Lösung zum Problem Y08

1. IR-Spektrum:

3460 cm^{-1}	vermutlich Oberton der Bande bei 1740
≈ 3000 cm^{-1}	C-H str
1740 cm^{-1}	C=O str

sonst wenig Information
Kein OH, NH, C≡C, C≡N, C=C

2. Massenspektrum

- m/z 258 = $M^{+\cdot}$? keine Widersprüche. M+1 nicht ablesbar
- Isotopenmuster: Br_2
- Starkes Signal bei 106: Br-Isotopenmuster
- Signale bei 179, 151: Br-Isotopenmuster
- Starkes Signal bei m/z = 55 (C_4H_7 / C_3H_3O)
- Massendifferenzen
  - Δm = 28 (258 –> 230) (- CO)
  - Δm = 45 (258 –> 213) (- C_2H_5O)
  - Δm = 73 (258 –> 185) (?, Verlust von 28 aus 213)
  - Δm = 79 (258 –> 179) (- Br)

3. ^{13}C NMR-Spektrum

Signalgruppe bei 77 ppm = Lösungsmittel.

δ =	169.6	62.7	41.2	29.8	13.9	ppm
aus DEPT:	C–X	CH_2	CH	CH_2	CH_3	
	II	I	I			
	O	Y	Z	(X, Y, Z: Heteroatome)		

=> ≥ C_5H_8O

4. ^{1}H NMR-Spektrum

δ =	4.43	4.30	3.93	3.68	1.33	ppm
Integral:	1	2	1	1	3	=> H_8
Mult:	dxD	Q	Dxd	Dxd	T	
HSQC:	CH	CH_2		CH_2	CH_3	

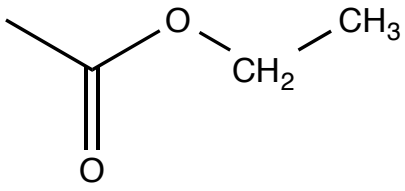
Kopplg: diastereotop!

6. Bilanz:

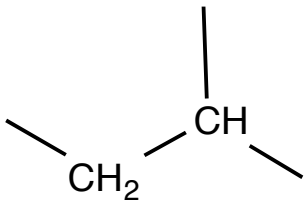
$C_5H_8OBr_2$ = 242, es fehlen 16 (1 x O; X = Y = O)

=> $C_5H_8O_2Br_2$ Molekulargewicht = 258, DBE = 1 (C=O)

7. Strukturelemente:



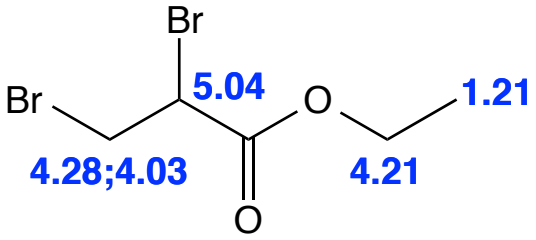
Chem. Verschiebungen
Kopplungen: CH_2–CH_3

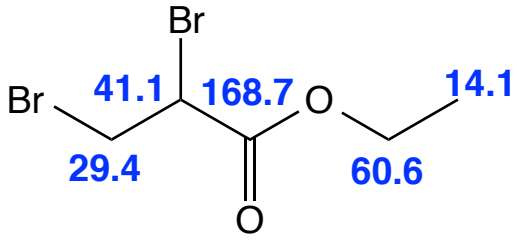


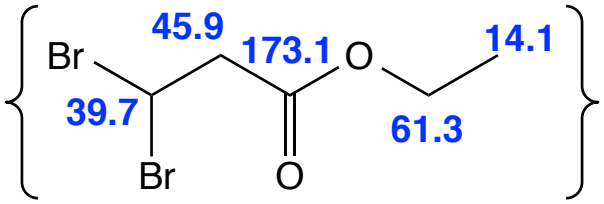
Kopplungen
CH-Gruppe: Chiralitätszentrum =>
Diastereotope CH_2

2 x –Br

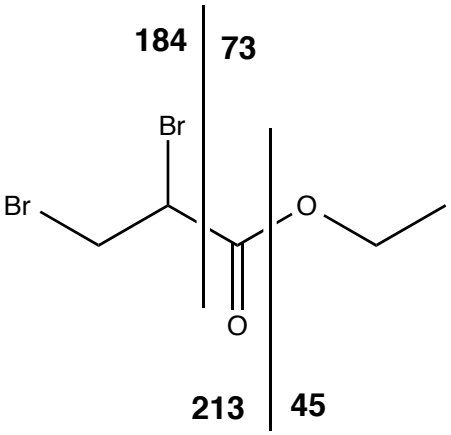
8. Verifizierung

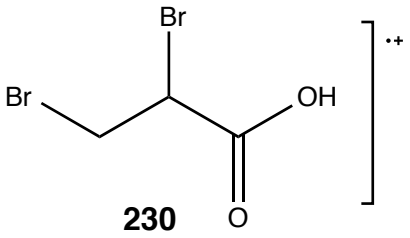




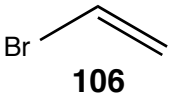


MS-Abspaltungen:





McLafferty-Produkt



C_3H_3O = m/z 55