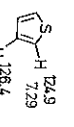
Furan



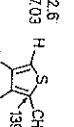
1,4-Dioxan



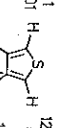
Thiiran (Ethylen-sulfid)



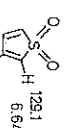
Tetrahydrothiophen



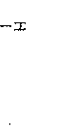
Sulfolan



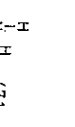
Thiophen-1,1-dioxyd (nicht isolierbar)



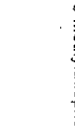
Thiophen



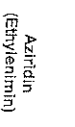
2-Methylthiophen



3-Methylthiophen



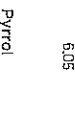
Adiridin (Ethylenimin)



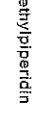
Pyrolidin



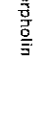
Pyrrrol

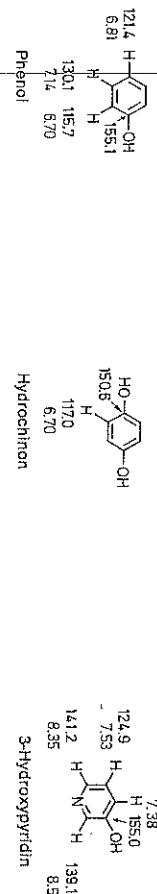
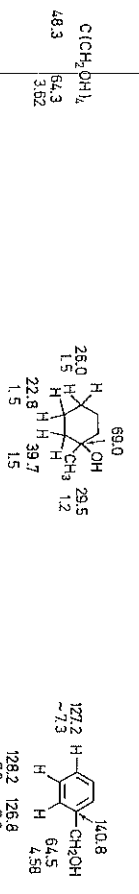


N-Methylpiperdin

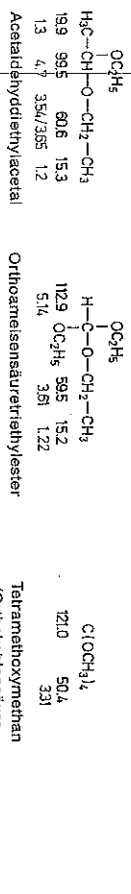
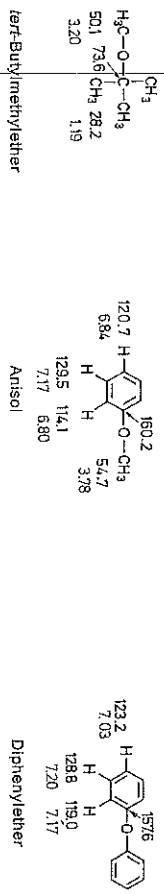
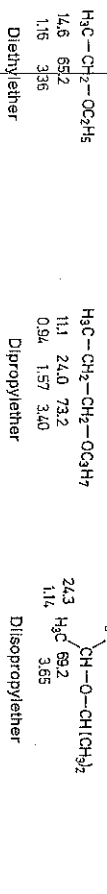


Morpholin

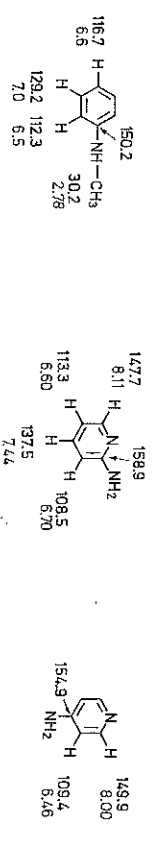
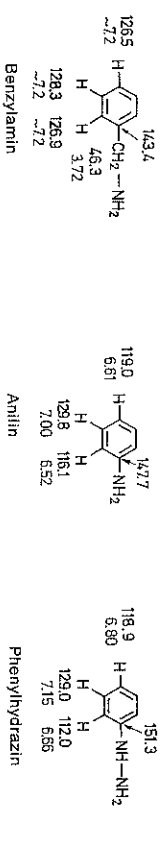
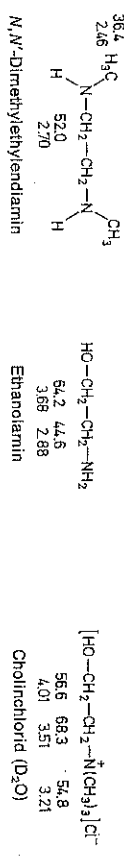
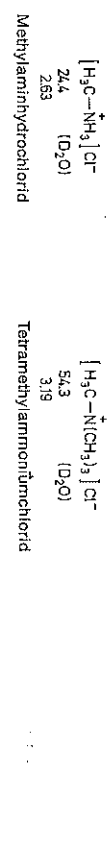
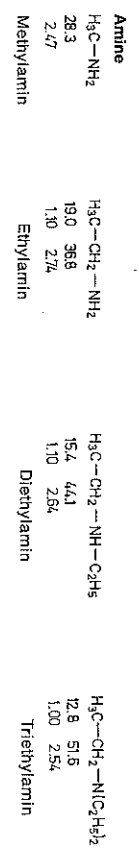
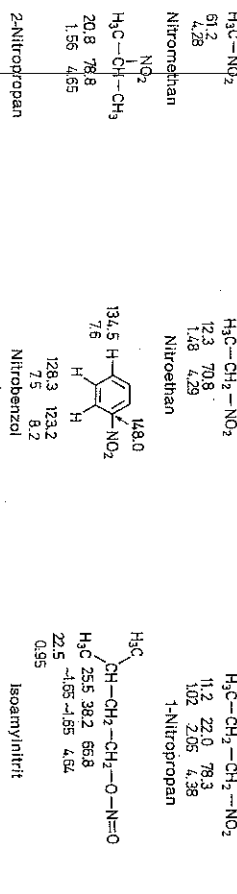




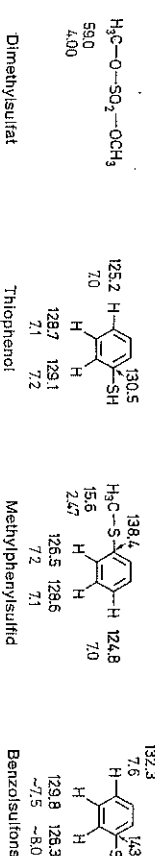
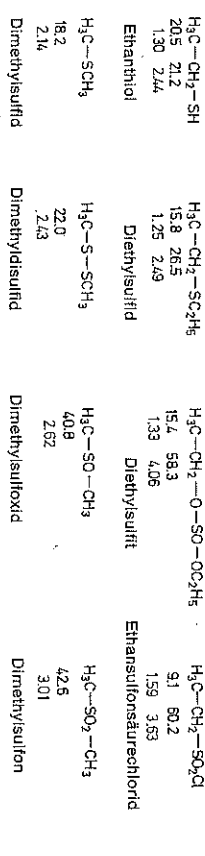
Ether (Acetale, Orthoester)



Nitro-Verbindungen, Salpetersäureester



Schwefel-Verbindungen



Phosphor-Verbindungen

<chem>H3C-CH2-P(C2H5)2</chem> 10.3, 19.5 0.99, 1.27	<chem>H3C-CH2-P(C2H5)Cl</chem> 8.9, 27.6 0.98, 1.56	<chem>H3C-CH2-PCl2</chem> 7.2, 36.2 0.95, 1.82
Triethylphosphin	Chlor(diethyl)phosphin	Dichlor(ethyl)phosphin

<chem>H3C-CH2-O-P(OC2H5)2</chem> 17.4, 58.0 1.28, 3.91	<chem>H3C-CH2-O-P(OC2H5)2</chem> 15.9, 63.4 1.35, 4.12
Triethylphosphit (Phosphordigäsuretriethyl ester)	Triethylphosphat (Phosphorsäuretriethyl ester)

<chem>H-C6H4-P(C6H5)2</chem> 128.5, 137.2 128.4, 133.6 7.2-7.3	<chem>H-C6H4-P(C6H5)2</chem> 132.0, 132.0 7.5	<chem>H-C6H4-P(OC2H5)2</chem> 132.7, 132.7 128.6, 132.2 7.5, 7.75	<chem>H-C6H4-P(OC2H5)2</chem> 125.5, 150.4 7.25
Triphenylphosphin	Triphenylphosphinioxid (Phosphorsäuretriphenyl ester)	Triphenylphosphat (Phosphorsäuretriphenyl ester)	Triphenylphosphat (Phosphorsäuretriphenyl ester)

<chem>H3C-CHO</chem> 30.8, 199.9 2.20, 9.80	<chem>H3C-CH2-CHO</chem> 13.3, 15.7, 45.7 0.99, 1.52, 2.42, 9.80	<chem>H3C-CHO</chem> 18.2, 2.03 153.7, 134.9 6.87, 9.80	<chem>H3C-CHO</chem> 127.5, 132.0 7.3
Acetaldehyd	Butanal	(E)-Crotonaldehyd	Phenylacetaldehyd

<chem>H-C6H5-CHO</chem> 134.2, 137.5 7.55	<chem>H-C6H5-CHO</chem> 136.4, 110.0 128.5, 152.5 131.0, 131.0 7.45, 7.45	<chem>H-C6H5-CHO</chem> 134.6, 143.3 7.78, 7.78 128.1, 136.4 7.22, 7.78	<chem>H-C6H5-CHO</chem> 127.3, 137.1 7.18, 7.18 124.9, 136.4 7.41, 7.41
Benzaldehyd	(E)-Zimtaldehyd	Triphenyl-2-aldehyd	Triphenyl-3-aldehyd

<chem>H3C-CO-CH3</chem> 30.6, 205.6 2.09	<chem>H3C-CO-CH2-CH3</chem> 27.1, 205.3, 35.2, 7.0 2.13	<chem>H3C-CO-CH(CH3)-CH3</chem> 27.1, 21.2, 41.3, 17.6 2.13	<chem>H3C-CO-CH(CH3)-CH2-CH3</chem> 24.5, 31.2, 8.0 2.11
Aceton	2-Butanon (Methyl-ethyl-keton)	3-Methyl-2-butanon (Methyl-isopropyl-keton)	3,3-Dimethyl-2-butanon (Pivalon)

<chem>F3C-CO-CH3</chem> 115.6, 187.4, 23.1 2.43	<chem>H3C-CO-CH(OH)-CH3</chem> 24.9, 211.2, 73.1, 19.4 2.20, 4.22, 1.36	<chem>H3C-CO-CH(OH)-CH3</chem> 18.0, 208.6 197.0, 26.6 162.7, 133.2 5.99, 6.18
1,1,1-Trifluoressig	3-Hydroxy-2-butanon (Aceton)	(E)-3-Penten-2-on

<chem>Cyclopentanone</chem> 213.5, 22.0, 20.2, 36.7, 2.06	<chem>Cyclohexanone</chem> 238.8, 208.5, 28.5, 40.4, 2.22	<chem>Bicyclo[2.2.1]heptan-2-on (Norcampher)</chem> 150.6, 129.5, 6.0, 199.5, 25.3, 22.3, 37.7, 1.4-2.7
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<chem>H3C-CO-CH2-CHO</chem> 23.3, 197.7, 2.33	<chem>HO-CO-CH=CH-CO-OH</chem> (Male C) 189.5	<chem>H3C-CO-CH2-CH2-CO-CH3</chem> 134.7, 194.3 128.9, 129.7 7.5, 7.88
2,3-Butandion (Diaceyl)	Quadratsäure	Benzil

<chem>H3C-CO-CH3</chem> 19.4, 201.9 5.82, 3.62, 30.2, 2.17	<chem>H3C-CO-CH3</chem> 191.4, 100.3, 5.57	<chem>H3C-CO-CH2-CH2-CO-CH3</chem> 29.6, 206.9, 37.0, 2.72
Acetylacetone (2,4-Pentandion)	Acetophenon	2,5-Hexandion

<chem>H3C-CO-CH2-Ph</chem> 134.3, 206.0, 50.7, 2.15	<chem>H3C-CO-CH2-Ph</chem> 131.3, 174.5, 195.7, 24.6, 2.55	<chem>H3C-CO-CH2-Ph</chem> 132.2, 137.9, 7.8, 195.2
Phenyl-2-propanon (Benzylmethylketon)	Acetophenon	Benzophenon

<chem>1,4-Naphthochinon</chem> 187.0, 136.4, 6.78	<chem>1,4-Naphthochinon</chem> 139.7, 70.9, 130.8, 6.34	<chem>1,4-Naphthochinon</chem> 133.7, 7.71, 131.8, 136.2, 139.5, 184.7, 7.03
p-Benzochinon	o-Benzochinon	1,4-Naphthochinon

