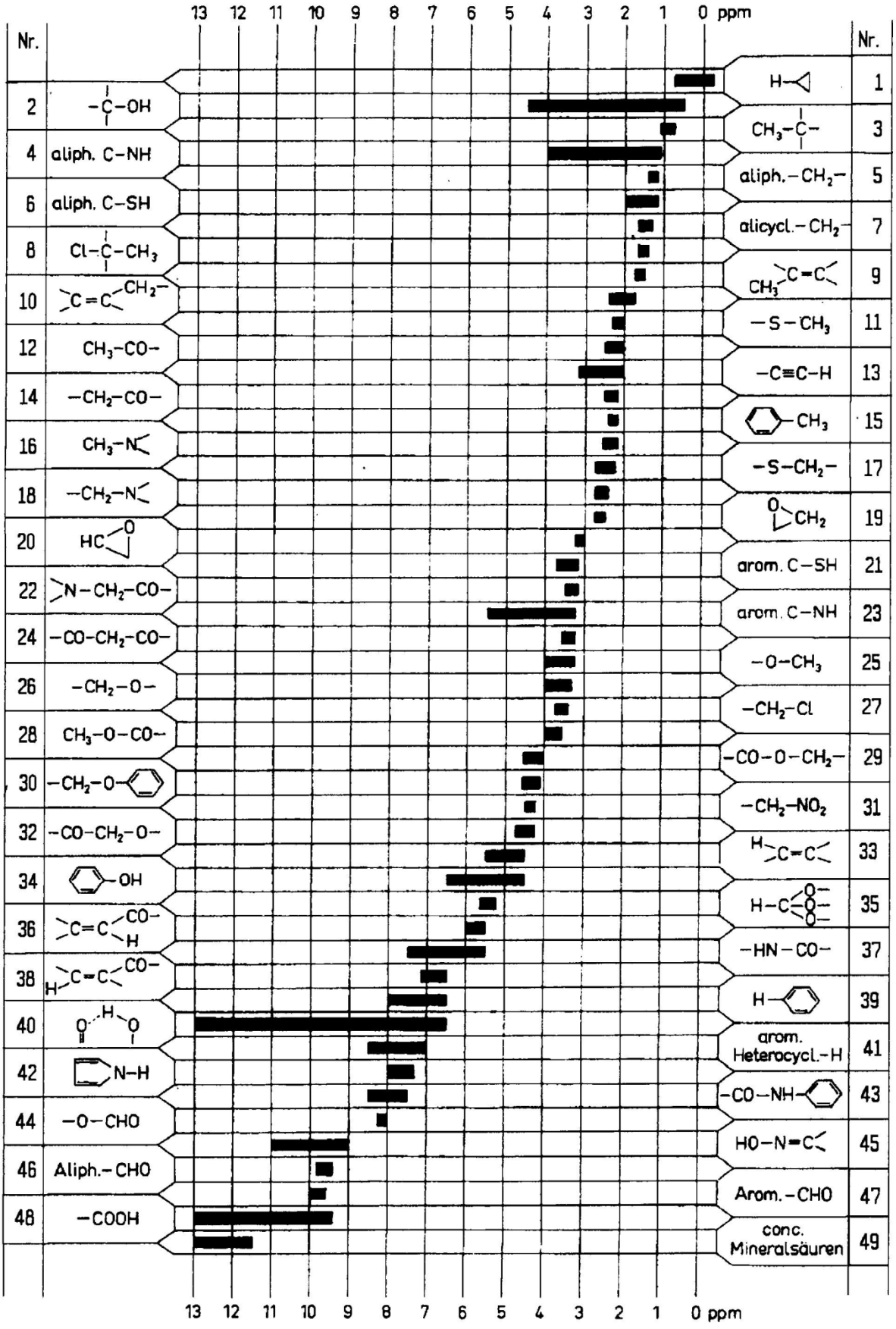
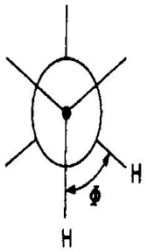
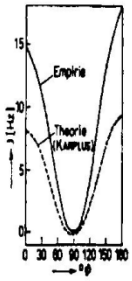
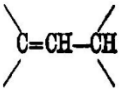
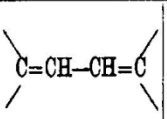
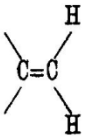
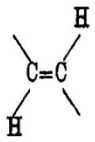
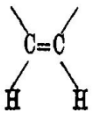
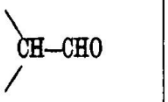
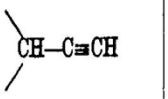
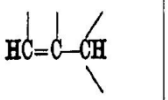
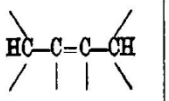
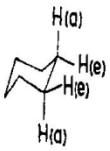
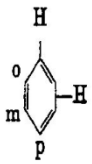
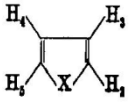
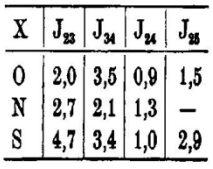
## $^1$H-NMR - Spektroskopie - Chemische Verschiebungen



## $^1$H Kopplungskonstanten

| Struktur | J | Bemerkungen |
|---|---|---|
|  | 10…18 | $J_{gem}$ hängt unter anderem vom Winkel $\Phi$ ab:<br>  <br>$CH_4$: $\|J\| = 12{,}4$ Hz $\Phi = 109°$<br>  : $\|J\| = 4$ Hz $\Phi = 118°$ |
|  | 2… 9 | J hängt vom Winkel $\Phi$ ab[2]:<br>  <br>  |
| | 6… 7 | Wenn frei drehbar |
|  | 4…10 | |

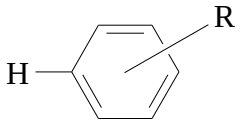
| Struktur | J | Bemerkungen |
|---|---|---|
|  | 10…13 | |
|  | 0… 3,5 | $J_{gem}$, $J_{cis}$ und $J_{trans}$ hängen stark von der Elektronegativität der Substituenten ab. |
|  | 12… 18 | |
|  | 5… 14 | |
|  | 1… 3 | |
|  | 2… 3 | Übersicht über Long-range Kopplung[3] |
|  | 0… 3 | |
|  | 0… 1,6 | |
|  | $J_{ee}$: 2… 4<br>$J_{ea}$: 2… 4<br>$J_{aa}$: 6…13 | |

| Struktur | J | Bemerkungen |
|---|---|---|
|  | o: 7…10<br>m: 2… 3<br>p: 0… 1 | |
|  | 0,9…4,7 |  |

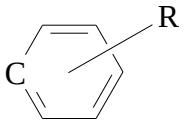
| X | $J_{23}$ | $J_{34}$ | $J_{24}$ | $J_{25}$ |
|---|---|---|---|---|
| O | 2,0 | 3,5 | 0,9 | 1,5 |
| N | 2,7 | 2,1 | 1,3 | – |
| S | 4,7 | 3,4 | 1,0 | 2,9 |

## $^{1}H$ und $^{13}C$-NMR- Spektroskopie: Chemische Verschiebung der aromatischen Kerne

$\delta = 7.26 + \Sigma I$




$\delta = 128.5 + \Sigma I$




| | $^{1}H$ | | | $^{13}C$ | | | |
|---|---|---|---|---|---|---|---|
| Substituent | $I_{ortho}$ | $I_{meta}$ | $I_{para}$ | $I_{direkt}$ | $I_{ortho}$ | $I_{meta}$ | $I_{para}$ |
| -H | 0.00 | 0.00 | 0.00 | 0.0 | 0.0 | 0.0 | 0.0 |
| $-CH_3$ | -0.18 | -0.10 | -0.20 | 9.3 | 0.6 | 0.0 | -3.1 |
| $-C_2H_5$ | -0.15 | -0.06 | -0.18 | 15.7 | -0.6 | -0.1 | -0.8 |
| $-CH(CH_3)_2$ | -0.13 | -0.08 | -0.18 | 20.1 | -2.0 | 0.0 | -2.5 |
| $-C(CH_3)_3$ | 0.02 | -0.09 | -0.22 | 22.1 | -3.4 | -0.4 | -3.1 |
| $-C=CH_2$ | 0.06 | -0.03 | -0.10 | 7.6 | -1.8 | -1.8 | -3.5 |
| -C#CH | 0.15 | -0.02 | -0.01 | -6.1 | 3.8 | 0.4 | -0.2 |
| | | | | | | | |
| $-CH_2OH$ | -0.07 | -0.07 | -0.07 | | | | |
| $-CH_2NH_2$ | 0.01 | 0.01 | 0.01 | | | | |
| $-CH_2Cl$ | 0.00 | 0.01 | 0.00 | 9.1 | 0.0 | 0.2 | -0.2 |
| -COOH | 0.85 | 0.18 | 0.25 | 2.4 | 1.6 | -0.1 | 4.8 |
| -COOR | | | | 2.0 | 1.0 | 0.0 | 4.5 |
| $-COCH_3$ | 0.62 | 0.14 | 0.21 | 9.3 | 0.2 | 0.2 | 4.2 |
| $-CONH_2$ | 0.61 | 0.10 | 0.17 | | | | |
| -CHO | 0.56 | 0.22 | 0.29 | 7.5 | 0.7 | -0.5 | 5.4 |
| -C#N | 0.36 | 0.18 | 0.28 | -16.0 | 3.8 | 0.7 | 4.3 |
| -COCl | 0.84 | 0.20 | 0.36 | 4.6 | 2.9 | 0.6 | 7.0 |
| | | | | | | | |
| -OH | -0.56 | -0.12 | -0.45 | 26.9 | -12.6 | 1.6 | -7.6 |
| $-O-CH_3$ | -0.48 | -0.09 | -0.44 | 31.3 | -15.0 | 0.9 | -8.1 |
| $-O-C_6H_5$ | -0.29 | -0.05 | -0.23 | 29.1 | -9.5 | 0.3 | -5.3 |
| $-O-COCH_3$ | -0.25 | 0.03 | -0.13 | 23.0 | -6.0 | 1.0 | -2.0 |
| | | | | | | | |
| | | | | | | | |
| $-NH_2$ | -0.75 | -0.25 | -0.65 | 19.2 | -12.4 | 1.3 | -9.5 |
| $-NHCH_3$ | -0.80 | -0.22 | -0.68 | | | | |
| $-N(CH_3)_2$ | -0.66 | -0.18 | -0.67 | | | | |
| -NHCOR | 0.12 | -0.07 | -0.28 | 11.1 | -9.9 | 0.2 | -5.6 |
| $-NO_2$ | 0.95 | 0.26 | 0.38 | 19.6 | -5.3 | 0.8 | 6.0 |
| | | | | | | | |
| -SH | -0.08 | -0.16 | -0.22 | 2.2 | 0.7 | 0.4 | -3.1 |
| | | | | | | | |
| -F | -0.26 | 0.00 | -0.20 | 35.1 | -14.3 | 0.9 | -4.4 |
| -Cl | 0.03 | -0.02 | -0.09 | 6.4 | 0.2 | 1.0 | -2.0 |
| -Br | 0.18 | -0.08 | -0.04 | -5.4 | 3.3 | 2.2 | -1.0 |
| -I | 0.39 | -0.21 | -0.03 | -32.3 | 9.9 | 2.6 | -0.4 |

## $^{13}$C-NMR- Spektroskopie: Chemische Verschiebung