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# NMR Spektroskopie

## Lekce 3: Spin-spinové interakce, $^1\text{H}$ NMR



**Martin Dračinský**

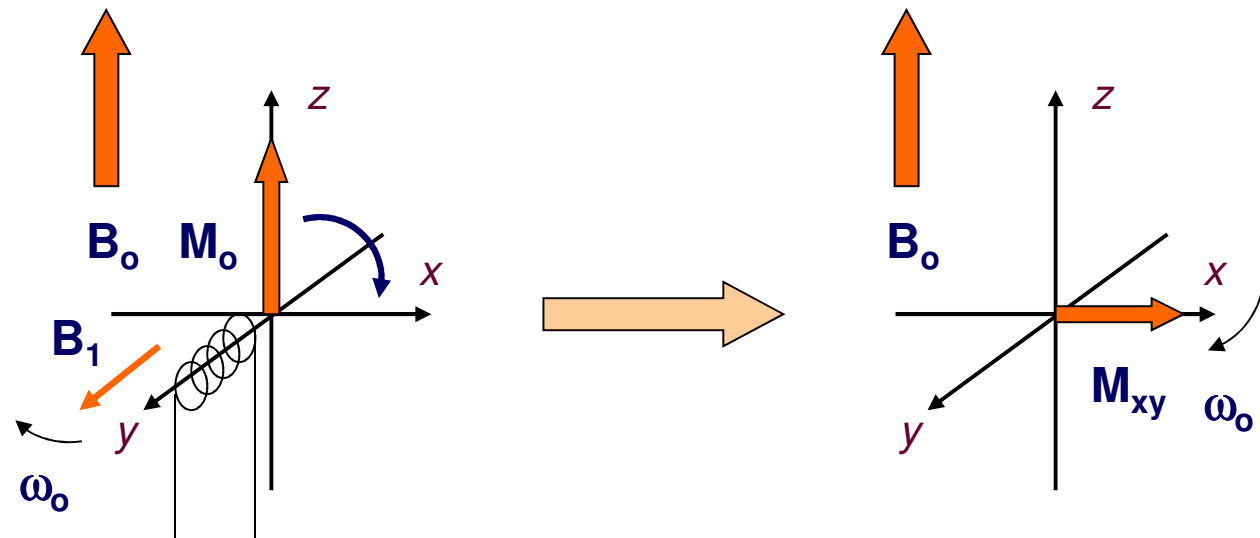
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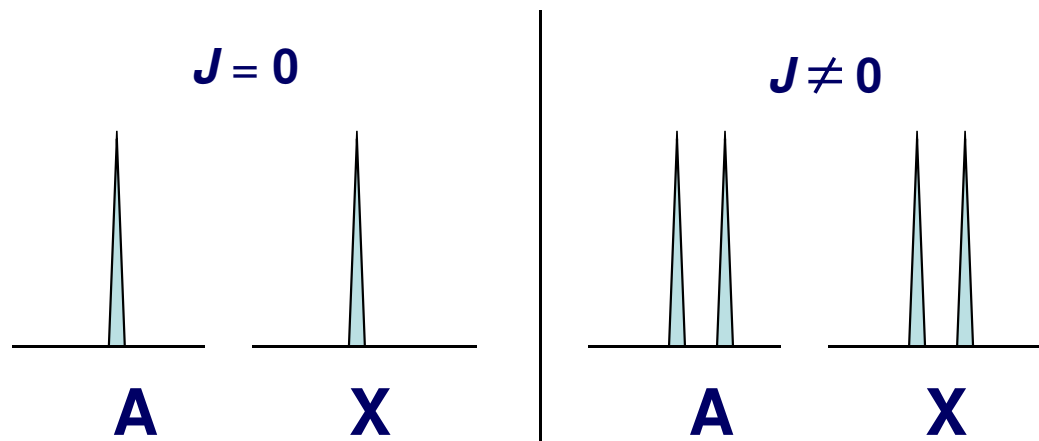
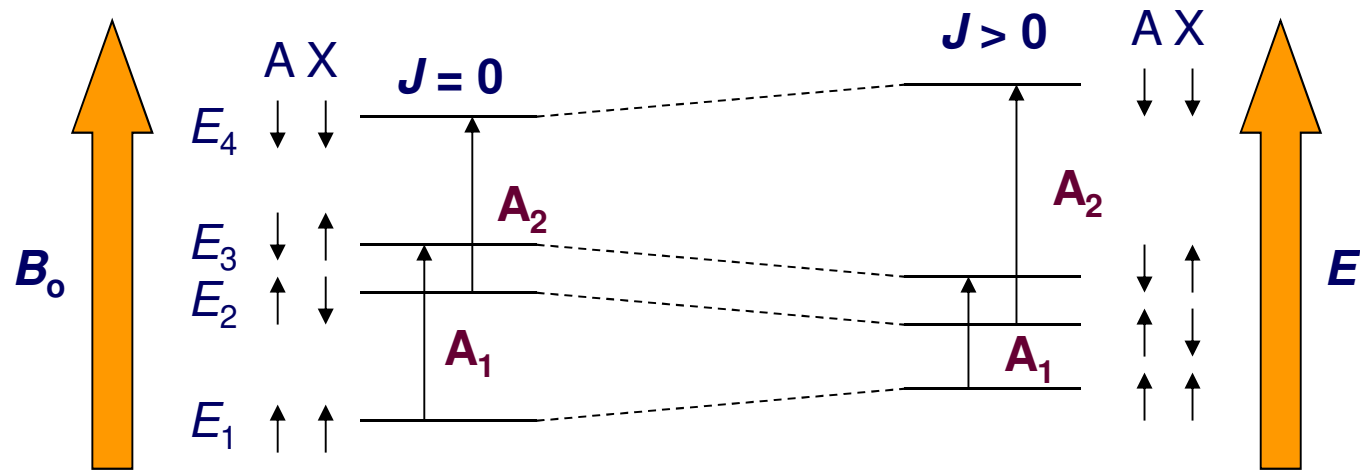
# Pulsní NMR spektroskopie

CW (continuous wave)

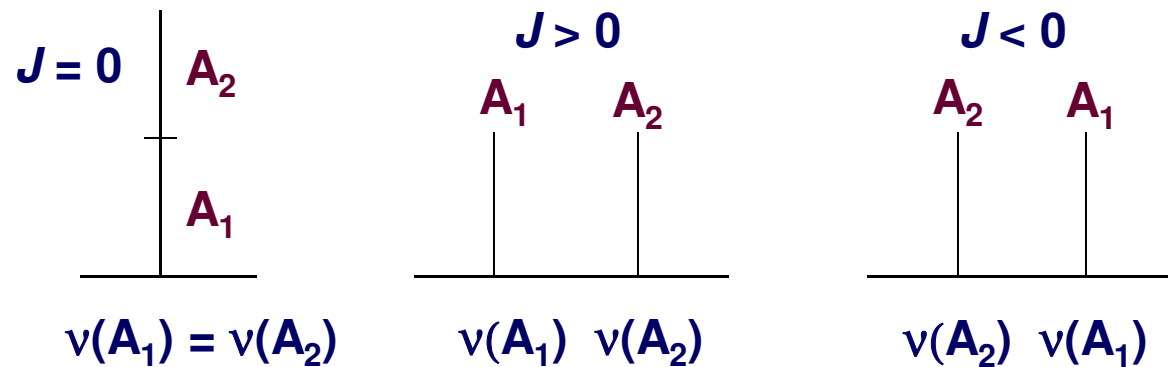
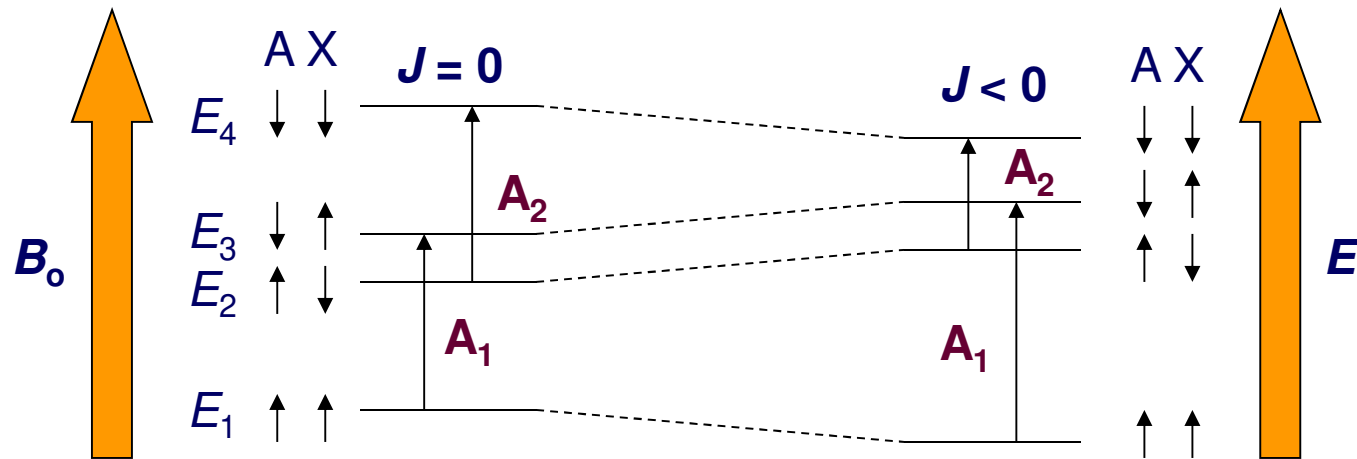
Pulsní NMR



# Spin-spinové interakce



# Spin-spinové interakce



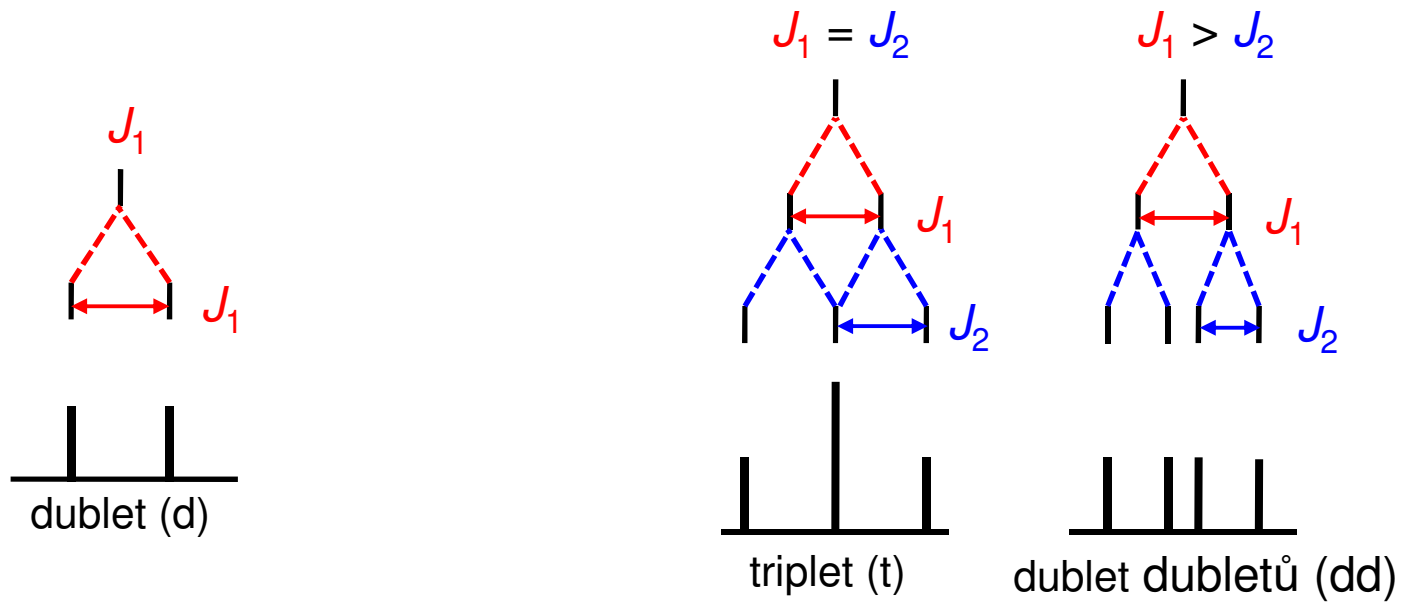
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# Spin-spinové interakce

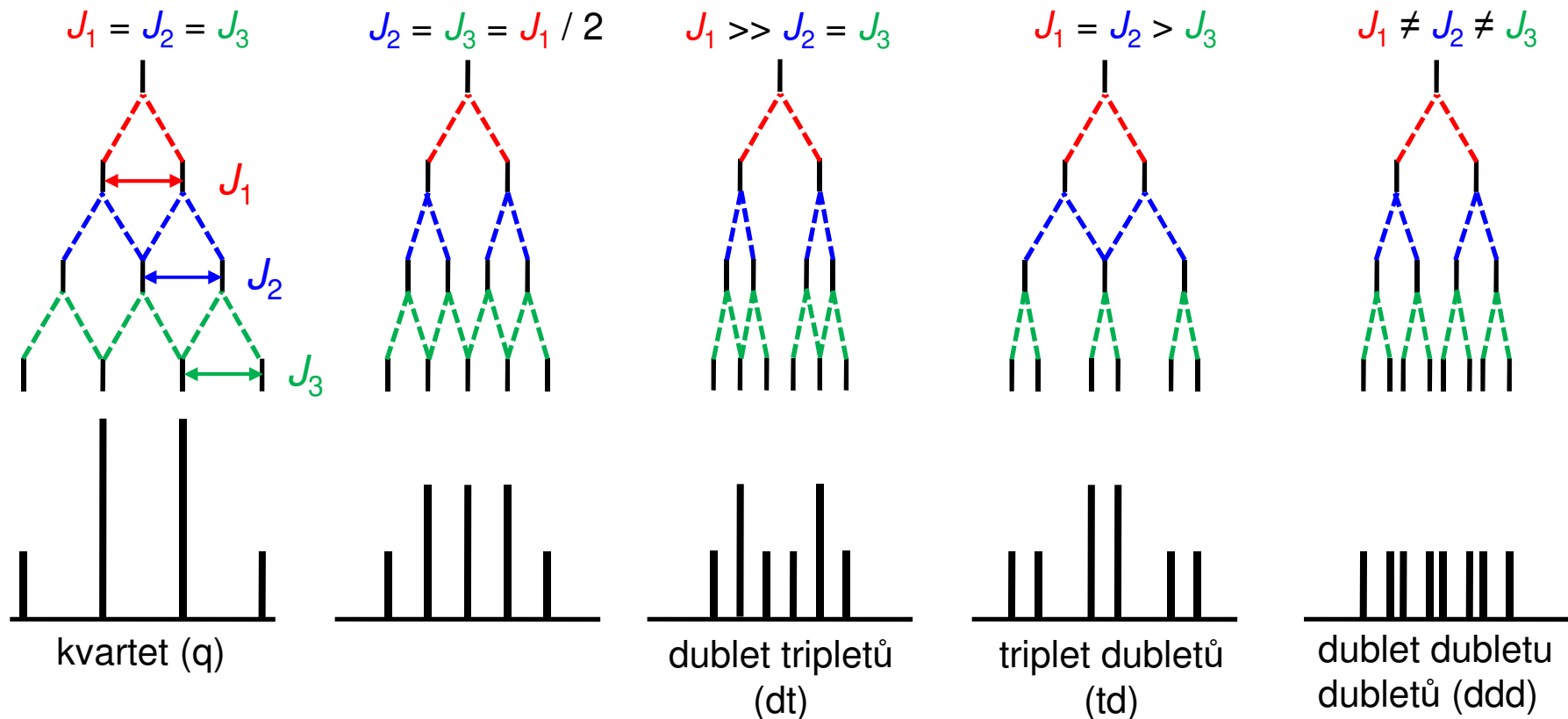
1	singlet	s
1 1	dublet	d
1 2 1	triplet	t
1 3 3 1	kvartet	q
1 4 6 4 1	pentet	p

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# Spin-spinové interakce

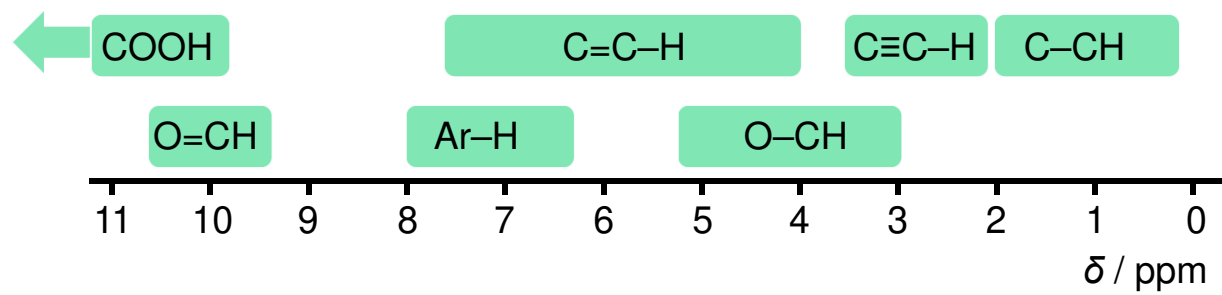


# Spin-spinové interakce



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# $^1\text{H}$ NMR

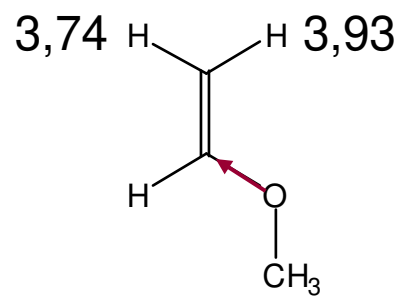
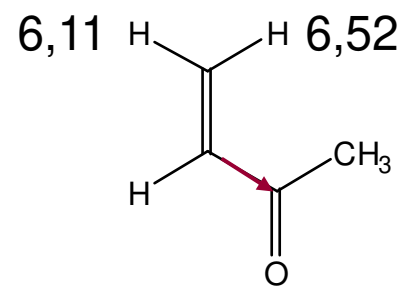
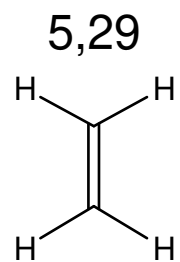




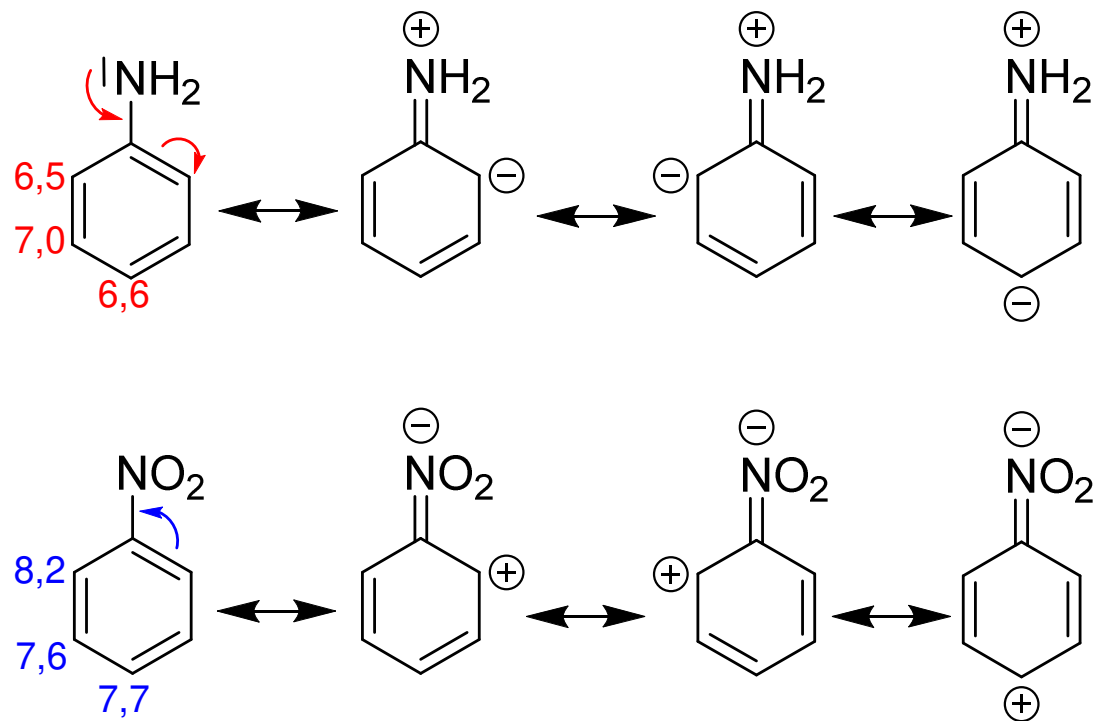
## <sup>1</sup>H NMR - alkany

X	$\delta(X-CH_3)$	elektronegativita
Li	-1	1,0
R <sub>3</sub> Si	0	1,8
H	0,4	2,1
CH <sub>3</sub>	0,8	2,5
NH <sub>2</sub>	2,36	3,0
OH	3,38	3,5
I	2,16	2,5
Br	2,70	2,8
Cl	3,05	3,0
F	4,25	4,0

## $^1\text{H}$ NMR – mezomerní efekt



# $^1\text{H}$ NMR - areny



## **<sup>1</sup>H NMR – alkeny**

$$\delta = 4\text{--}7,5 \text{ ppm}$$

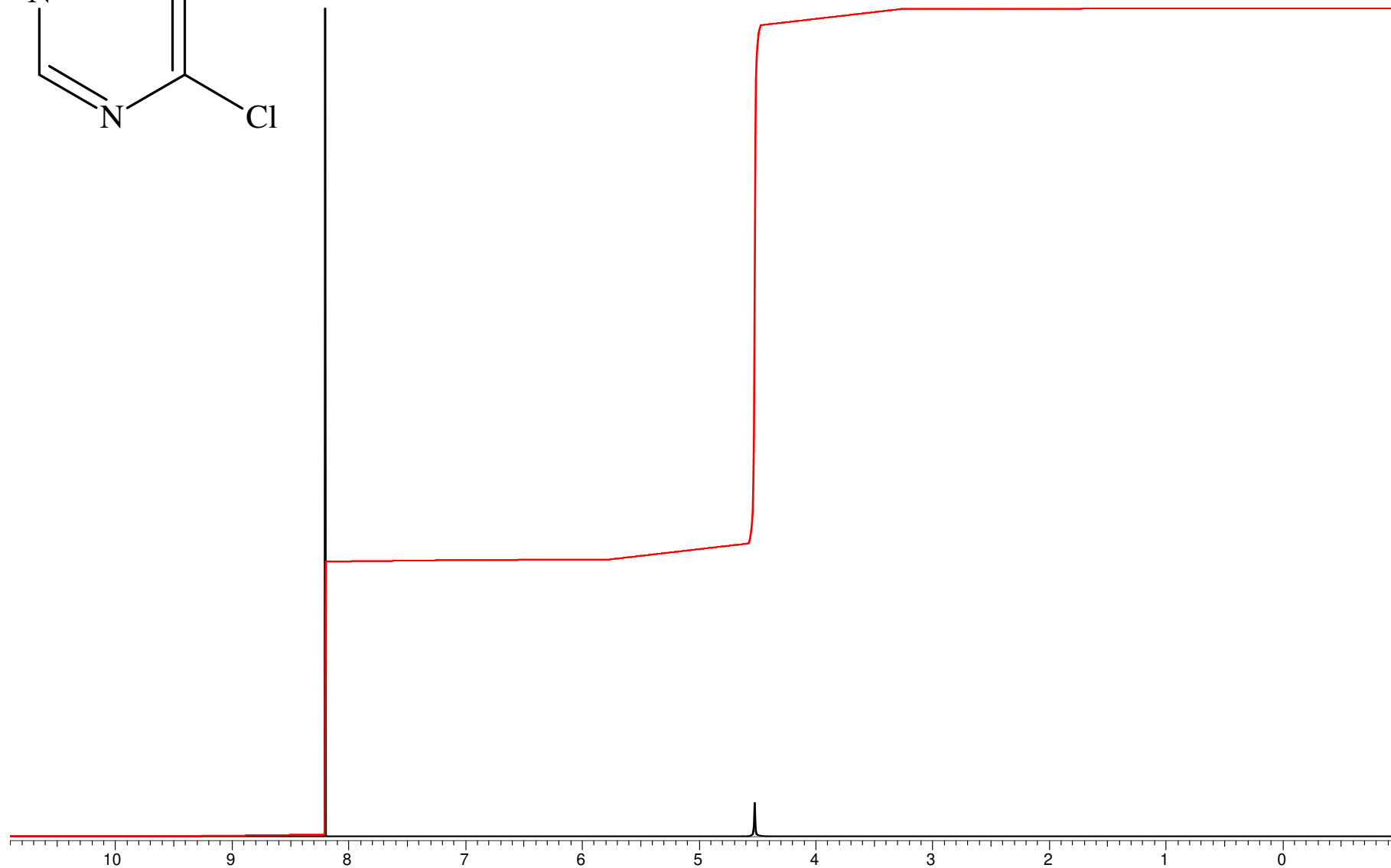
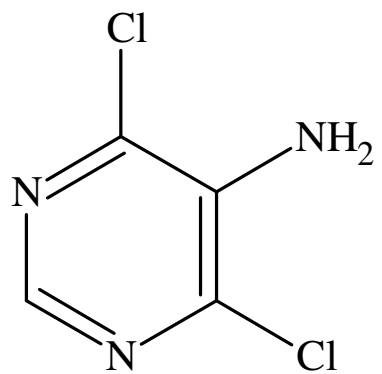
## **Alkyny**

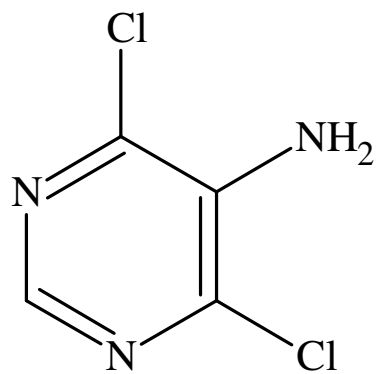
$$\delta = 2\text{--}3 \text{ ppm}$$

## **Aldehydy**

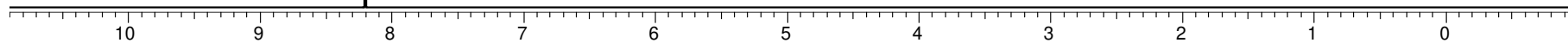
$$\delta = 9\text{--}11 \text{ ppm}$$

## **Vyměnitelné protony (OH, SH, NH)**

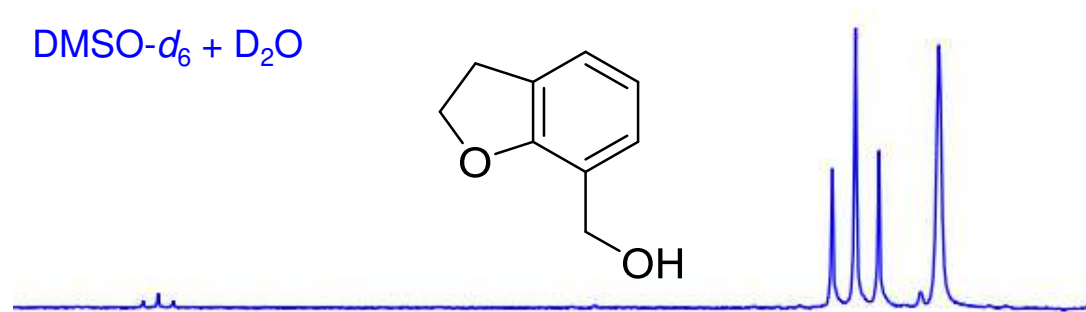
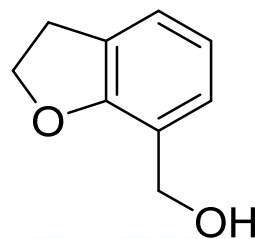




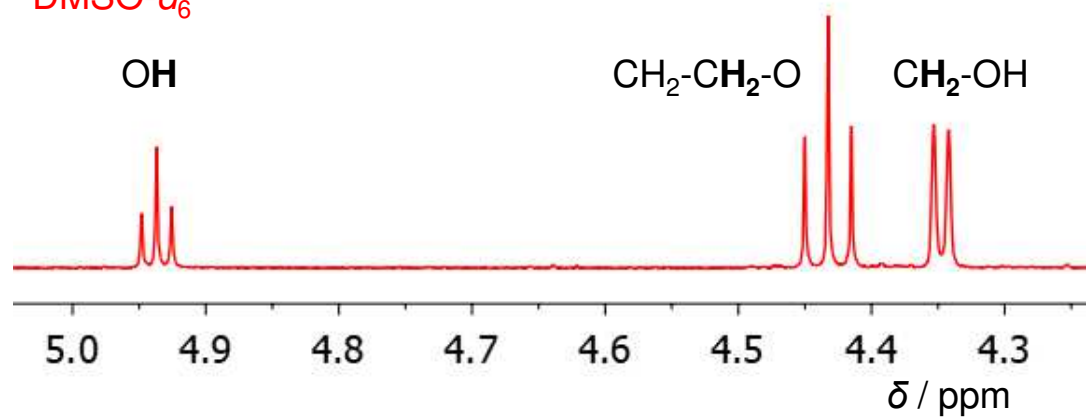
+ D<sub>2</sub>O

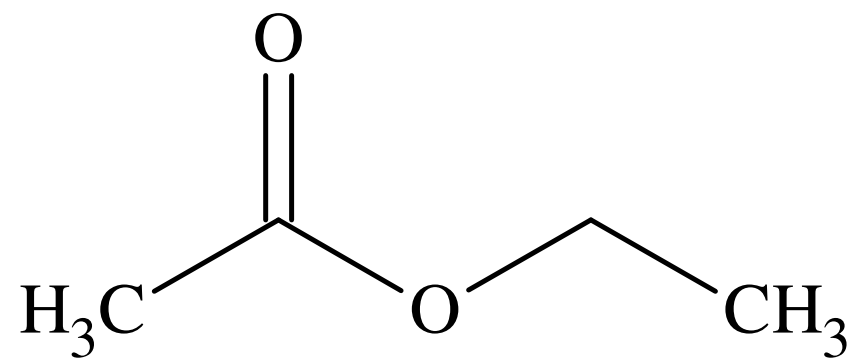


DMSO- $d_6$  + D $_2$ O



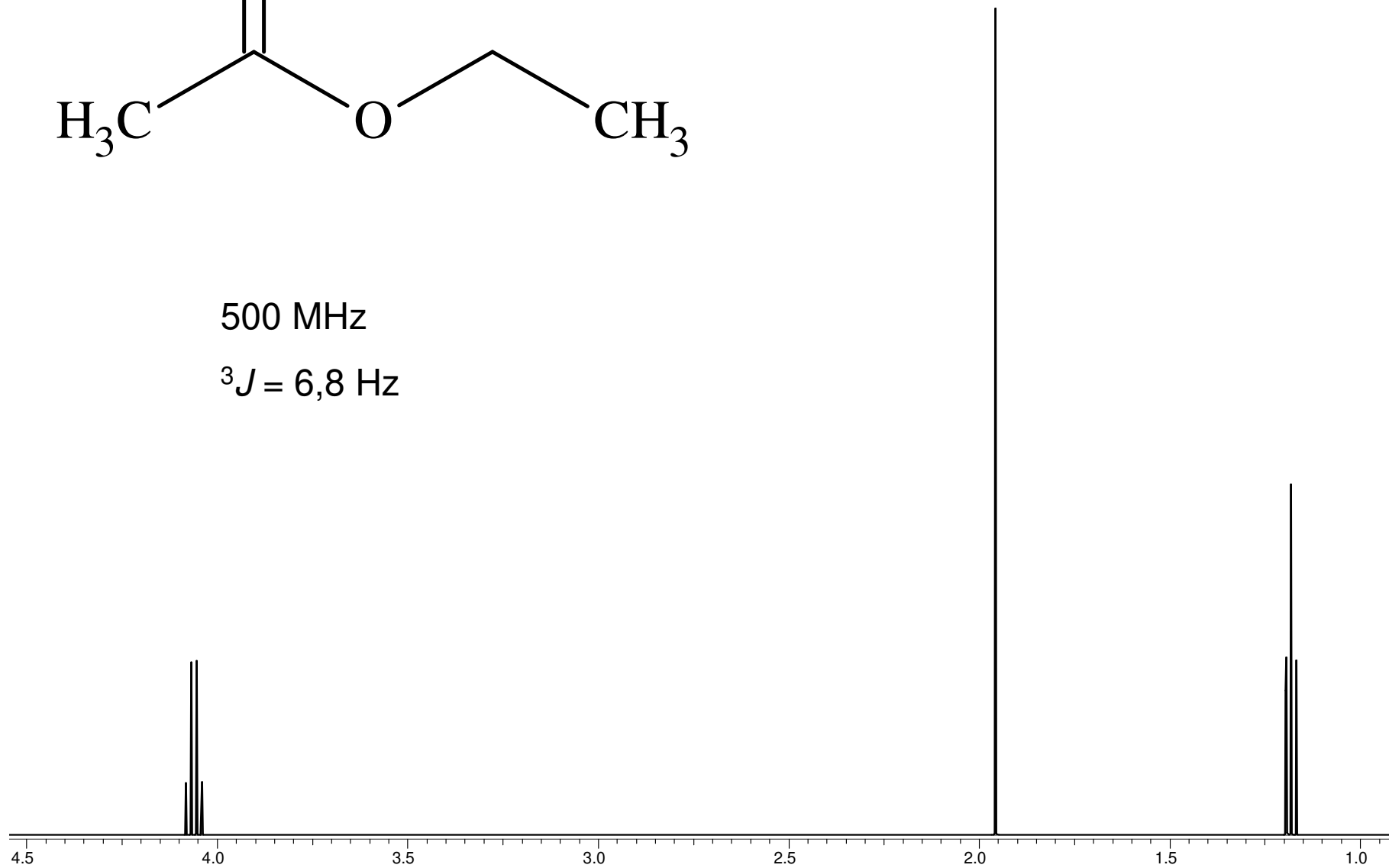
DMSO- $d_6$



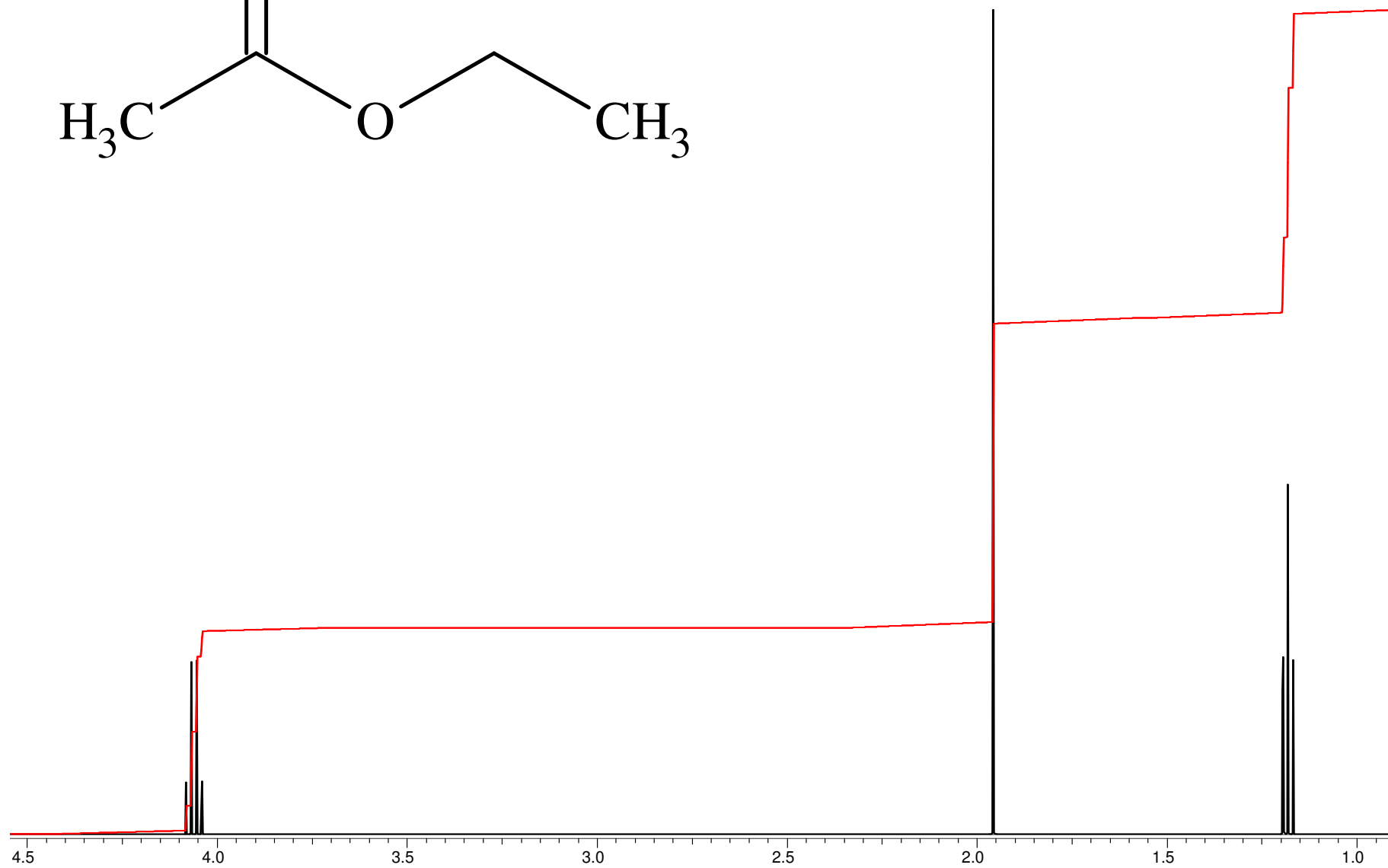
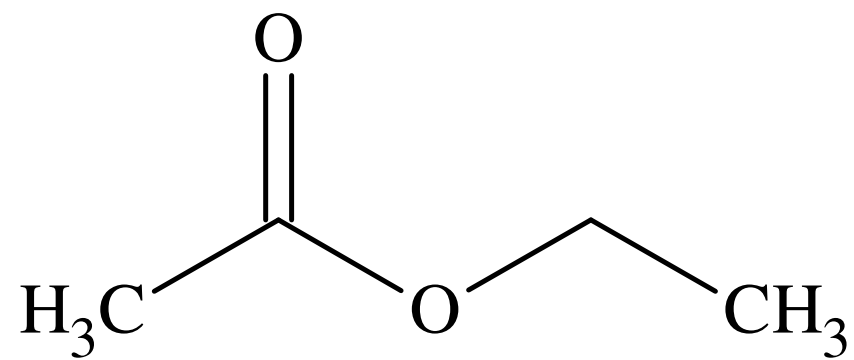


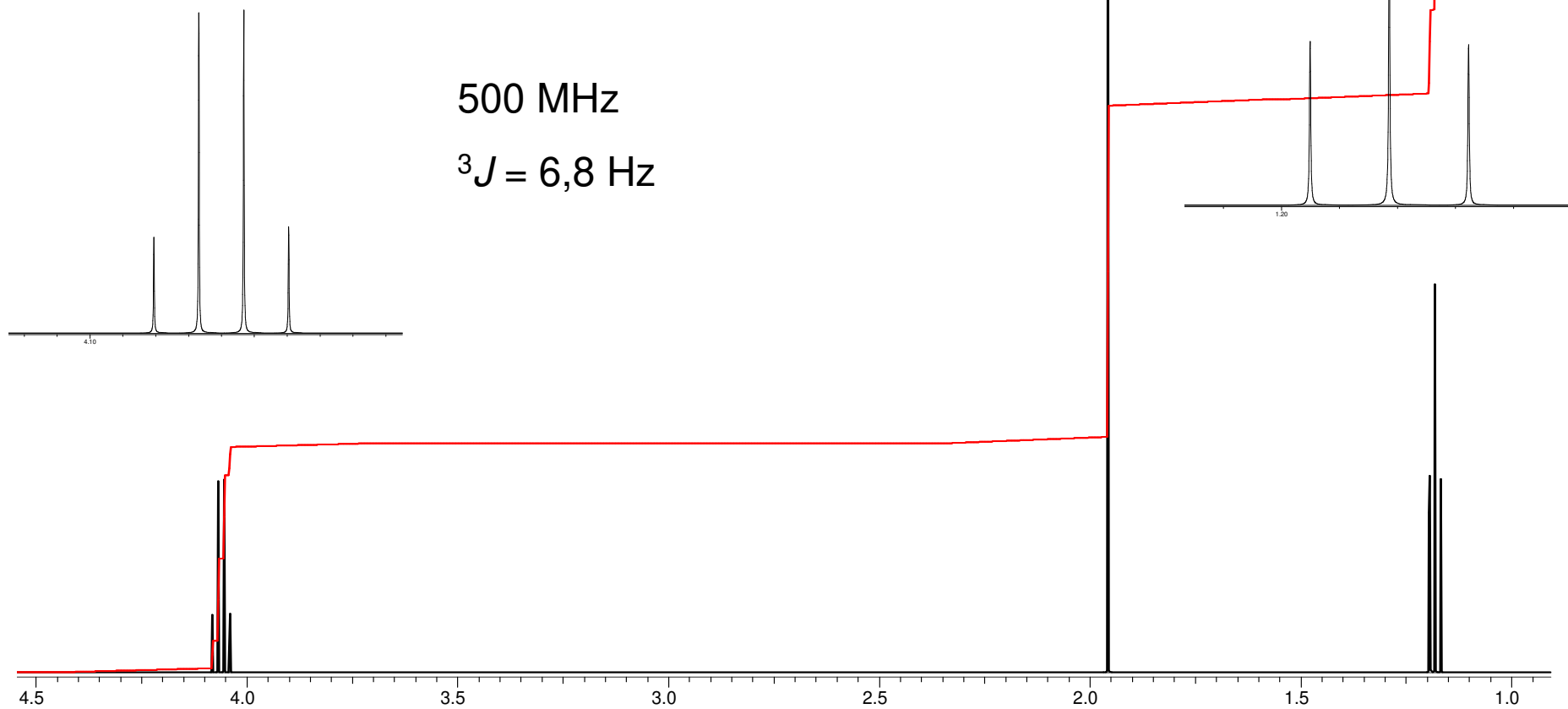
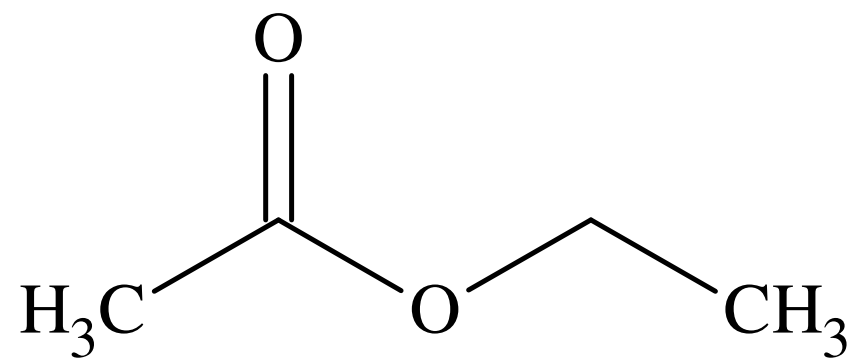
500 MHz

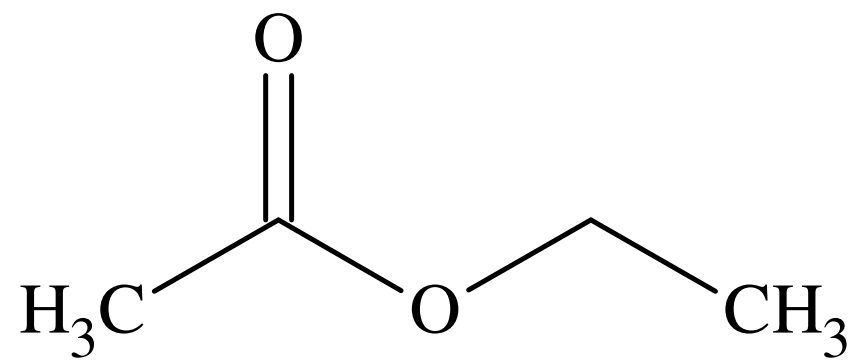
$^3J = 6,8$  Hz





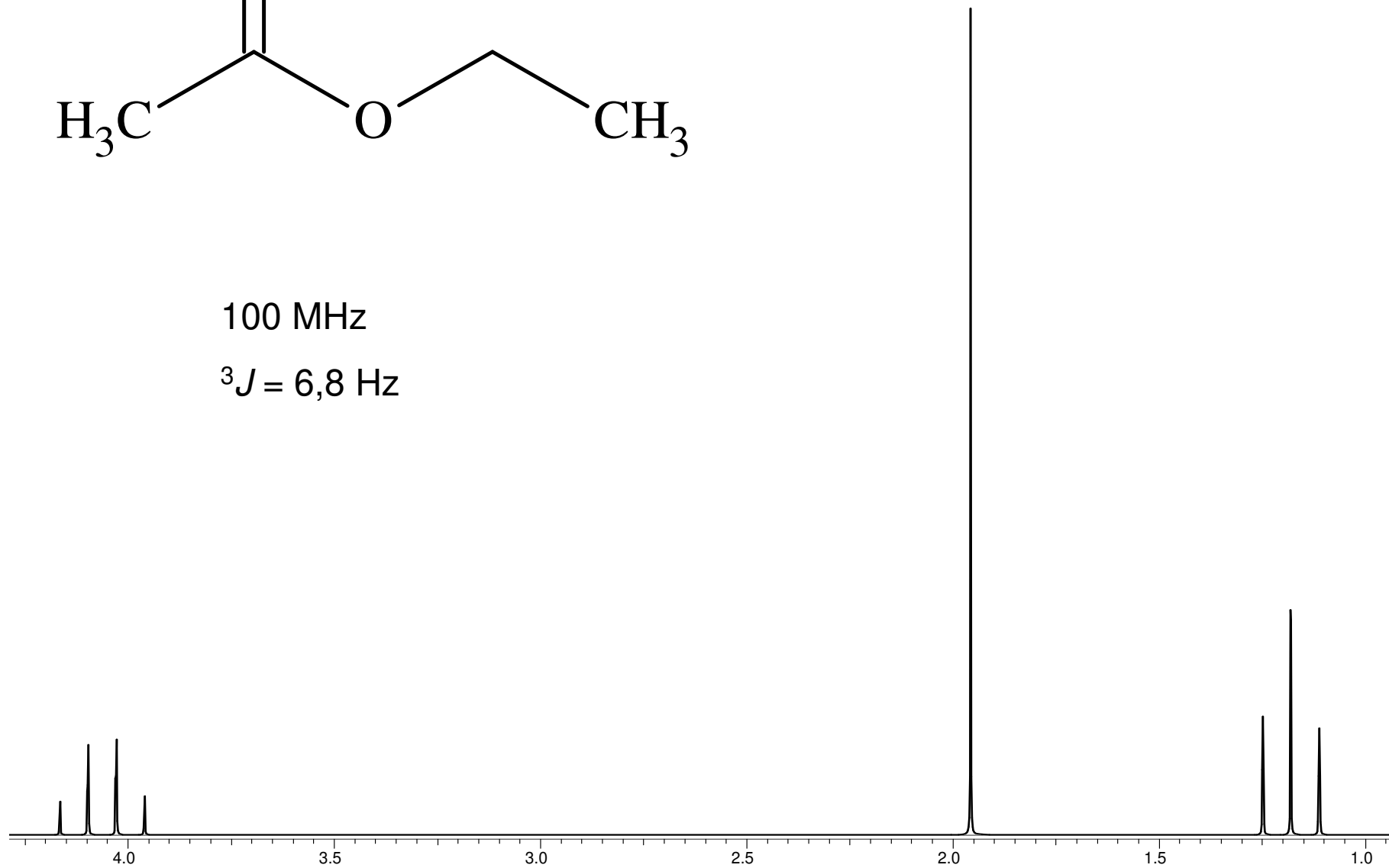


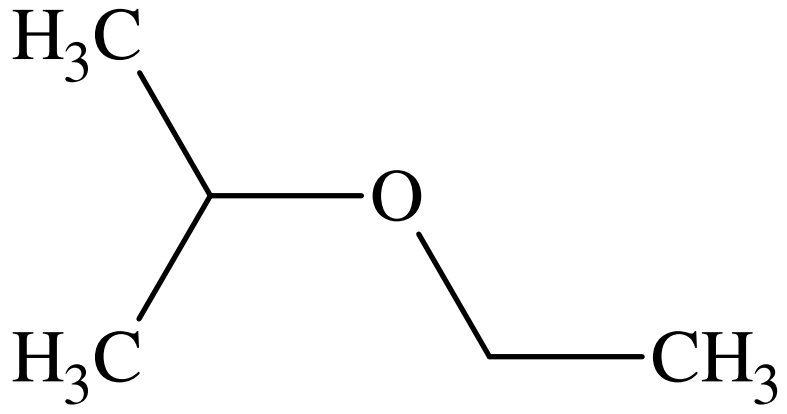




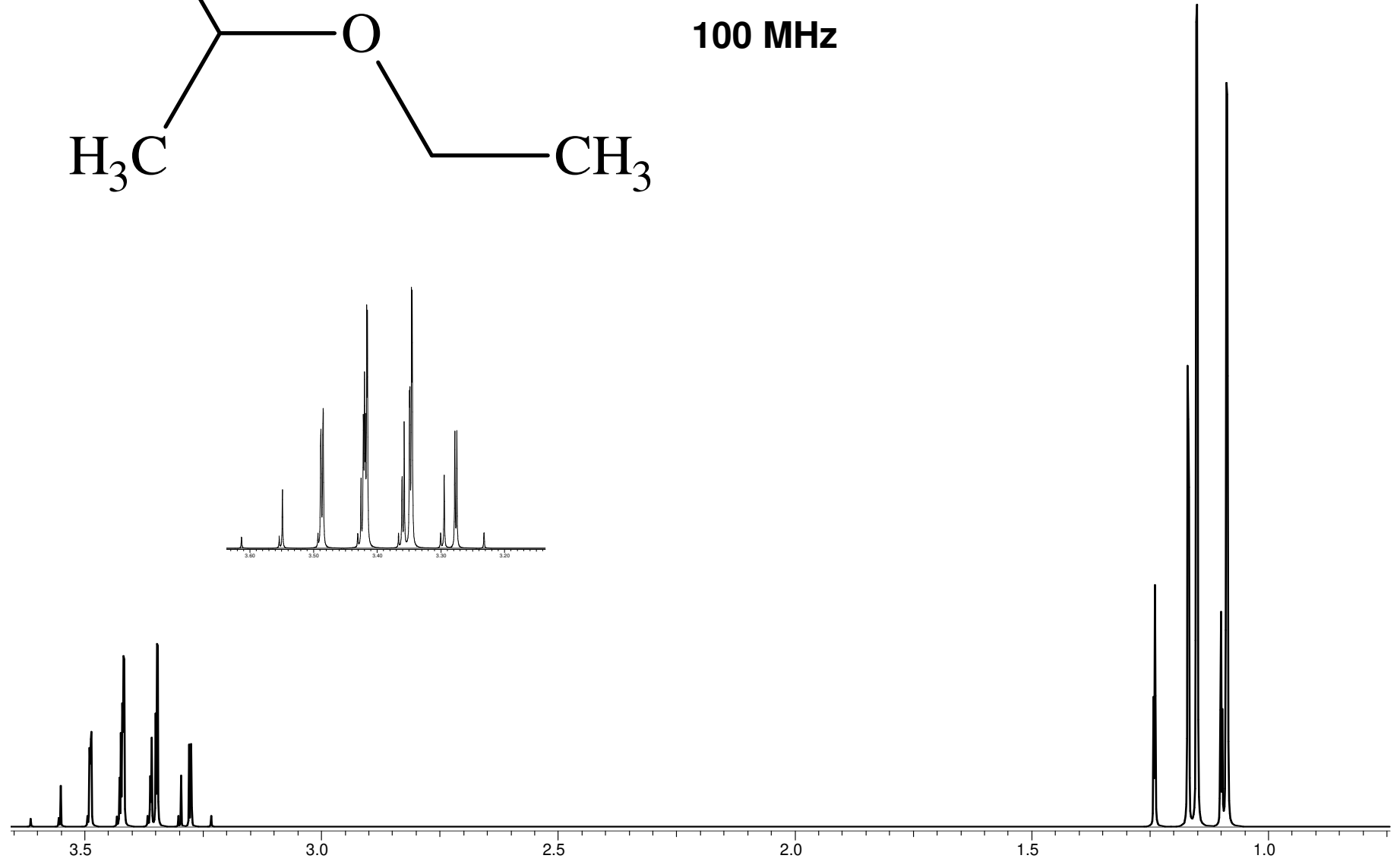
100 MHz

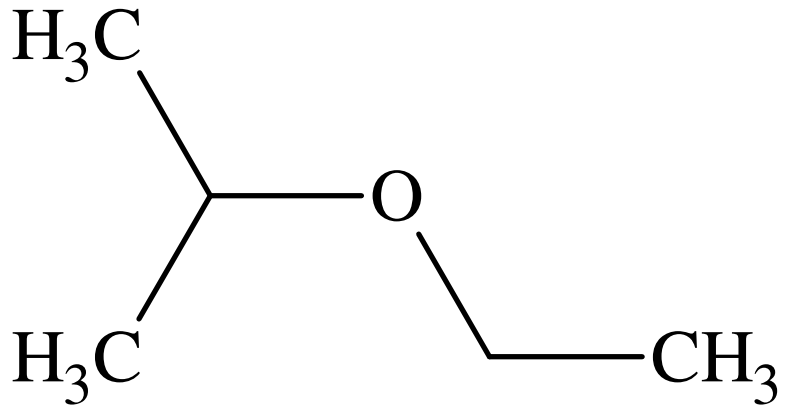
$^3J = 6,8$  Hz



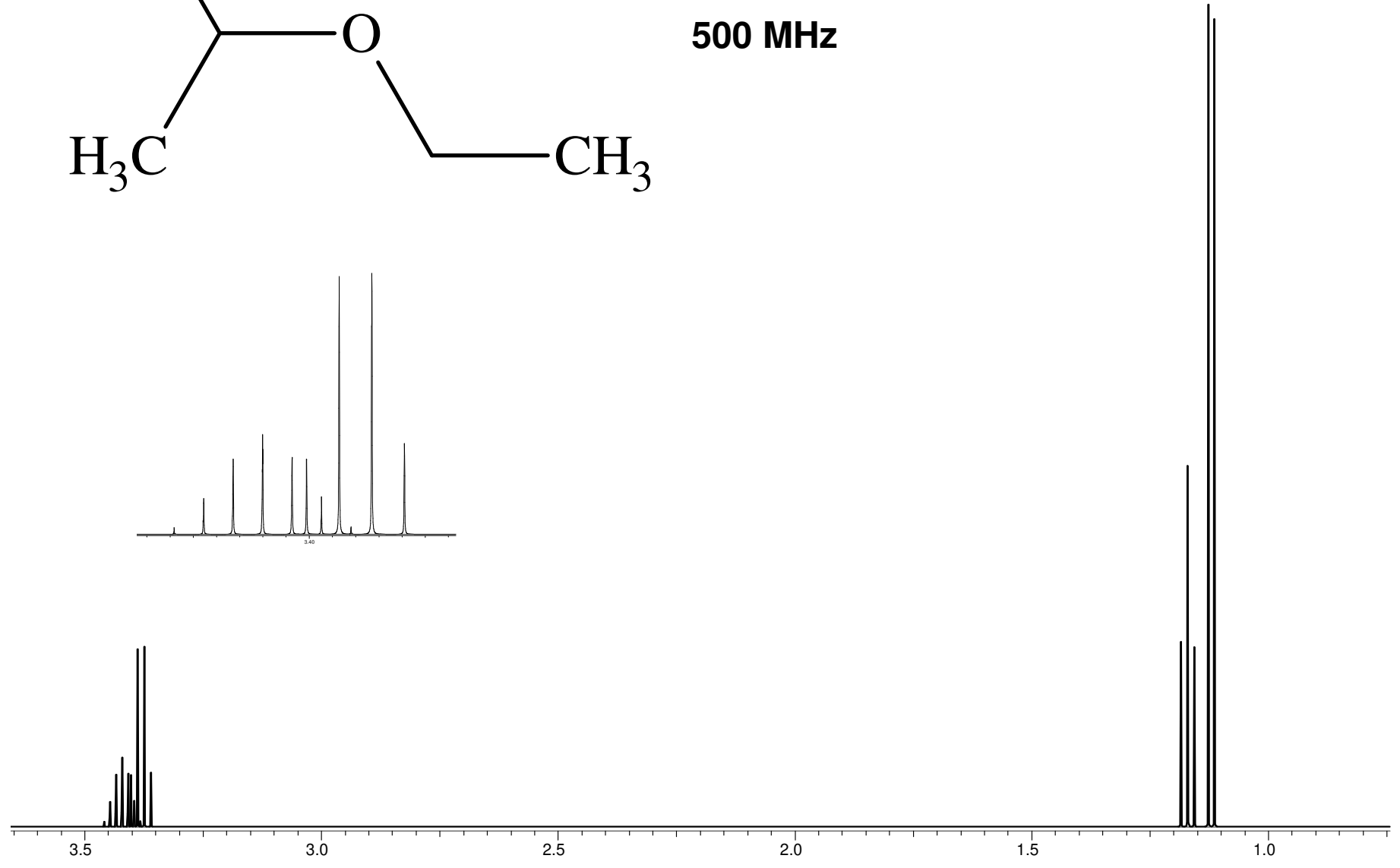


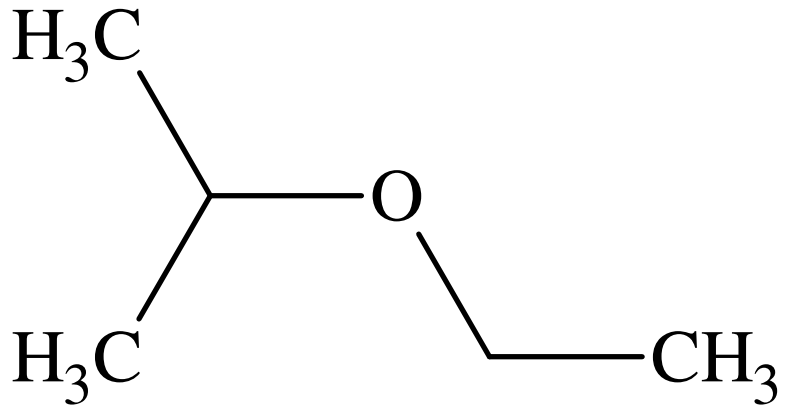
100 MHz





500 MHz





800 MHz

