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# NMR Spektroskopie

## Lekce 2: Pulsní NMR, spin-spinové interakce, $^{13}\text{C}$ NMR



**Martin Dračínský**

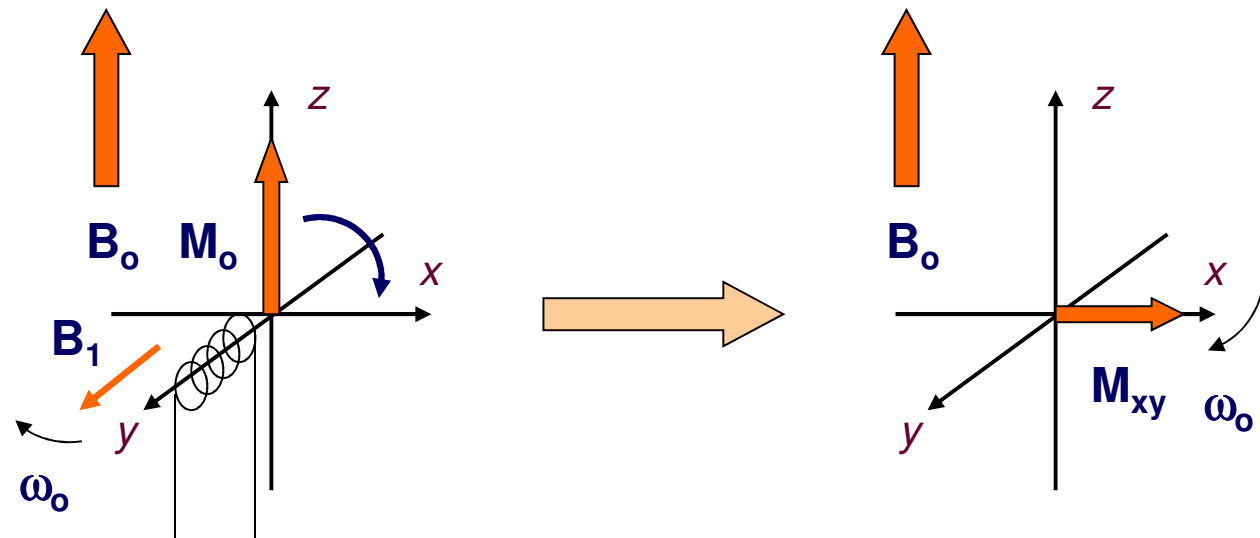
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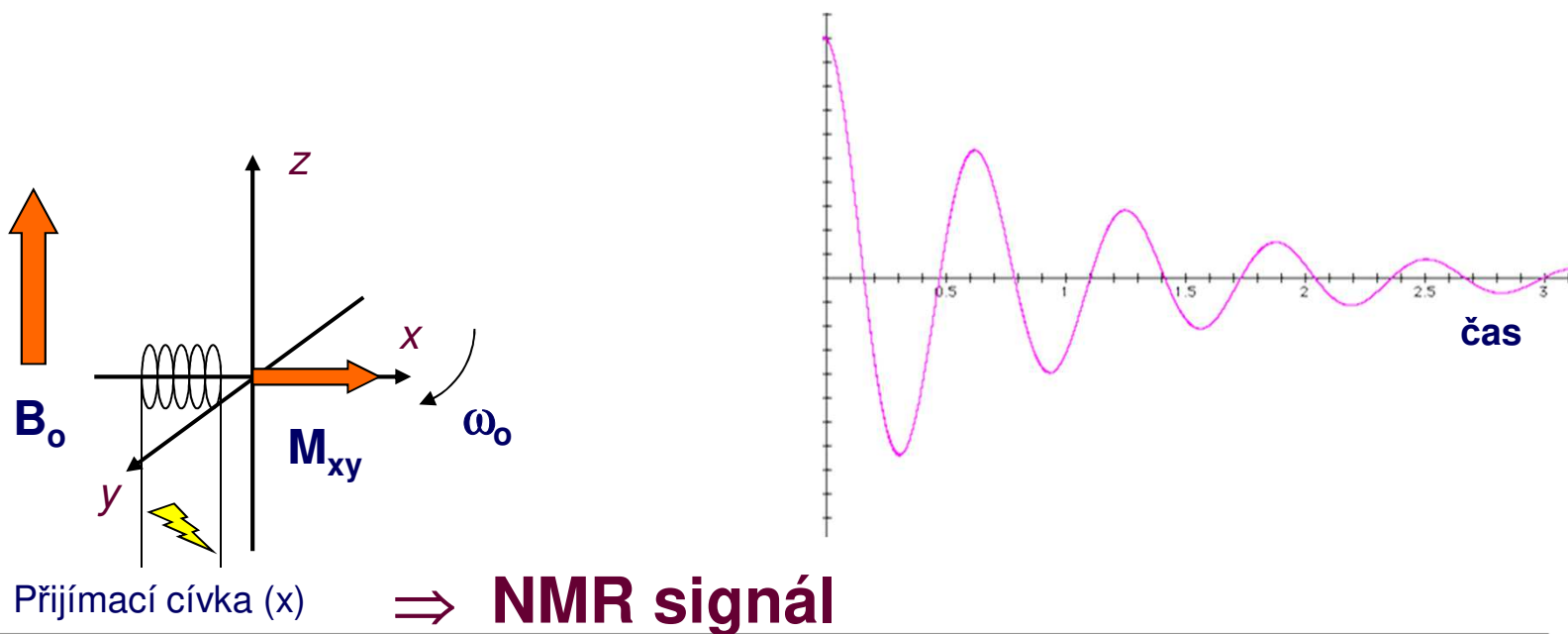
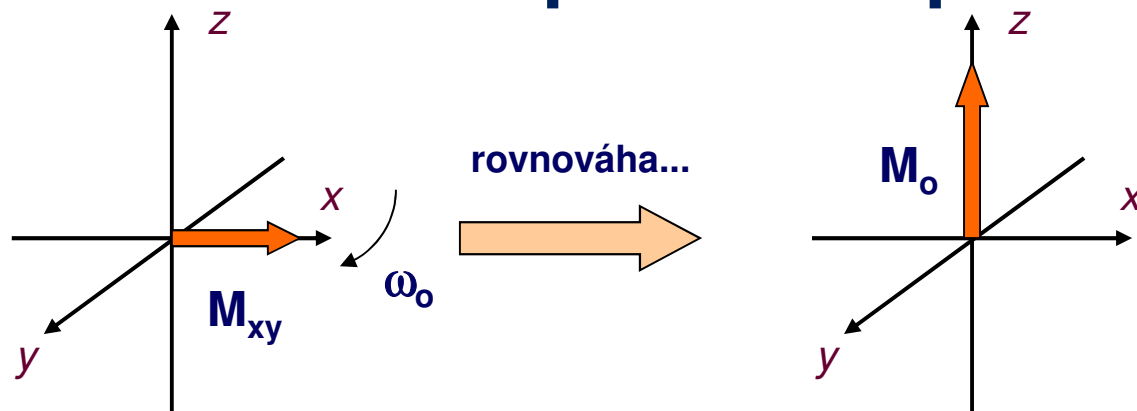
# Pulsní NMR spektroskopie

CW (continuous wave)

Pulsní NMR

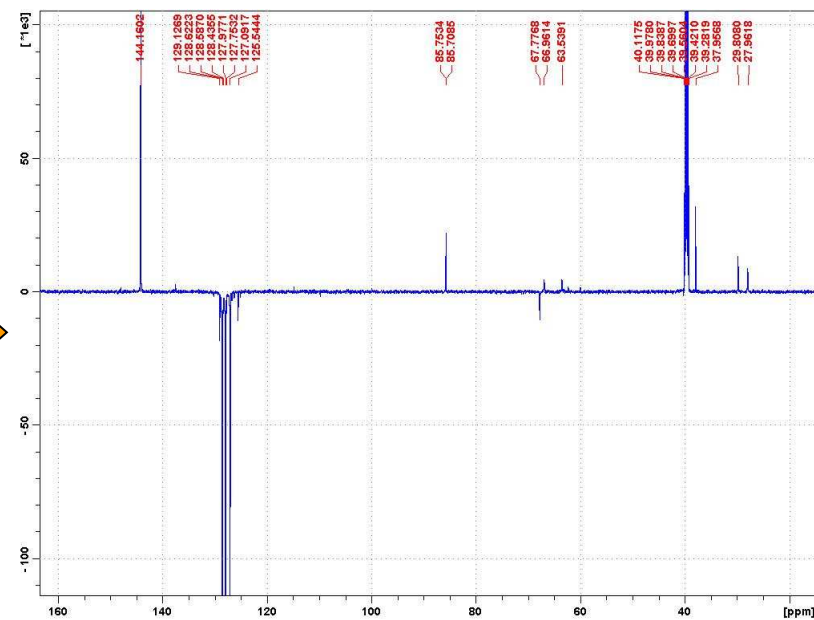
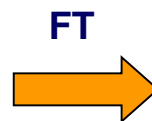
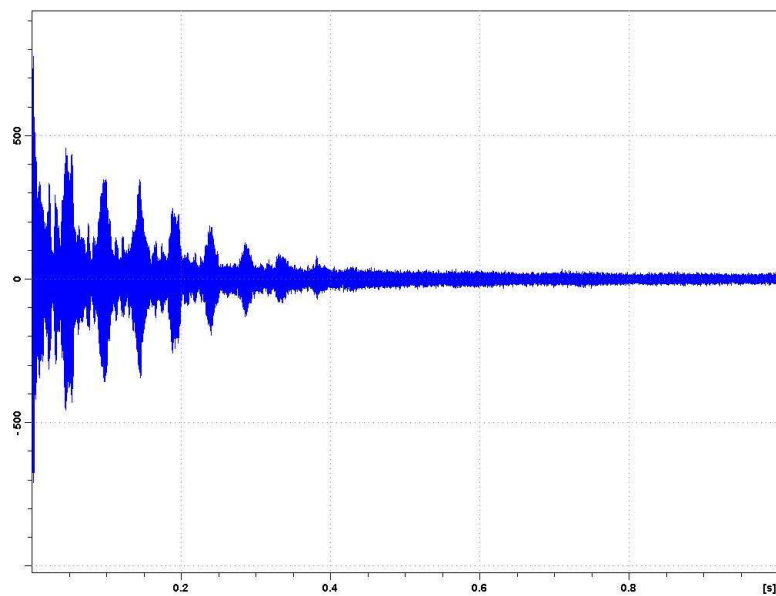
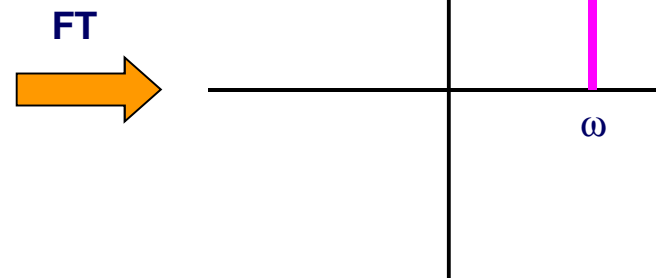
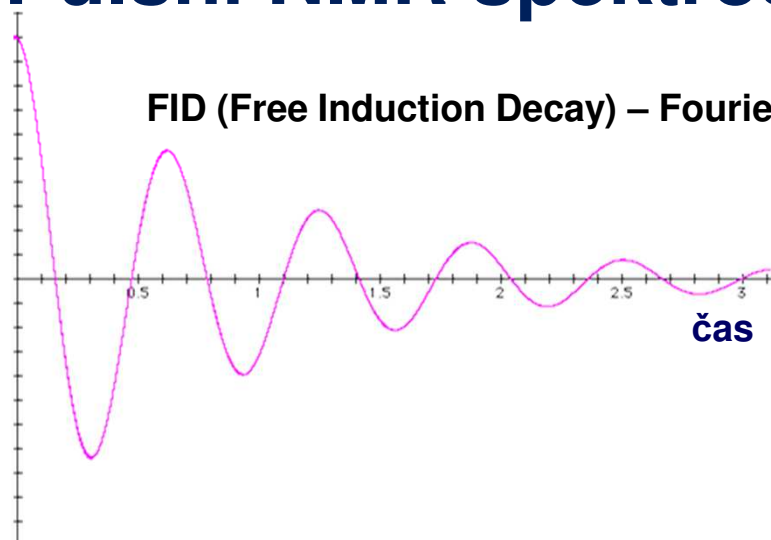


# Pulsní NMR spektroskopie

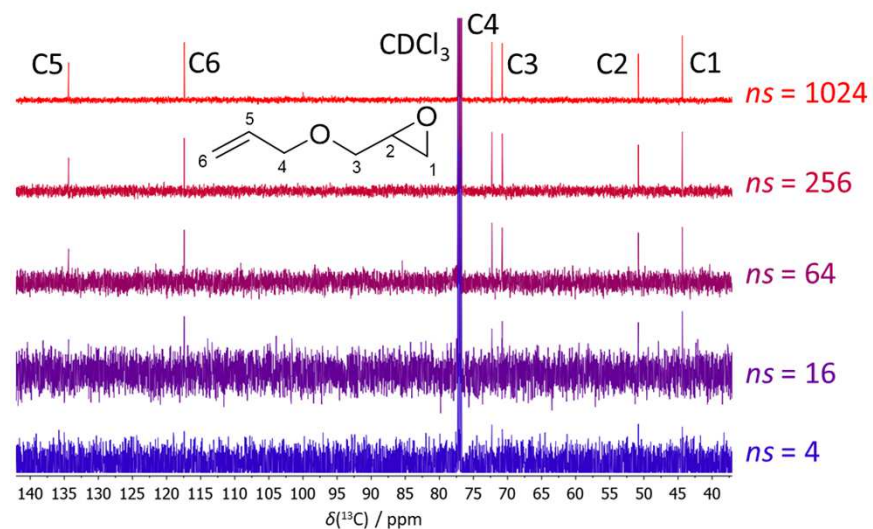
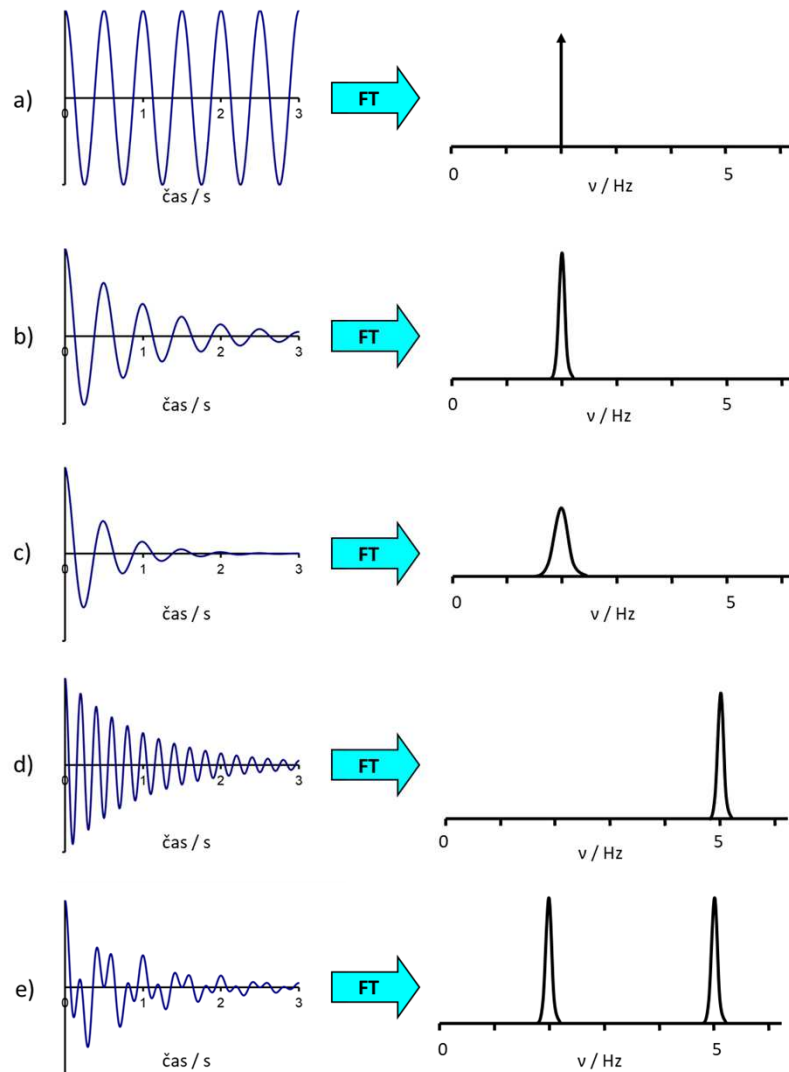


# Pulsní NMR spektroskopie

FID (Free Induction Decay) – Fourierova transformace - Spektrum

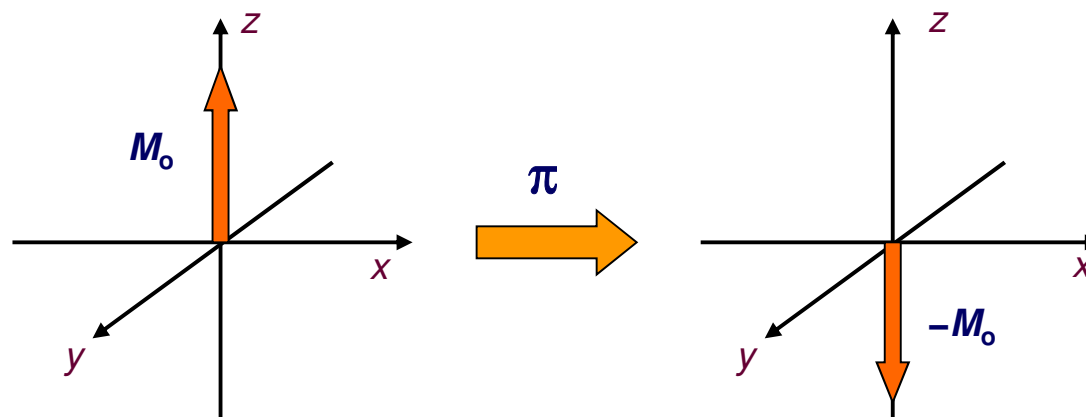
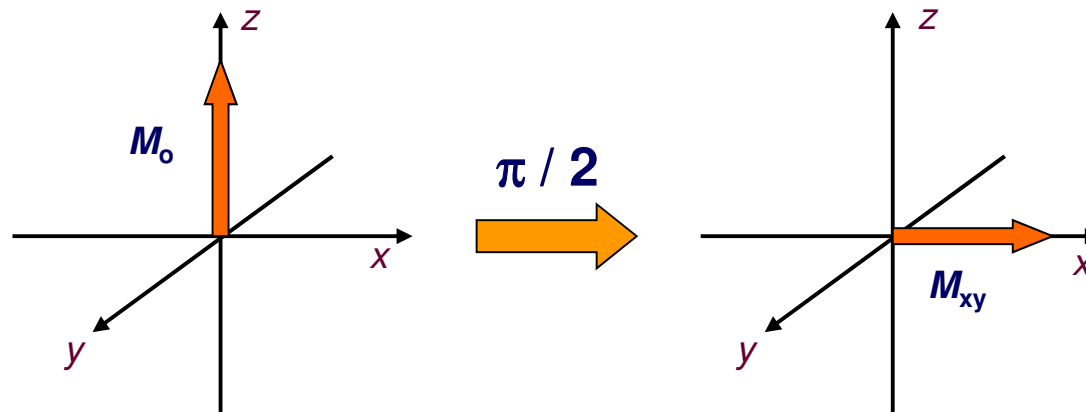


# Pulsní NMR spektroskopie

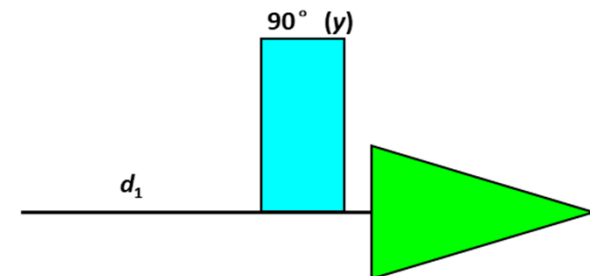
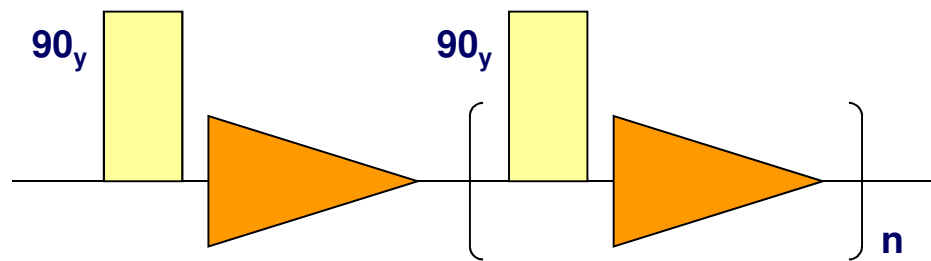
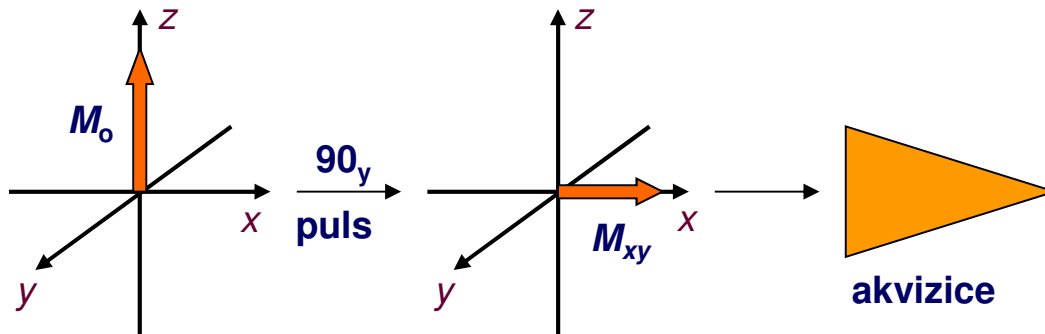


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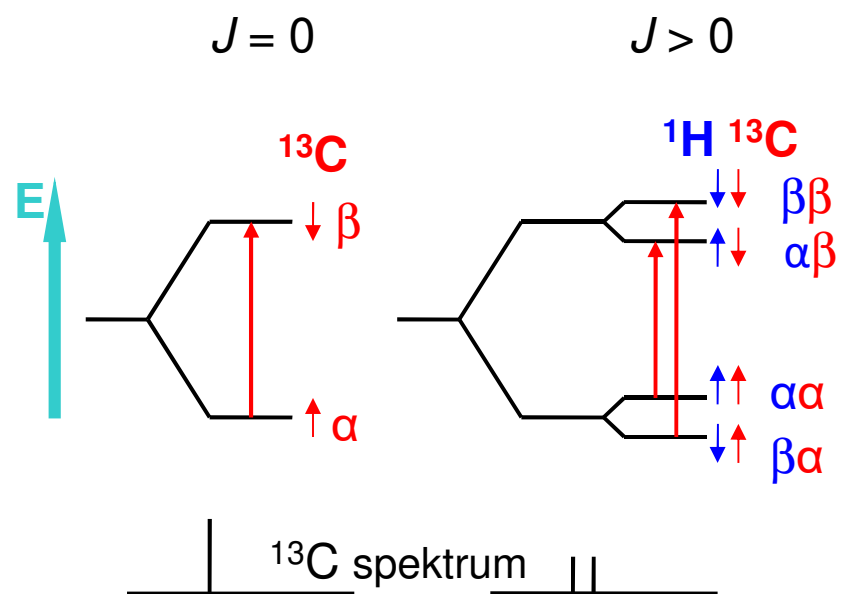
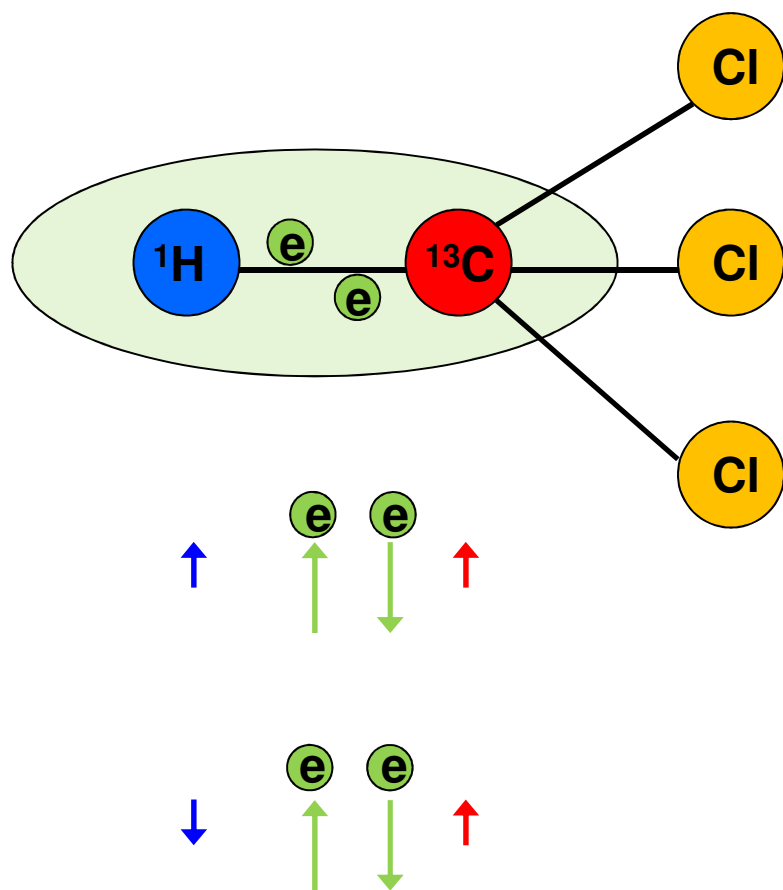
# Pulsní NMR spektroskopie



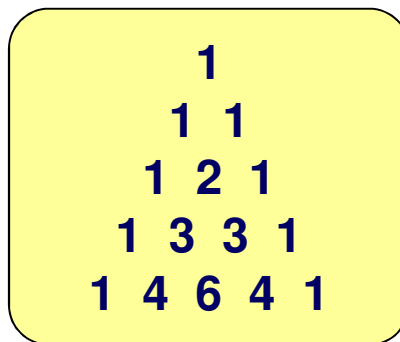
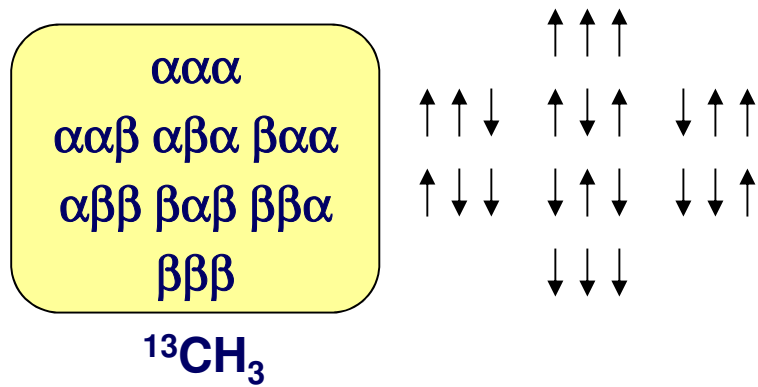
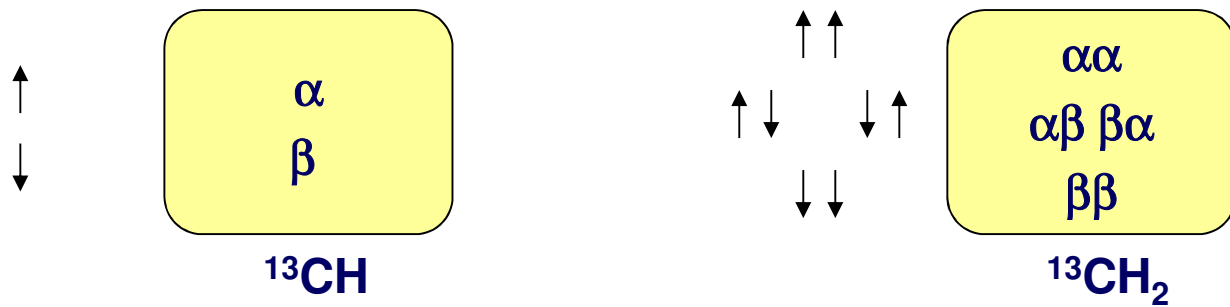
# Pulsní NMR spektroskopie



# Nepřímá spin-spinová interakce

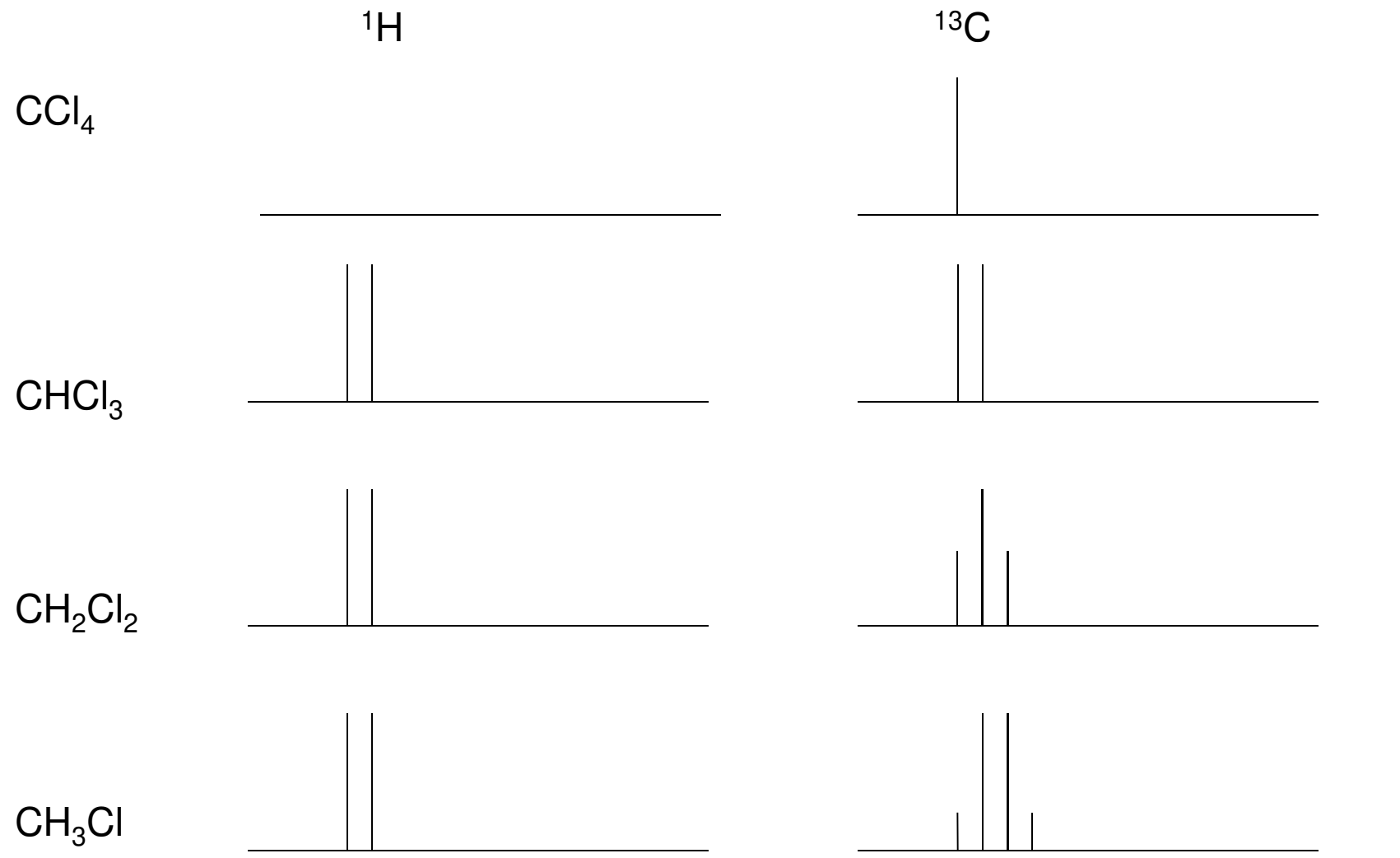


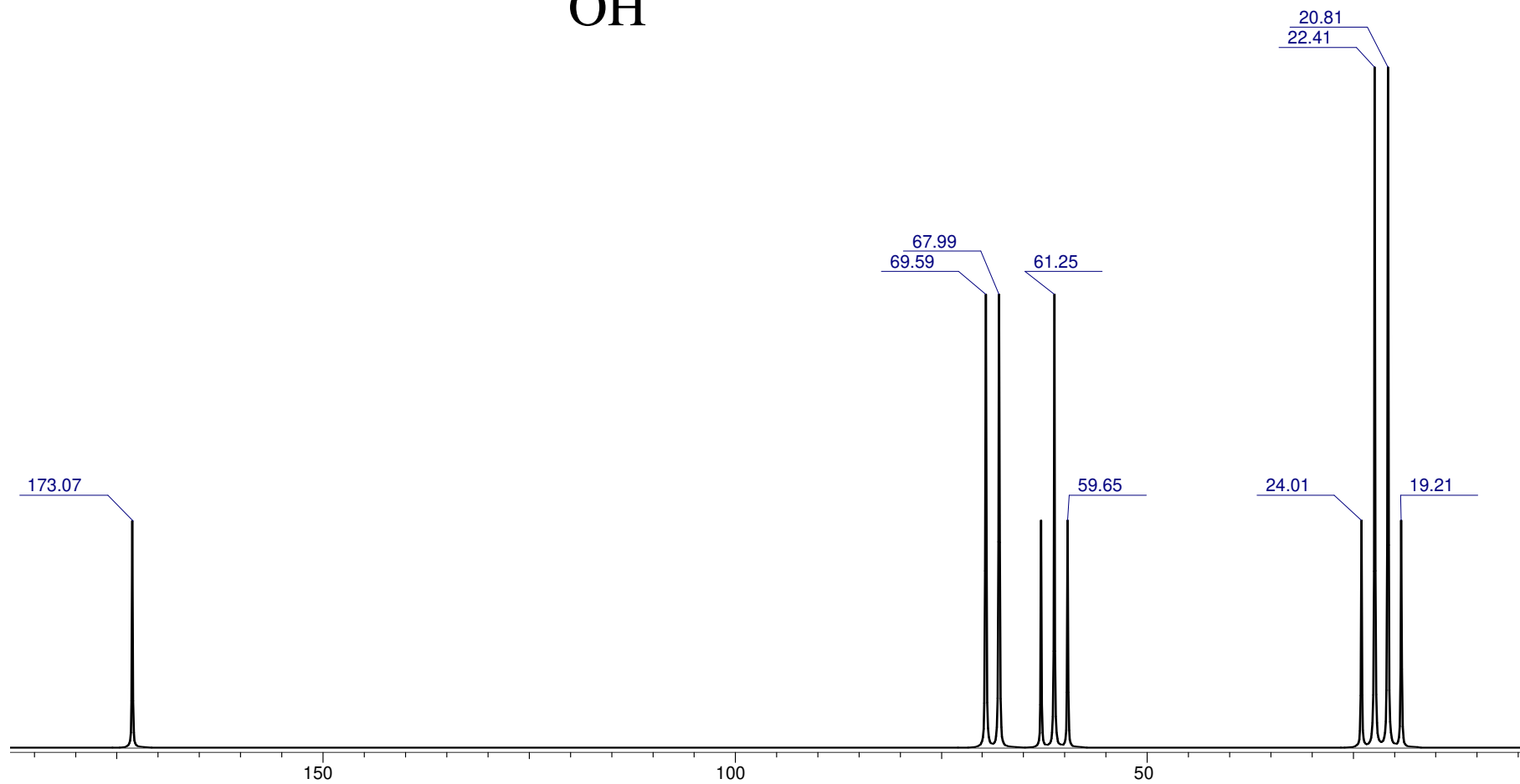
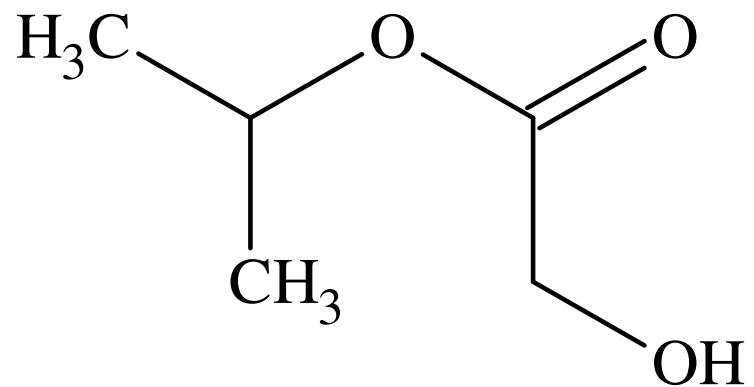




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# Nepřímá spin-spinová interakce

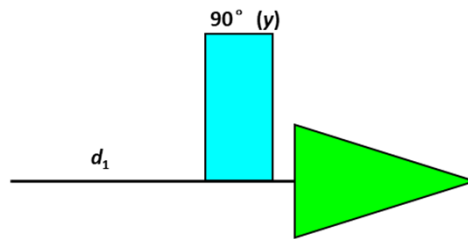




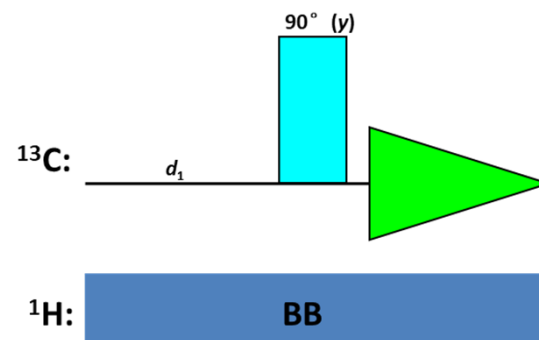
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# Základní 1D pulzní sekvence

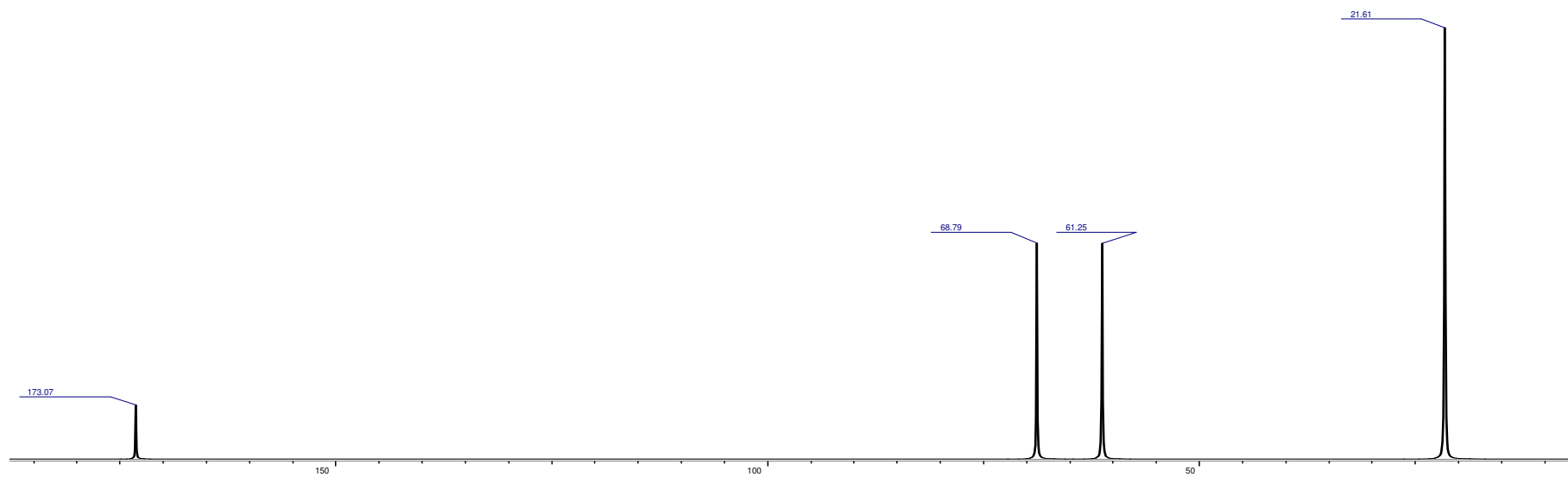
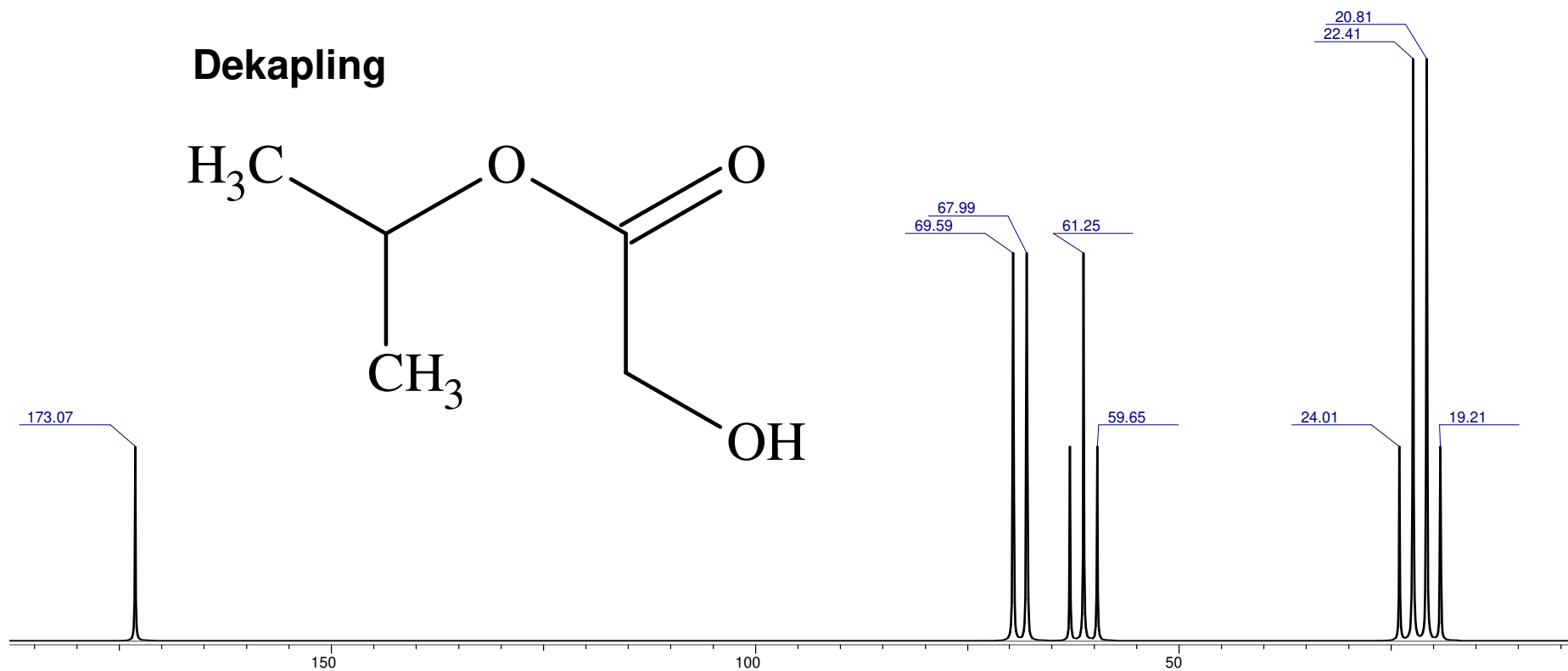
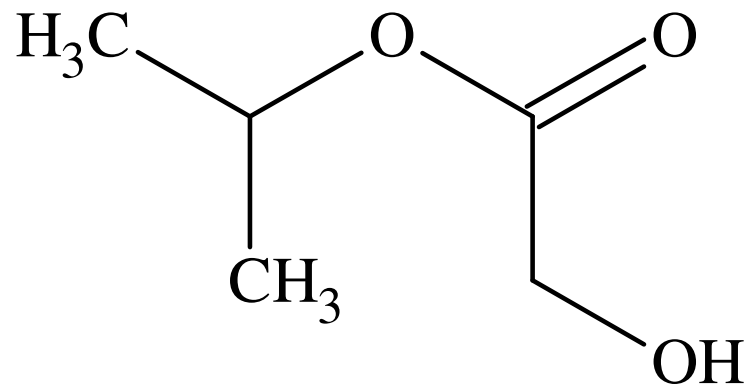
Měření  $^1\text{H}$ ,  $^{19}\text{F}$ , ...

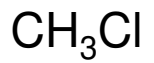


Dekapling – měření  $^{13}\text{C}$ ,  $^{31}\text{P}$ , ...

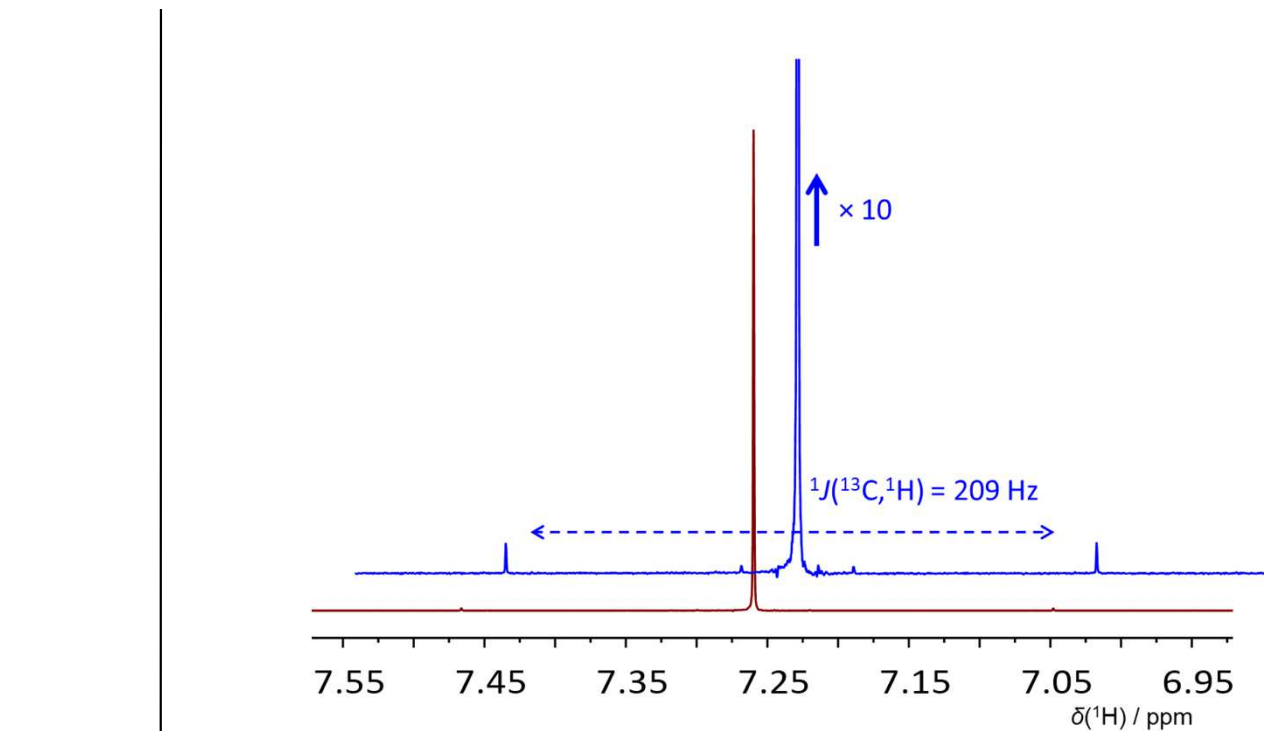


# Dekapling





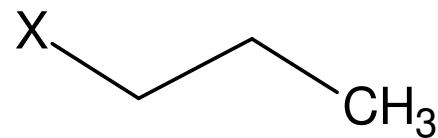
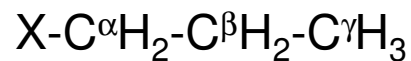
<sup>1</sup>H



<sup>13</sup>C satelity



## <sup>13</sup>C NMR - alkany



X	$\delta(C^{\alpha}) / \text{ppm}$	$\delta(C^{\beta}) / \text{ppm}$	$\delta(C^{\gamma}) / \text{ppm}$
H	16,1	16,3	16,1
CH <sub>3</sub>	24,9	24,9	13,1
NH <sub>2</sub>	44,6	27,4	11,5
OH	64,9	26,9	11,8
NO <sub>2</sub>	77,4	21,2	10,8
F	85,2	23,6	9,2
Cl	46,7	26,0	11,5
Br	35,4	26,1	12,7
I	9,0	26,8	15,2

Indukční efekt, mezomerní efekt,  $\gamma$ -efekt, efekt těžkého atomu

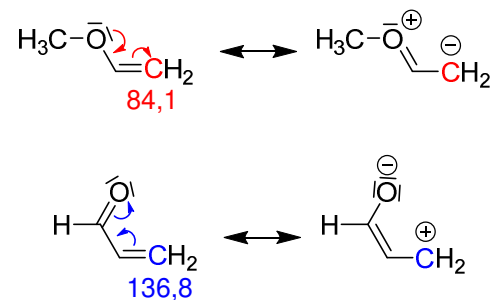
## <sup>13</sup>C NMR - cykloalkany

	$\delta$ / ppm
Cyklopropan	-2,8
Cyklobutan	22,4
Cyklopentan	25,8
Cyklohexan	27,0
cykloheptan	28,7



## <sup>13</sup>C NMR - alkeny

$\delta \approx 100\text{--}150$  ppm

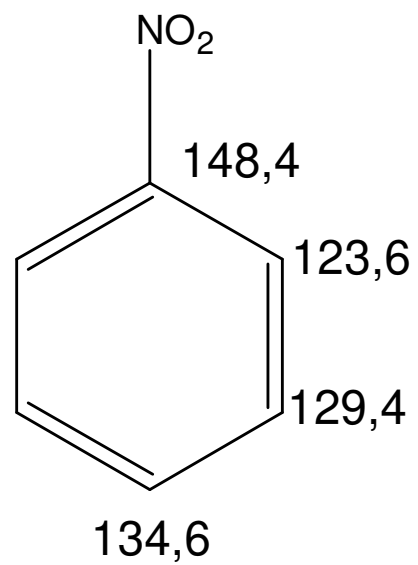
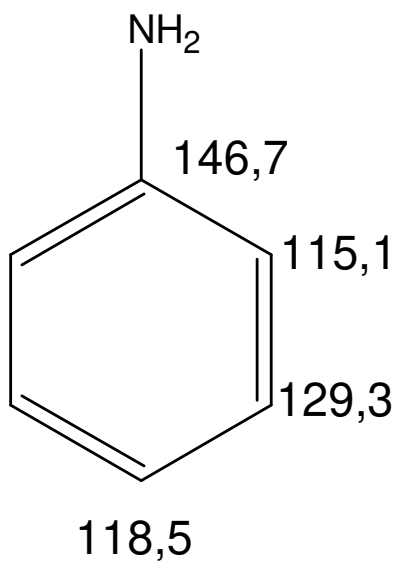


## <sup>13</sup>C NMR - alkyny

X — $\equiv$ C H		
H	71,9	71,9
Alkyl	84,0	68,6
CH <sub>3</sub> CH <sub>2</sub> O	89,6	23,4

# $^{13}\text{C}$ NMR - areny

$\delta \approx 120\text{--}140$  ppm

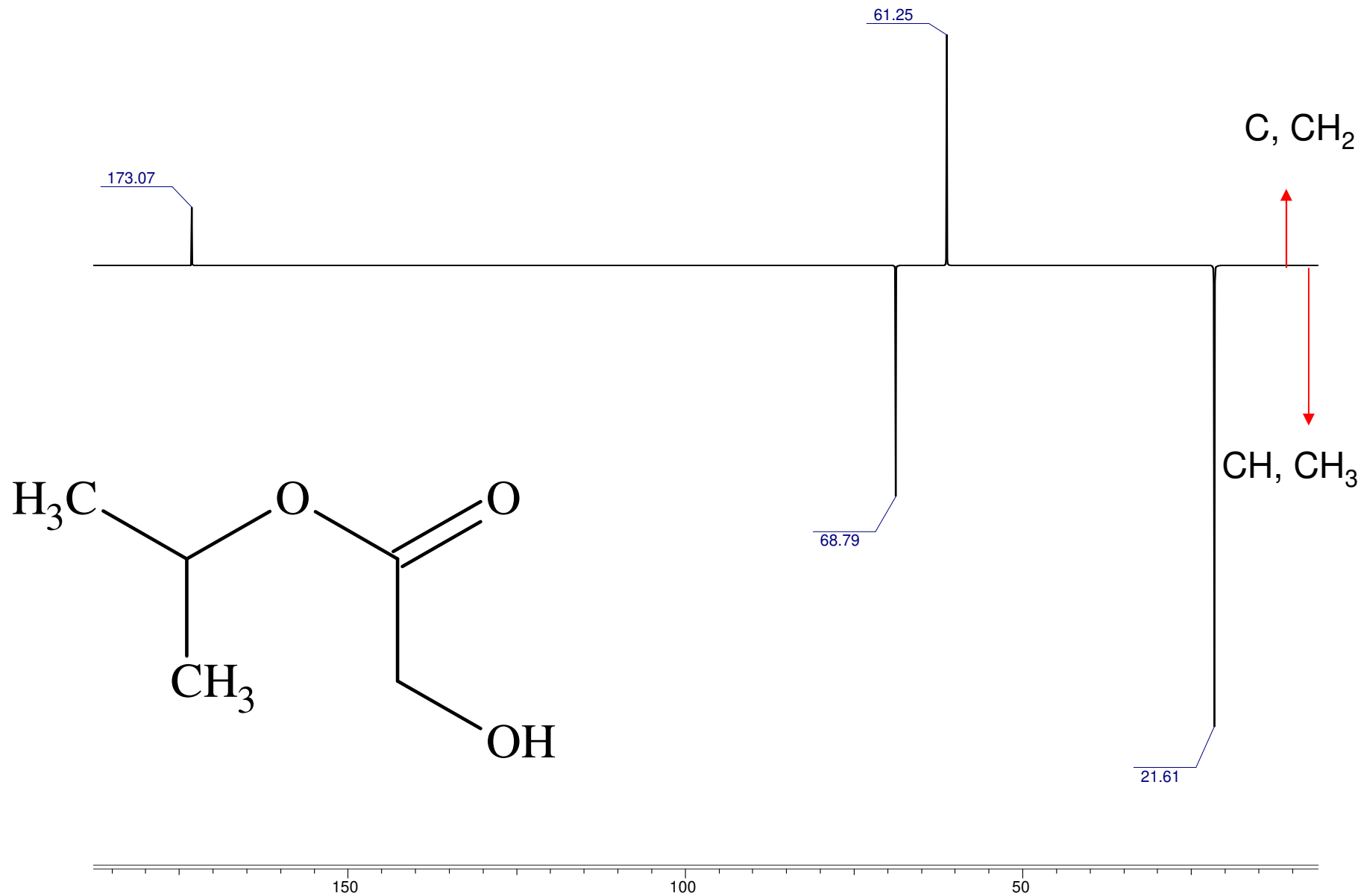


## **$^{13}\text{C}$ NMR – karbonylové a karboxylové sloučeniny**

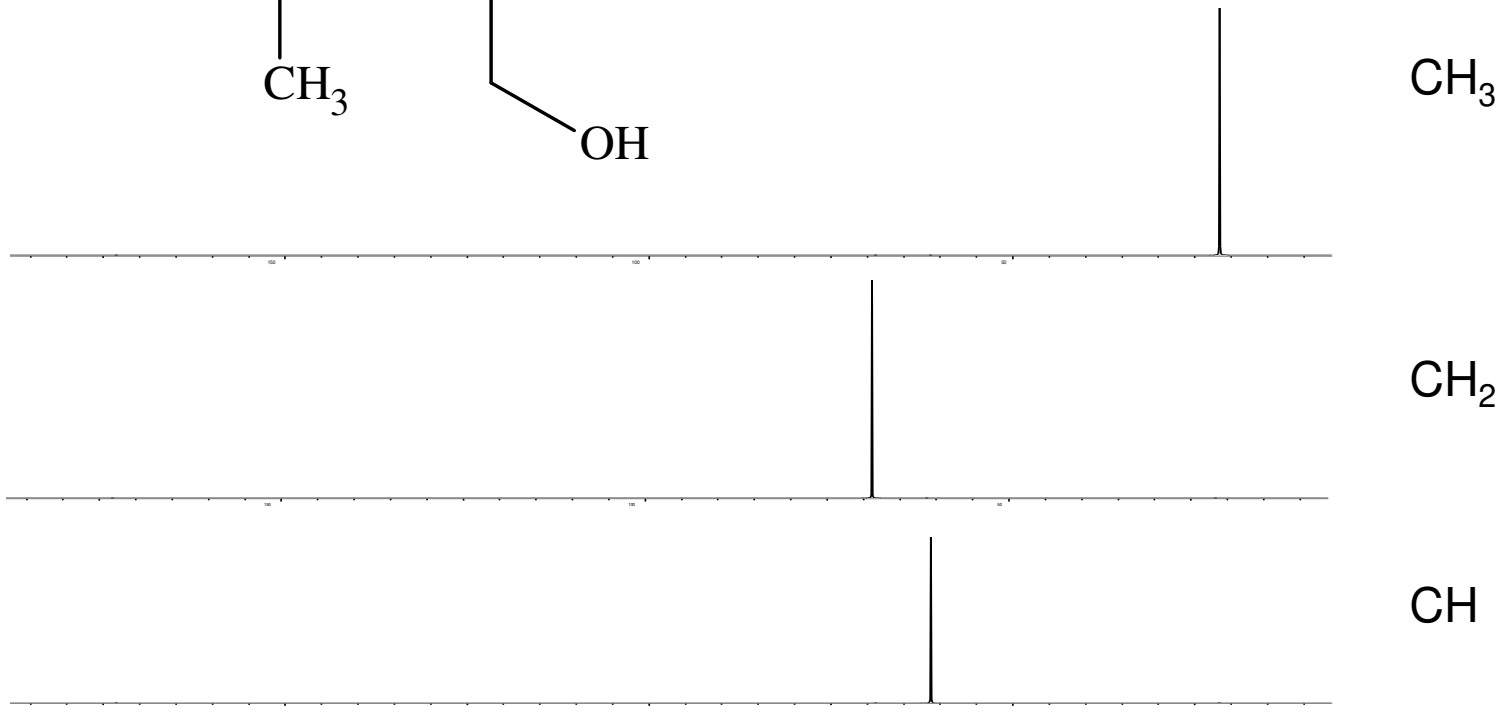
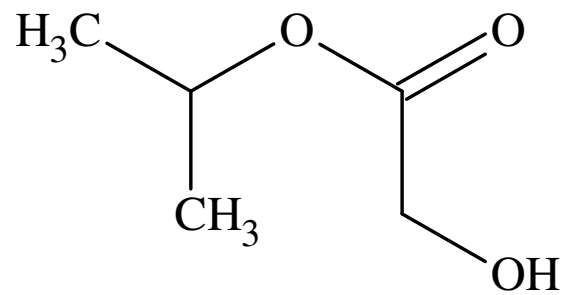
Aldehydy, ketony  $\delta \approx 190\text{--}220$  ppm

Deriváty karboxylových kyselin  $\delta \approx 160\text{--}180$  ppm

# APT



# DEPT



# DEPT

