

Übung Y29

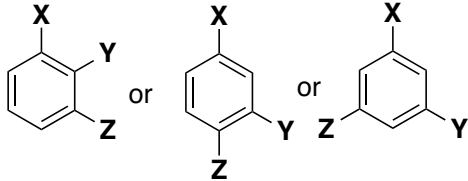
IR

Wavenumber [cm ⁻¹]	possible assignment
3100-3000 (m)	=C-H
3000-2800 (m)	C-H or O-H (H-bonded)
1800-2000 (w)	aromatic ring overtone
1680 (s)	C=O

EI-MS

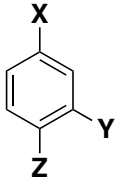
<i>m/z</i>		possible information
190	M ^{+•}	0 or even number of N M + 2, M + 4: 2xCl
173	M - 17	- OH (acid)
145	M - 45	- C ₂ H ₅ O or - COOH

^{13}C -NMR

#	δ [ppm]	multipl icity	possible information
1	165.4	C	C=O
2	135.7	C] aromatic region: 6-different carbons (3xquaternary and 3xCH) 
3	131.5	C	
4	131.4	C	
5	131.0	CH	
6	130.9	CH	
7	129.2	CH	

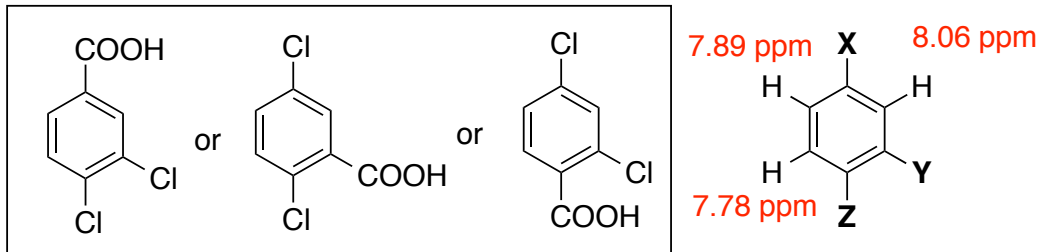
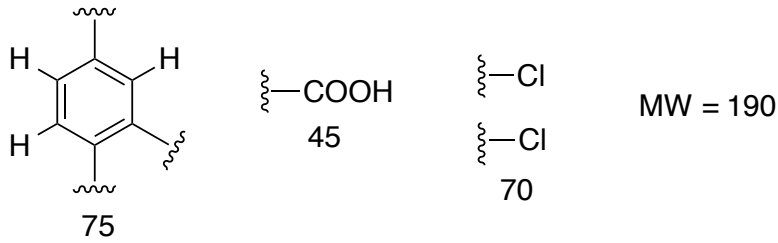
C \geq 7

^1H -NMR

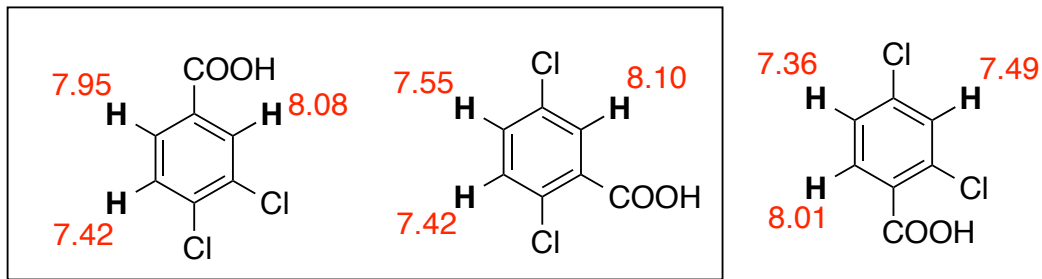
#	δ [ppm]	Integ.	shape	possible information
1	13.5	1H	br. s.	H-bonded O-H or N-H
2	8.06	1H	d ($J = 2$ Hz)] aromatic region 
3	7.89	1H	d ($J = 9, 2$ Hz)	
4	7.78	1H	d ($J = 9$ Hz)	

H \geq 4

partial structures



$^1\text{H-NMR}$ chemical shift estimation



$^{13}\text{C-NMR}$ chemical shift estimation

C peaks: 135.7, 131.5, 131.4 ppm
 CH peaks: 131.0, 130.9, 129.2 ppm

