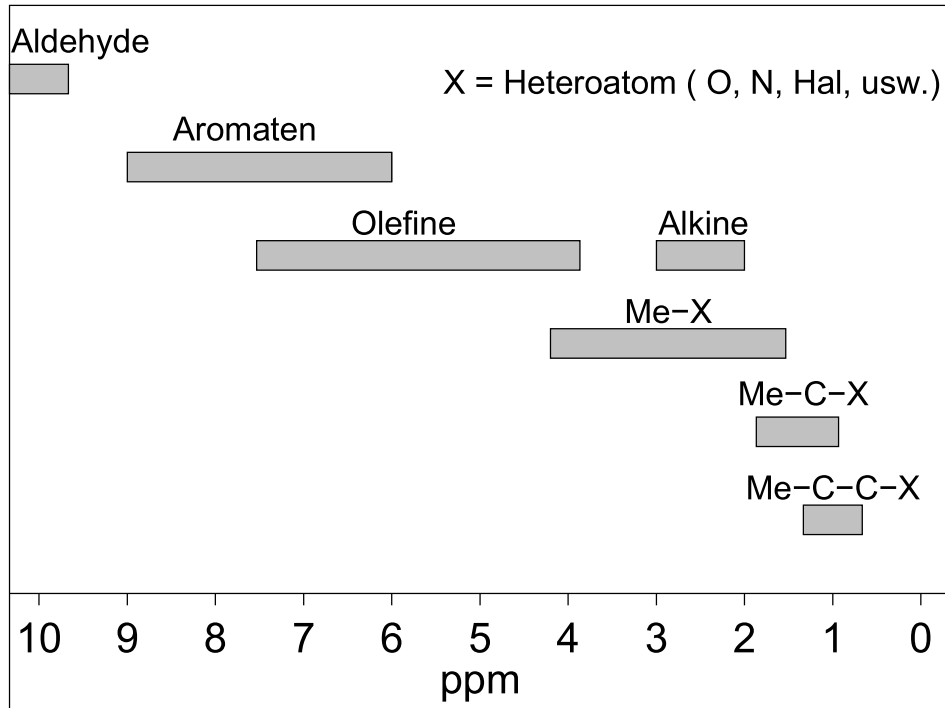
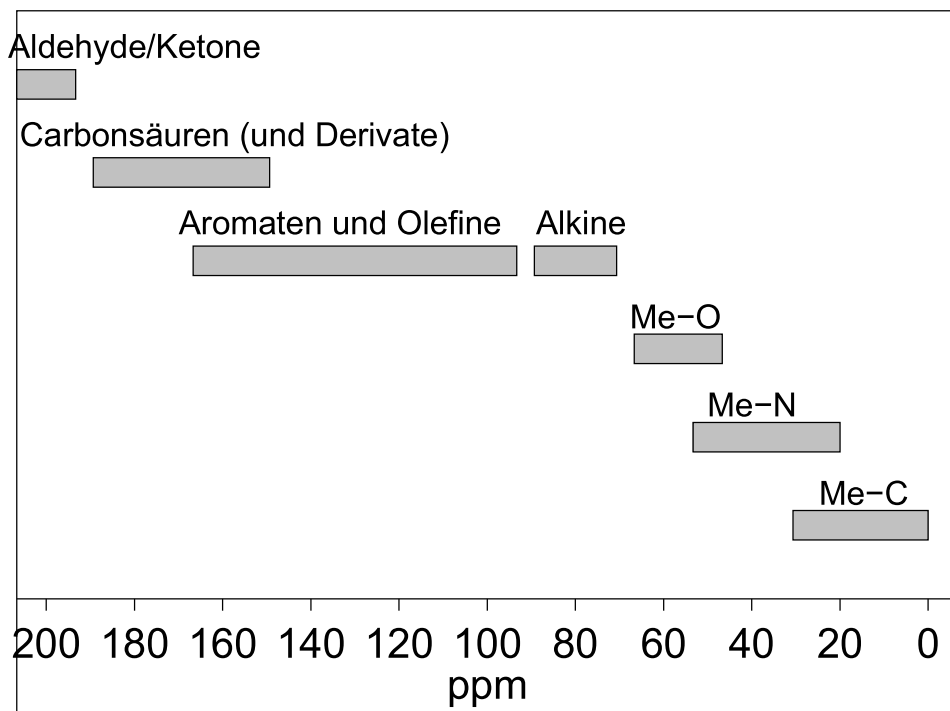


- Die ^1H chemischen Verschiebungen liegen meistens zwischen 0 ppm und 10 ppm.



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

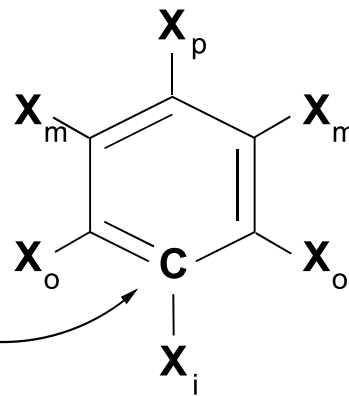


8. ¹³C - „Inkremente“

- Benzole

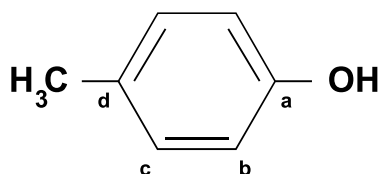
$$\delta_c = 128.5 + \sum_k S_k n_k$$

(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 ₂ CH 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 ₂ Cl	9.3	0.3	0.2	0
CH ₂ Br	9.5	0.7	0.3	0.2
CH ₂ OH	12.4	-1.2	0.2	-1.1
CH=CH ₂	8.9	-2.3	-0.1	-0.8
C ₆ H ₅	13.1	-1.1	0.4	-1.1
C≡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 ₂ CH 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



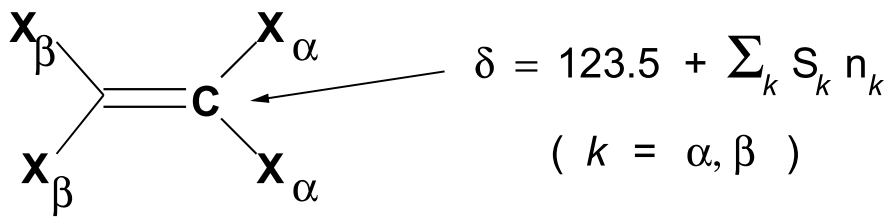
$$\delta_a = 128.5 + 26.9 - 3.1 = 152.3 \quad (\text{gem.: } 152.6)$$

$$\delta_b = 128.5 - 12.8 - 0.1 = 115.6 \quad (\text{gem.: } 115.3)$$

$$\delta_c = 128.5 + 1.4 + 0.7 = 130.6 \quad (\text{gem.: } 130.2)$$

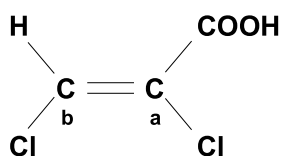
$$\delta_d = 128.5 - 7.4 + 9.2 = 130.3 \quad (\text{gem.: } 130.5)$$

• Olefine



X	S_α	S_β
CH ₃	10.6	-7.9
CH ₂ CH ₃	15.5	-9.7
CH ₂ CH ₂ CH ₃	14.0	-8.2
CH(CH ₃) ₂	20.4	-11.5
C(CH ₃) ₃	25.3	-13.3
CH ₂ Cl	10.2	-6.0
CH ₂ Br	10.9	-4.5
CH ₂ I	14.2	-4.0
CH ₂ OH	14.2	-8.4
CH=CH ₂	13.6	-7.0
C≡CH	-7.5	8.9
C ₆ H ₅	12.5	-11.0
CHO	13.1	12.7
COCH ₃	15.0	5.8
COOH	4.2	8.9
COOCH ₂ CH ₃	6.3	7.0
OCH ₃	29.4	-38.9
OCH ₂ CH 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



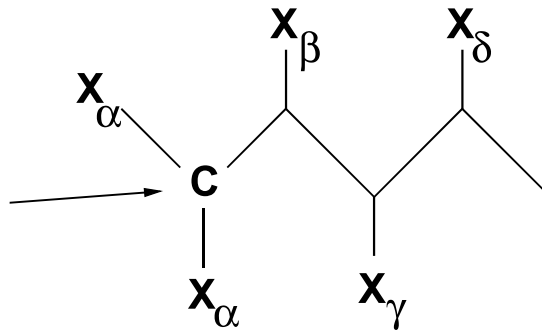
$$\delta_a = 123.5 + 4.2 + 2.6 - 6.1 = 124.2 \text{ (gem.: 129.3)}$$

$$\delta_b = 123.5 + 8.9 - 6.1 + 2.6 = 128.9 \text{ (gem.: 132.6)}$$

- Aliphaten

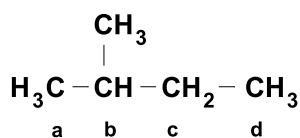
$$\delta = -2.3 + \sum_k S_k n_k$$

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



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(<i>cis</i>)	14.2	7.3	-1.5	0
CH=CH(<i>trans</i>)	19.7	7.2	-1.6	0
C≡CH	4.5	5.5	-3.5	0
C ₆ H 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(<i>prim</i>)	48.3	10.2	-5.8	0.3
OH(<i>sek</i>)	44.5	9.7	-3.3	0.2
OH(<i>tert</i>)	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: Isopentanon



$$\delta_a = -2.3 + 1 \cdot 9.1 + 2 \cdot 9.4 - 1 \cdot 2.5 = 23.1 \quad (\text{gem.: } 21.9)$$

$$\delta_b = -2.3 + 3 \cdot 9.1 + 1 \cdot 9.4 - 0 \cdot 2.5 = 34.4 \quad (\text{gem.: } 29.7)$$

$$\delta_c = -2.3 + 2 \cdot 9.1 + 2 \cdot 9.4 - 0 \cdot 2.5 = 34.7 \quad (\text{gem.: } 31.7)$$

$$\delta_d = -2.3 + 1 \cdot 9.1 + 1 \cdot 9.4 - 2 \cdot 2.5 = 11.2 \quad (\text{gem.: } 11.4)$$