Übungen zur Spektroskopie 2

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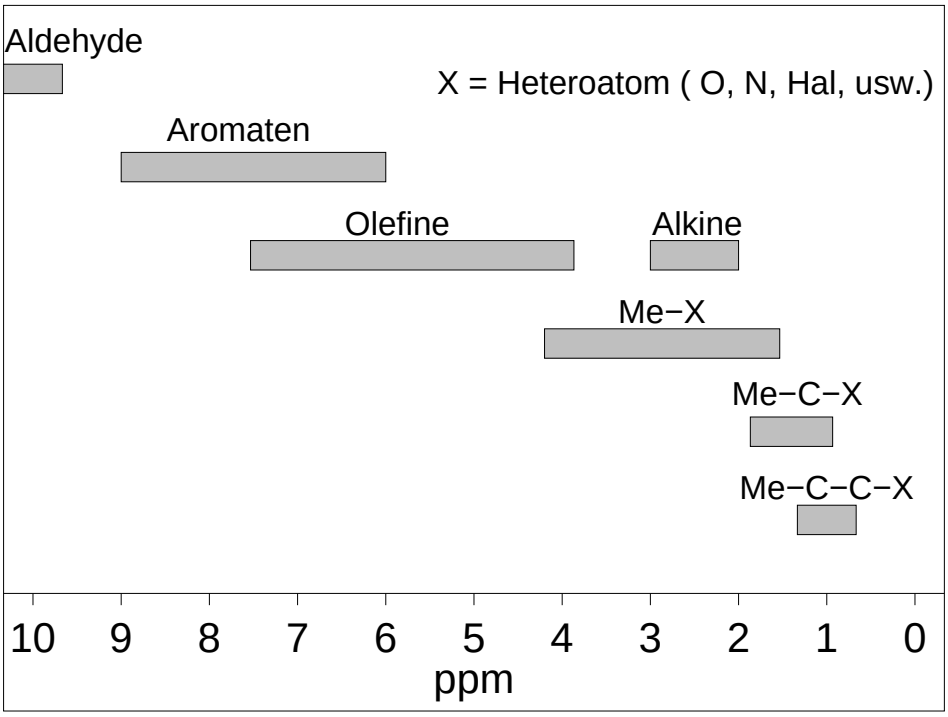
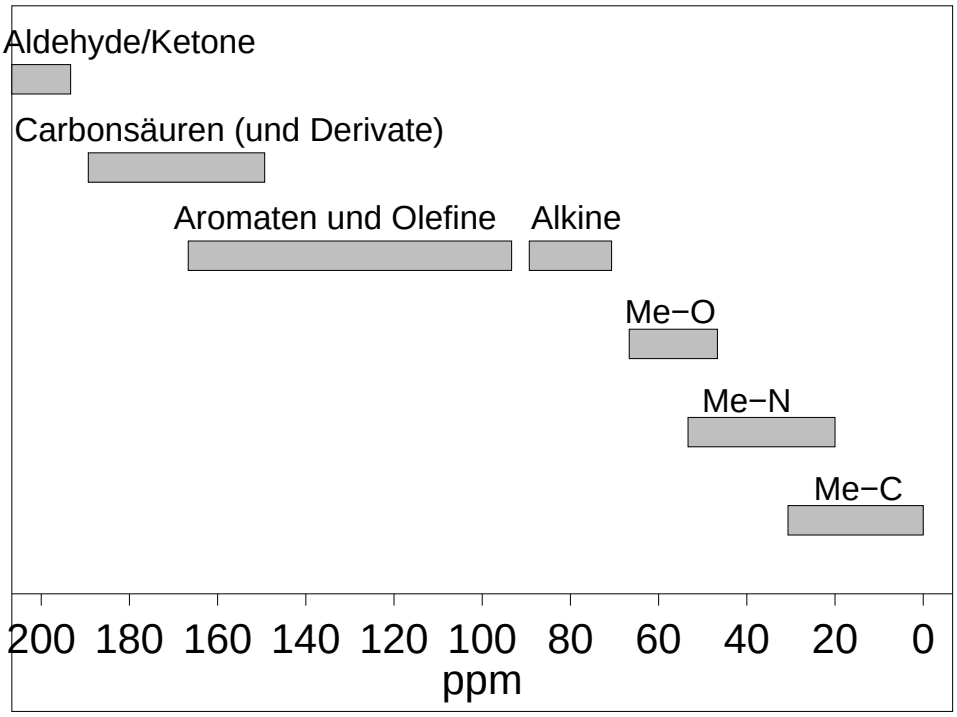
Sie finden diese Übungen und alte Klausuren (mit Lösung) auf unserer Homepage:

https://www.cup.uni-muenchen.de/oc/nmr/uebungen/
https://www.cup.uni-muenchen.de/oc/nmr/alte-klausuren/

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



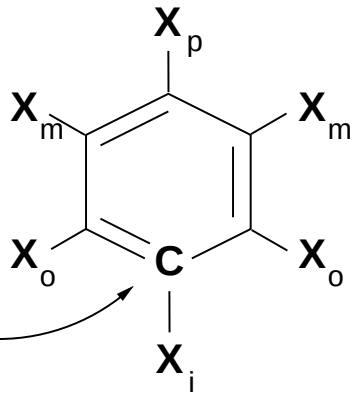
- Die ^{13}C chemischen Verschiebungen liegen meistens zwischen 0 ppm und 200 ppm.



8. ^{13}C - „Inkremente“

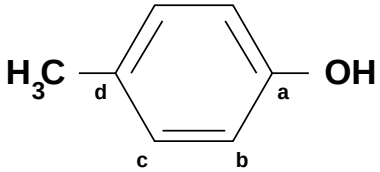
- Benzole

$$\delta_C = 128.5 + \sum_k S_k\, n_k \qquad (k = \text{i, o, m, p})$$



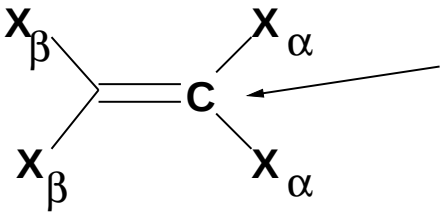
X	S_{ipso}	S_{ortho}	S_{meta}	S_{para}
CH_3	9.2	0.7	-0.1	-3.1
CH_2CH_3	15.6	-0.5	0.0	-2.7
$CH(CH_3)_2$	20.1	-2.0	0.0	-2.5
$C(CH_3)_3$	22.1	-3.4	-0.4	-3.1
CH_2Cl	9.3	0.3	0.2	0
CH_2Br	9.5	0.7	0.3	0.2
CH_2OH	12.4	-1.2	0.2	-1.1
$CH{=}CH_2$	8.9	-2.3	-0.1	-0.8
C_6H_5	13.1	-1.1	0.4	-1.1
$C{\equiv}CH$	-6.2	3.6	-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
$COOCH_2CH_3$	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



δ_a = 128.5 + 26.9 − 3.1 = 152.3 (gem.: 152.6)
δ_b = 128.5 − 12.8 − 0.1 = 115.6 (gem.: 115.3)
δ_c = 128.5 + 1.4 + 0.7 = 130.6 (gem.: 130.2)
δ_d = 128.5 − 7.4 + 9.2 = 130.3 (gem.: 130.5)

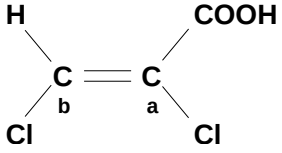
- Olefine



$$\delta = 123.5 + \sum_k S_k n_k \qquad (k = \alpha, \beta)$$

X	S_α	S_β
CH_3	10.6	-7.9
CH_2CH_3	15.5	-9.7
$CH_2CH_2CH_3$	14.0	-8.2
$CH(CH_3)_2$	20.4	-11.5
$C(CH_3)_3$	25.3	-13.3
CH_2Cl	10.2	-6.0
CH_2Br	10.9	-4.5
CH_2I	14.2	-4.0
CH_2OH	14.2	-8.4
$CH{=}CH_2$	13.6	-7.0
$C{\equiv}CH$	-7.5	8.9
C_6H_5	12.5	-11.0
CHO	13.1	12.7
$COCH_3$	15.0	5.8
COOH	4.2	8.9
$COOCH_2CH_3$	6.3	7.0
OCH_3	29.4	-38.9
OCH_2CH_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

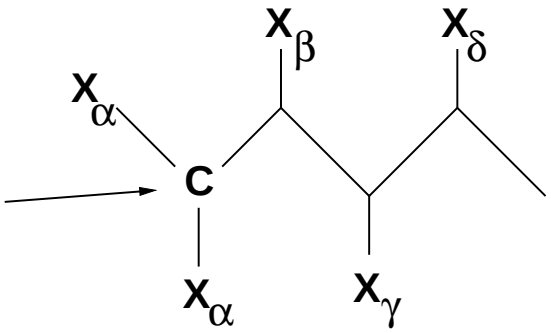


δ_a = 123.5 + 4.2 + 2.6 −6.1 = 124.2 (gem.: 129.3)

δ_b = 123.5 + 8.9 −6.1 + 2.6 = 128.9 (gem.: 132.6)

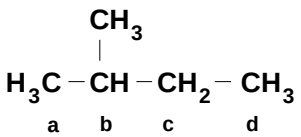
- Aliphaten

$$\delta = -2.3 + \sum_k S_k \, n_k \qquad (k = \alpha, \beta, \gamma, \delta)$$



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
$CH{=}CH(cis)$	14.2	7.3	-1.5	0
$CH{=}CH(trans)$	19.7	7.2	-1.6	0
$C{\equiv}CH$	4.5	5.5	-3.5	0
C_6H_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
$OH(prim)$	48.3	10.2	-5.8	0.3
$OH(sek)$	44.5	9.7	-3.3	0.2
$OH(tert)$	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: Isopentan



$\delta_a = -2.3 + 1 * 9.1 + 2 * 9.4 - 1 * 2.5 = 23.1$ (gem.: 21.9)

$\delta_b = -2.3 + 3 * 9.1 + 1 * 9.4 - 0 * 2.5 = 34.4$ (gem.: 29.7)

$\delta_c = -2.3 + 2 * 9.1 + 2 * 9.4 - 0 * 2.5 = 34.7$ (gem.: 31.7)

$\delta_d = -2.3 + 1 * 9.1 + 1 * 9.4 - 2 * 2.5 = 11.2$ (gem.: 11.4)