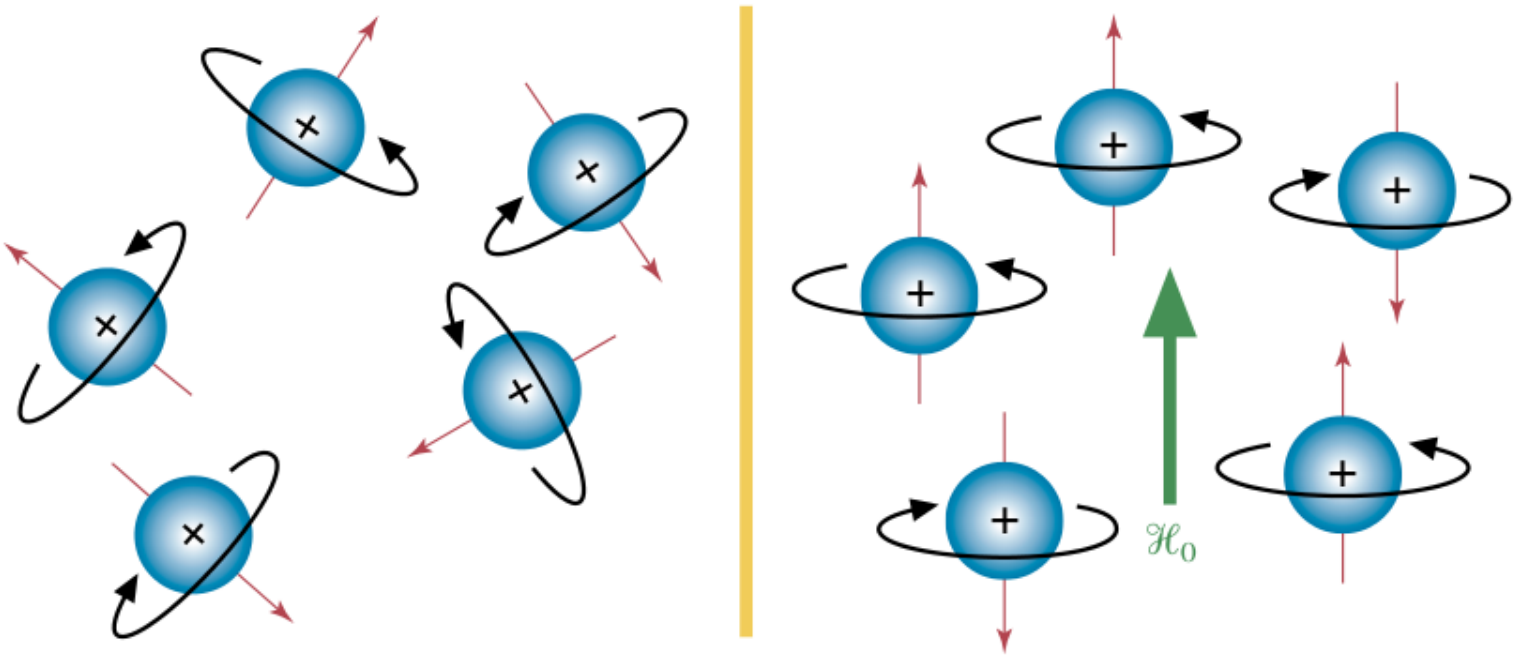
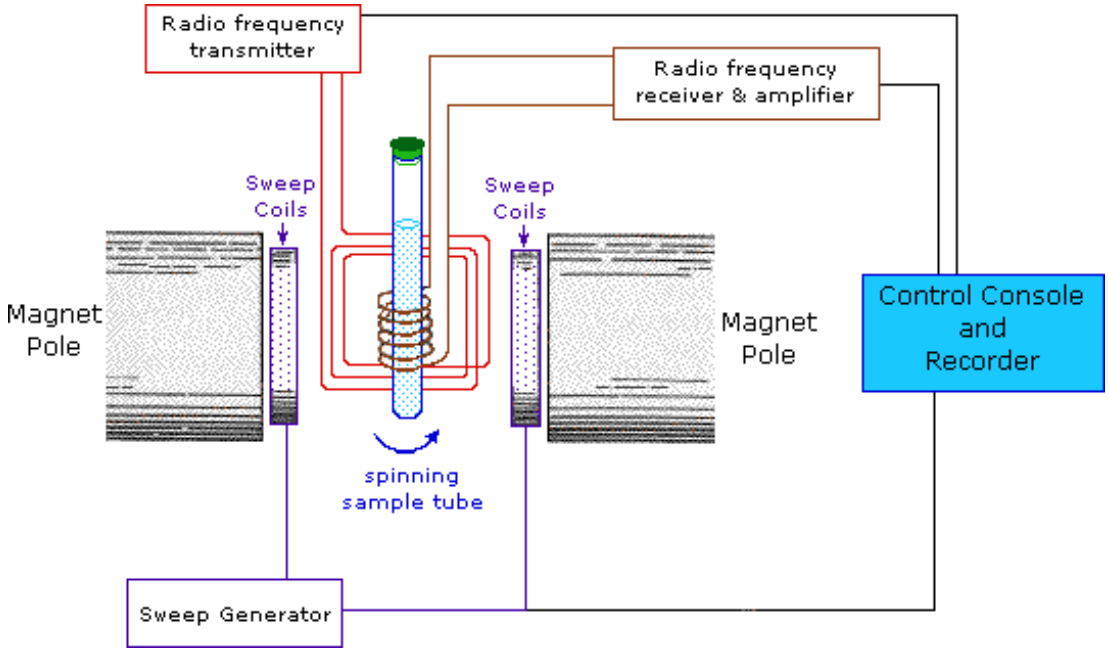
Nukleární magnetická rezonance



Jádra s $I = 1/2$, např.:

^{1}H (99,99 %), ^{13}C (1,1 %), ^{15}N (0,37 %), ^{19}F (100 %), ^{29}Si (4,67 %), ^{31}P (100 %)...

Nukleární magnetická rezonance



Rezonanční frekvence:

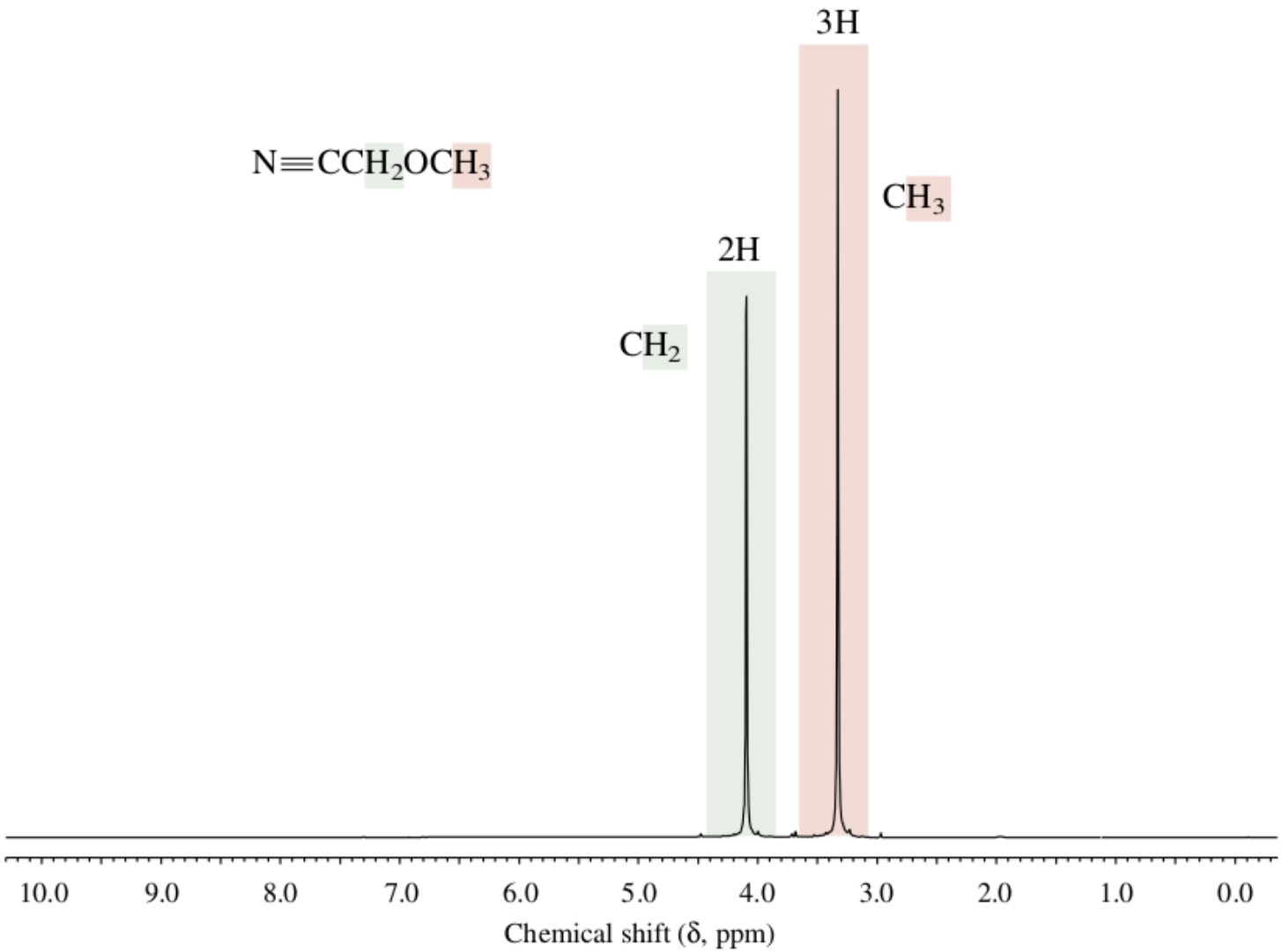
$$\nu = \frac{-\gamma B}{2\pi}$$

Chemický posun:

$$\delta = \frac{\nu - \nu_{ref}}{\nu_{ref}} \times 10^6 \text{ ppm}$$

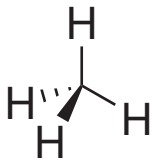
Nukleární magnetická rezonance

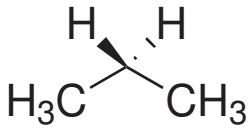
Nukleární magnetická rezonance

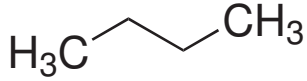


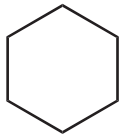
Nukleární magnetická rezonance

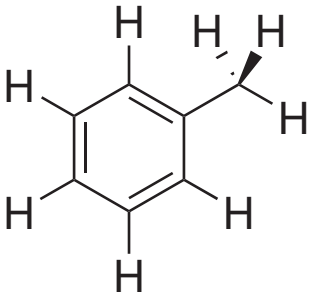
Počet chemicky neekvivalentních atomů vodíku?

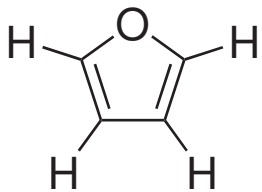


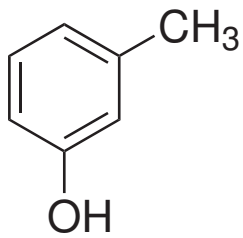


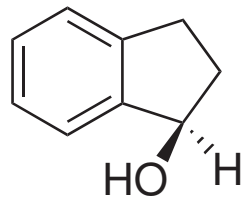




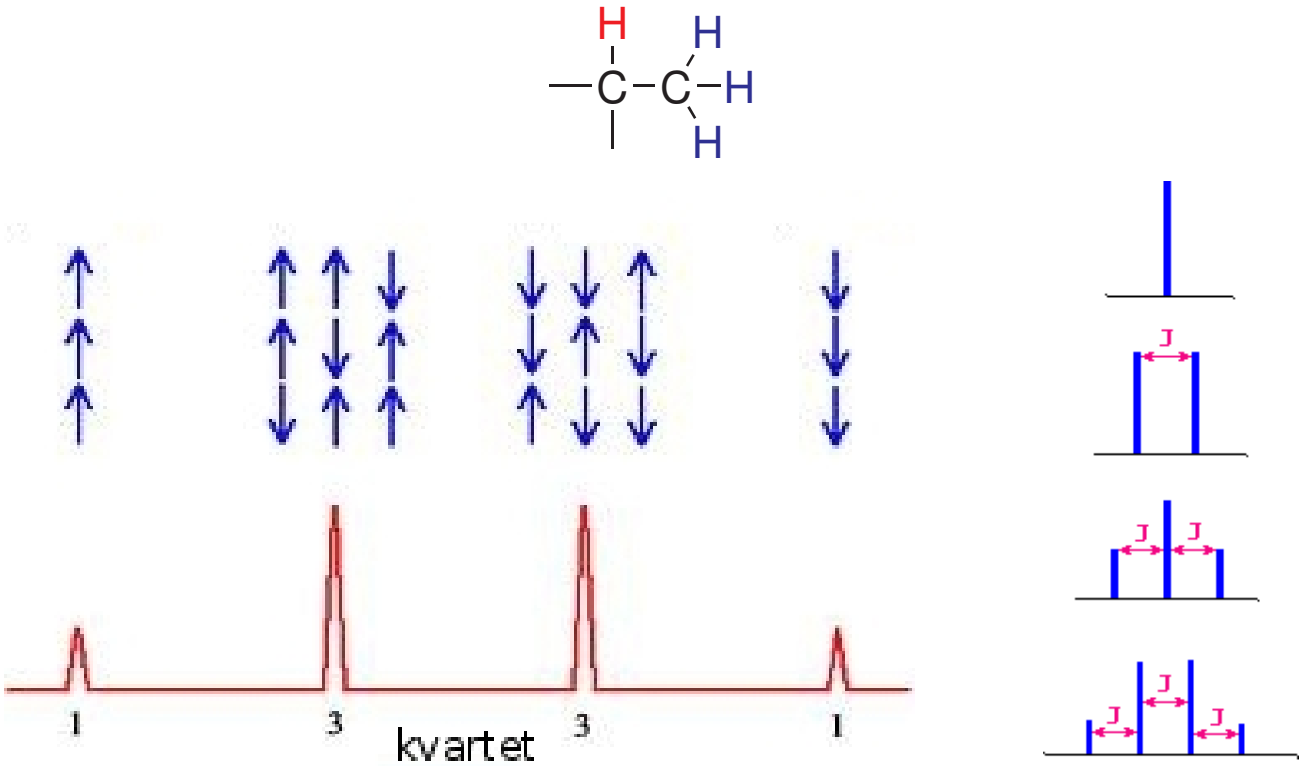








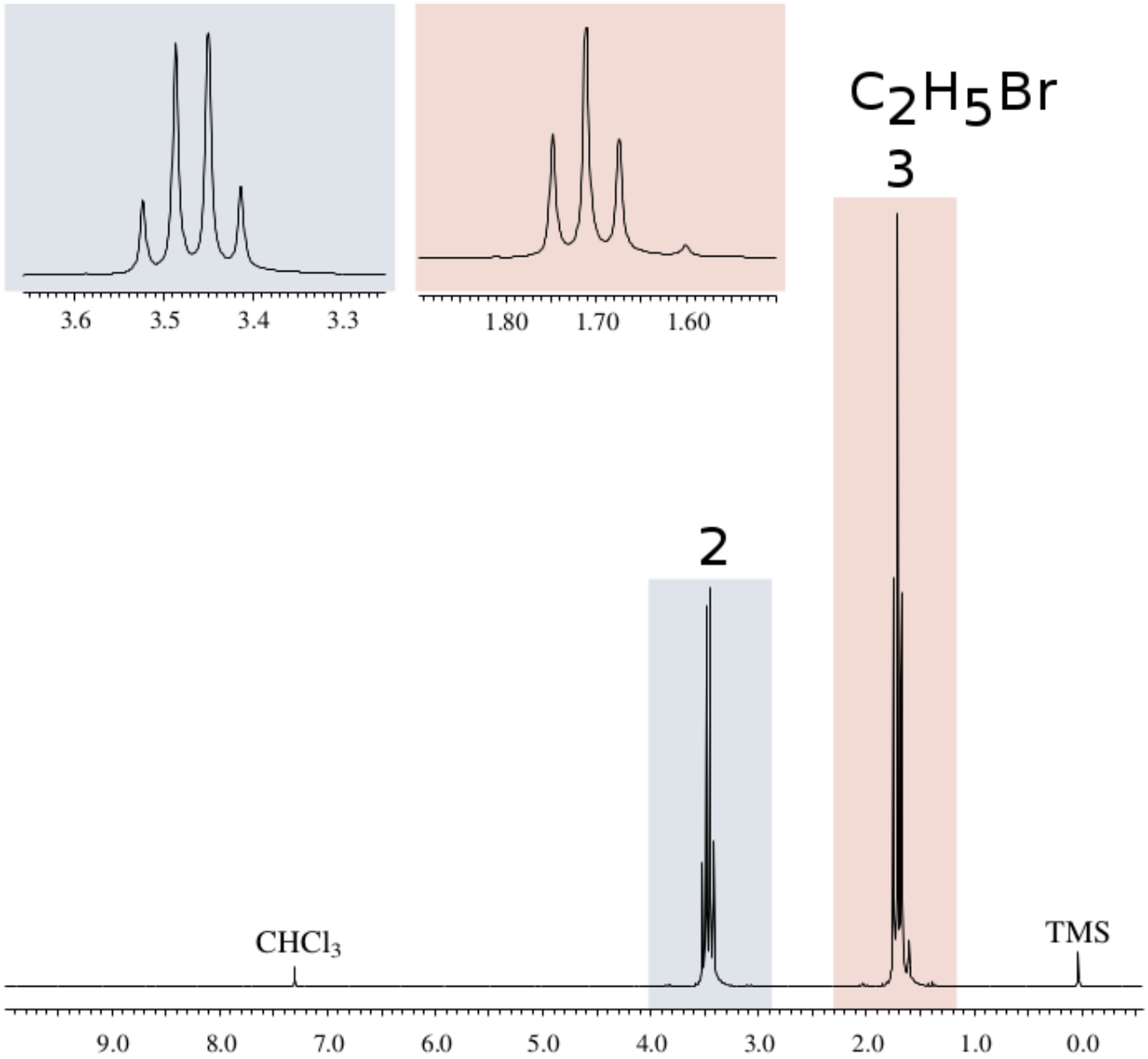
Nukleární magnetická rezonance



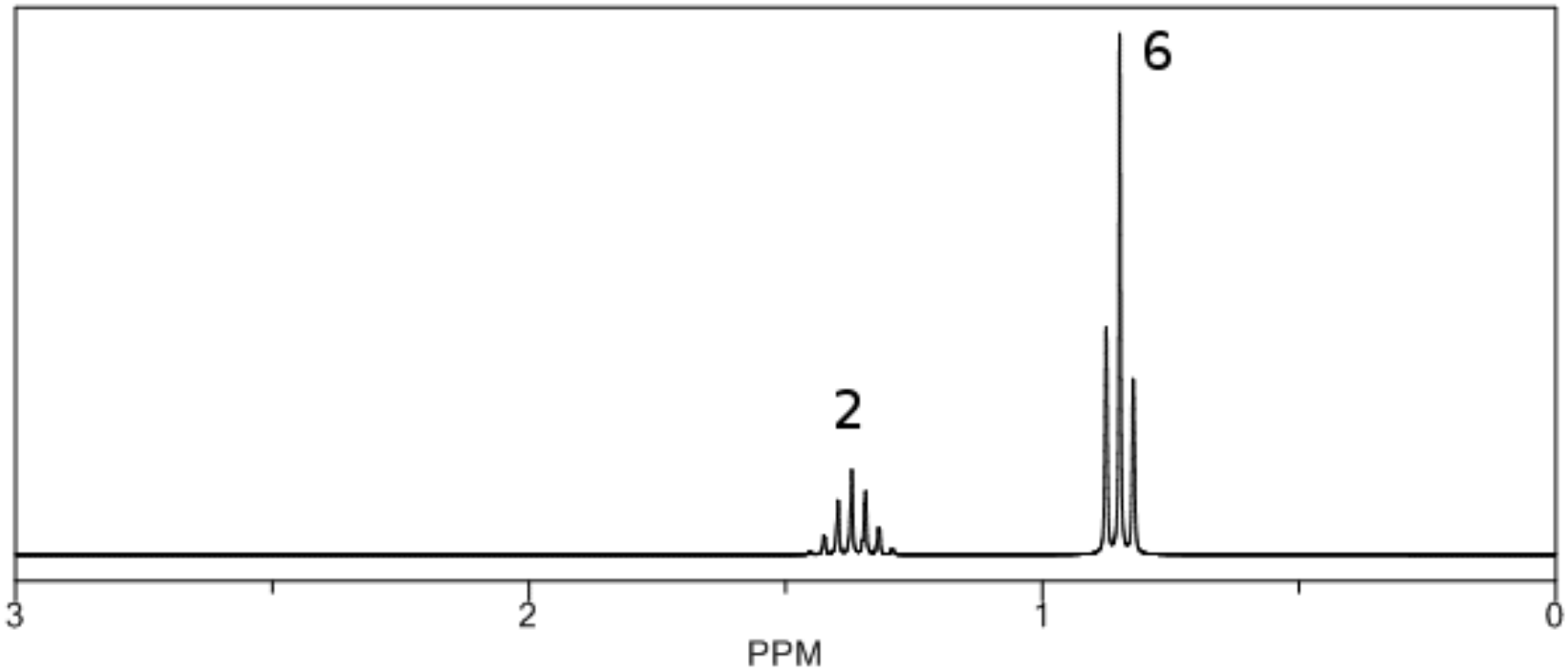
Počet linií:

$$N = 2\,n\,I + 1$$

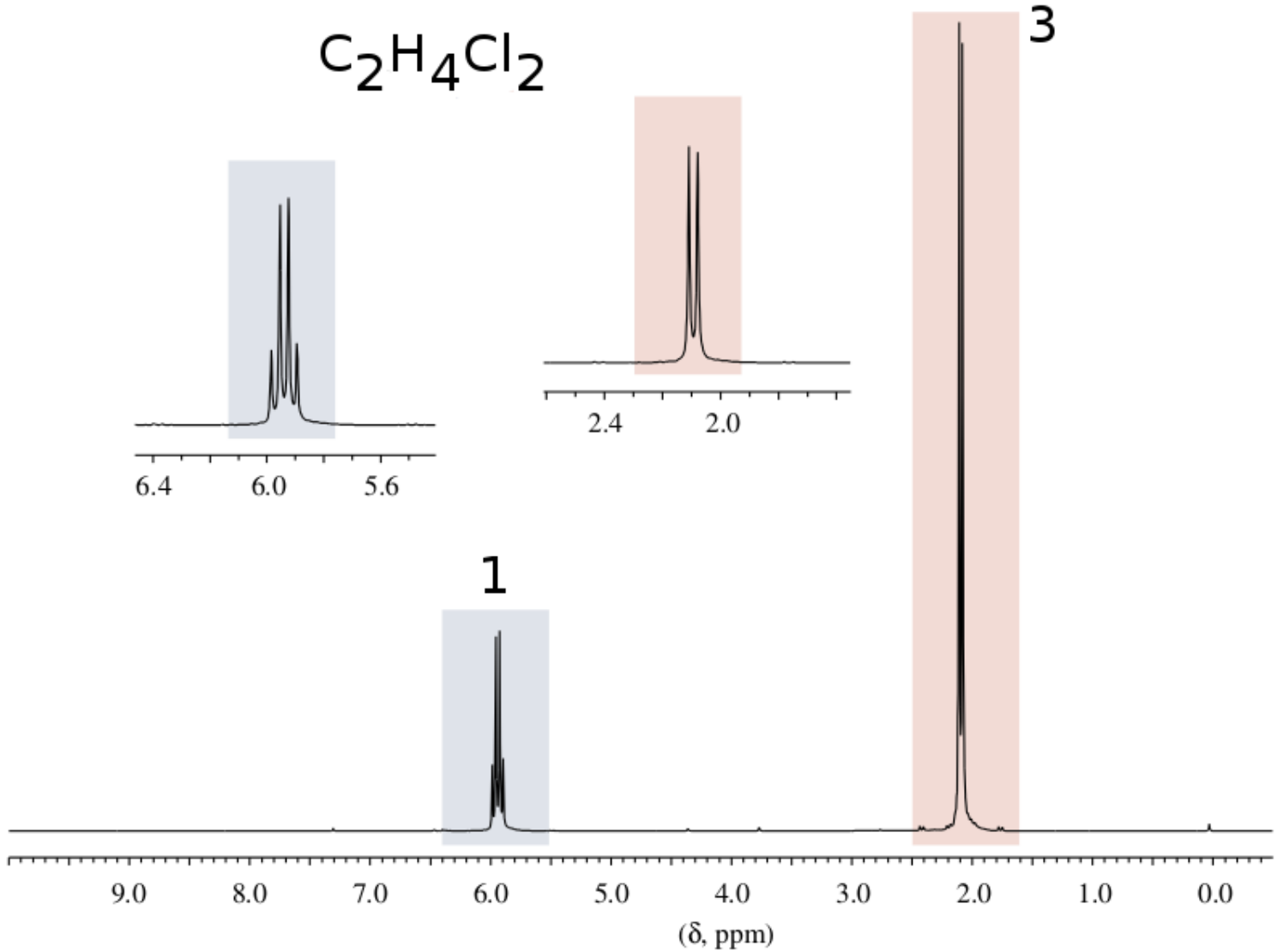
Nukleární magnetická rezonance



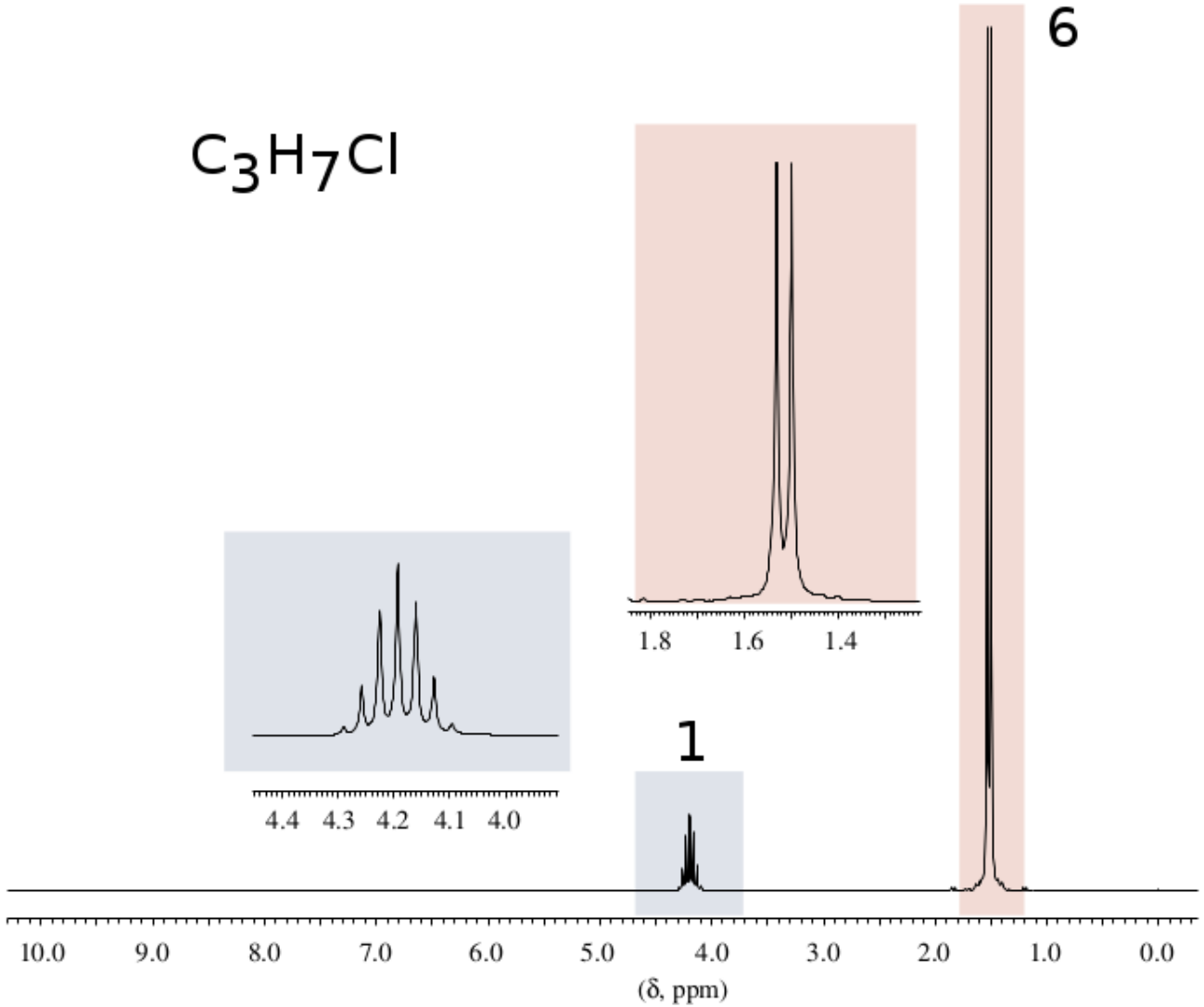
Nukleární magnetická rezonance



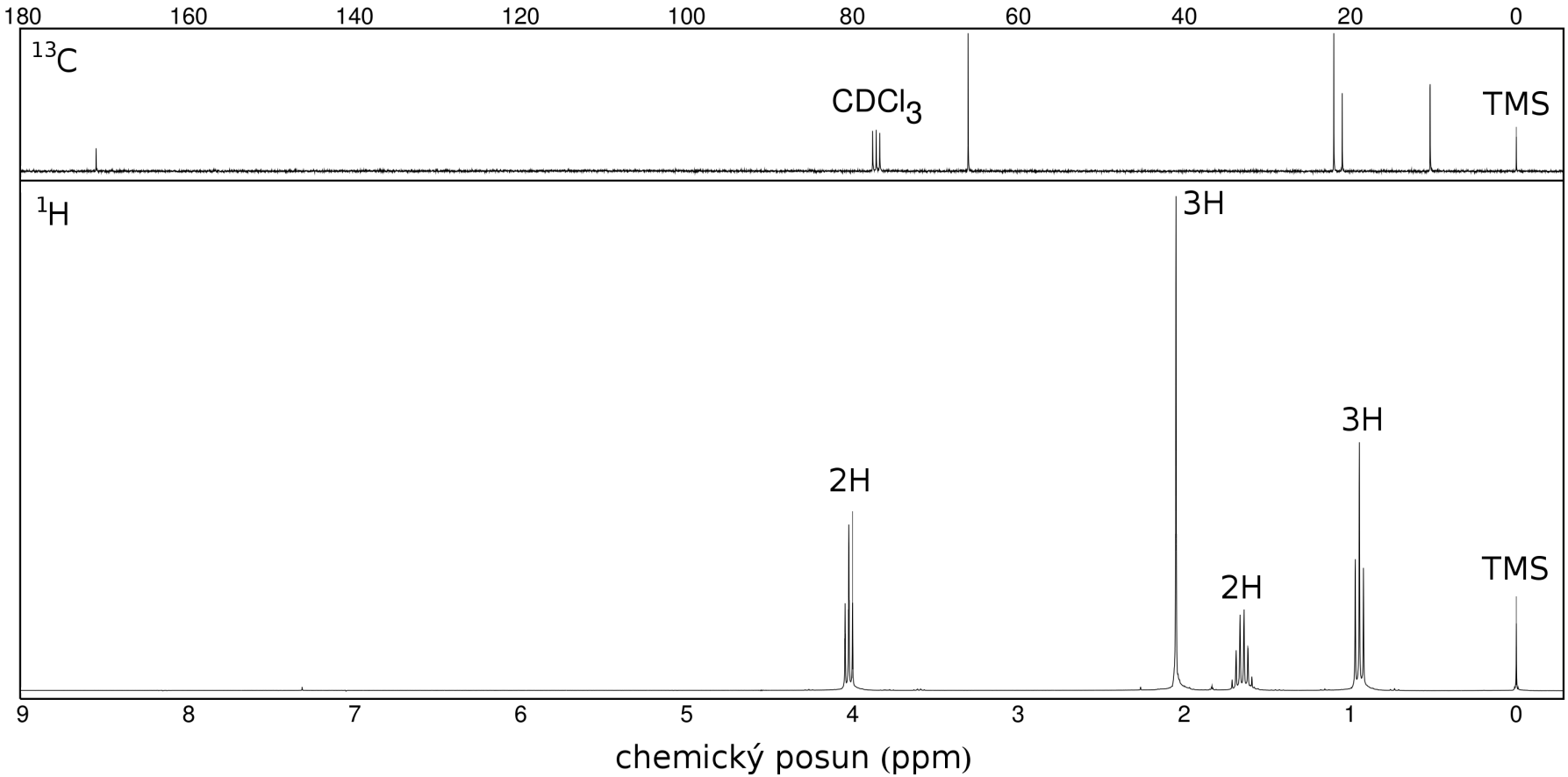
Nukleární magnetická rezonance



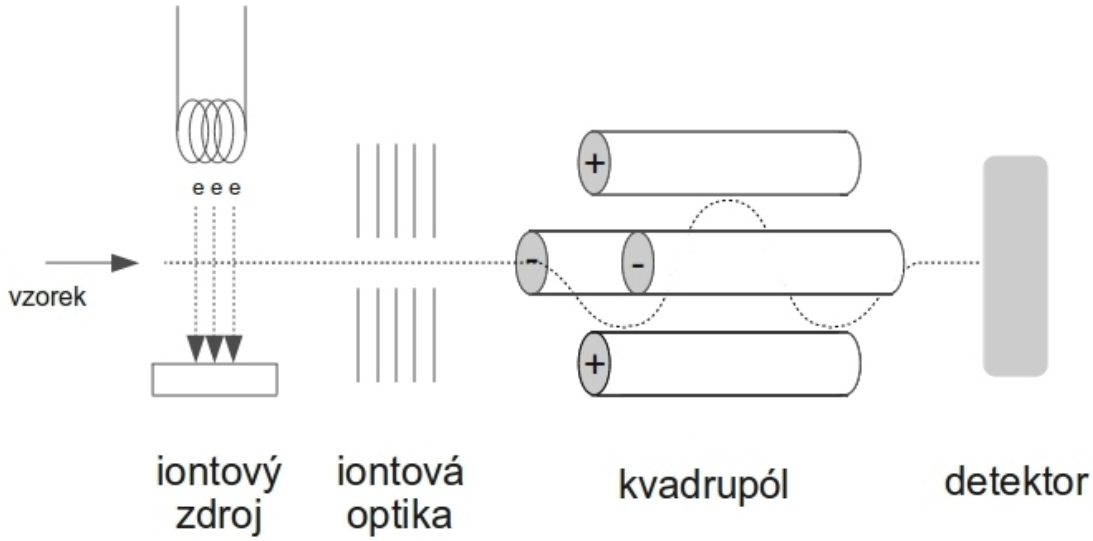
Nukleární magnetická rezonance



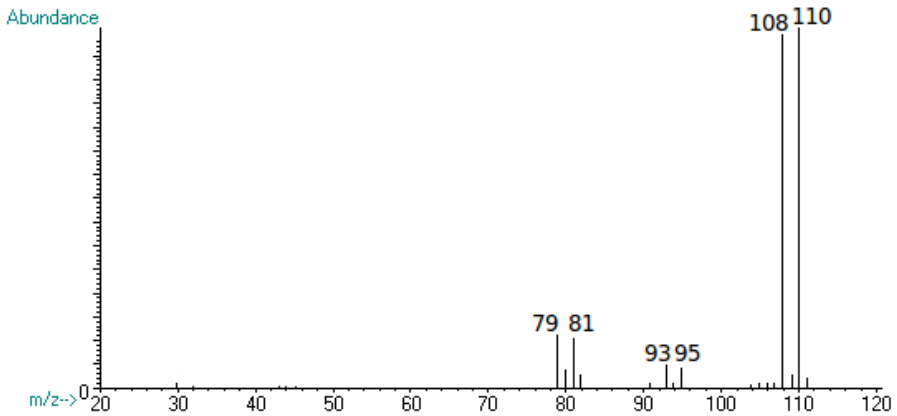
^{13}C NMR – propyl-acetát



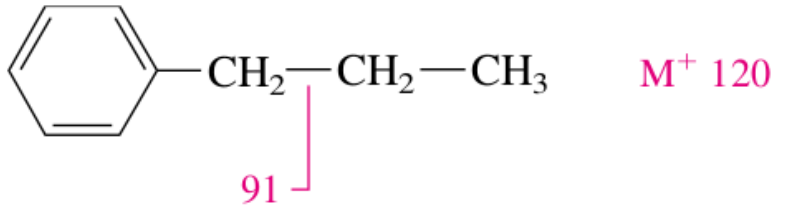
Hmotnostní spektroskopie

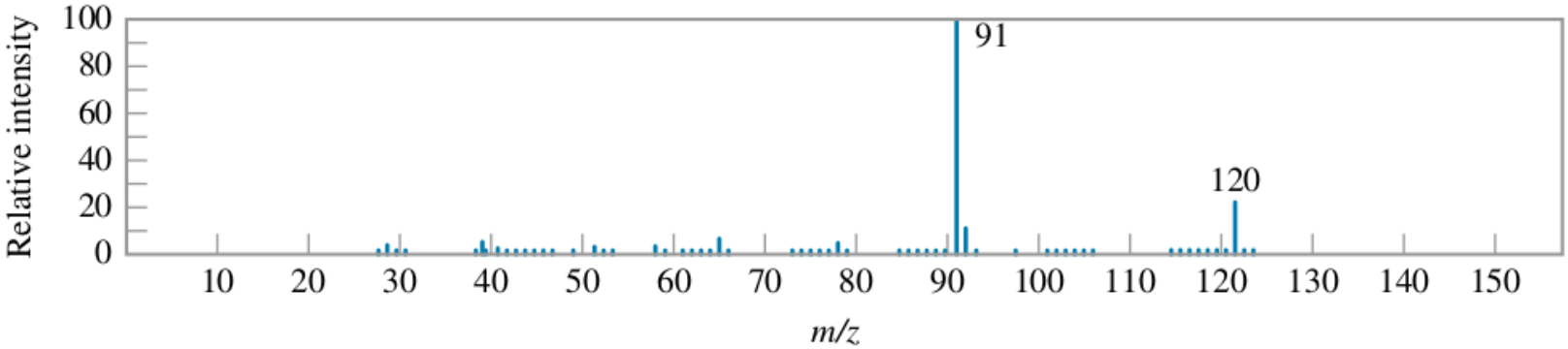


Bromethan:



Hmotnostní spektroskopie



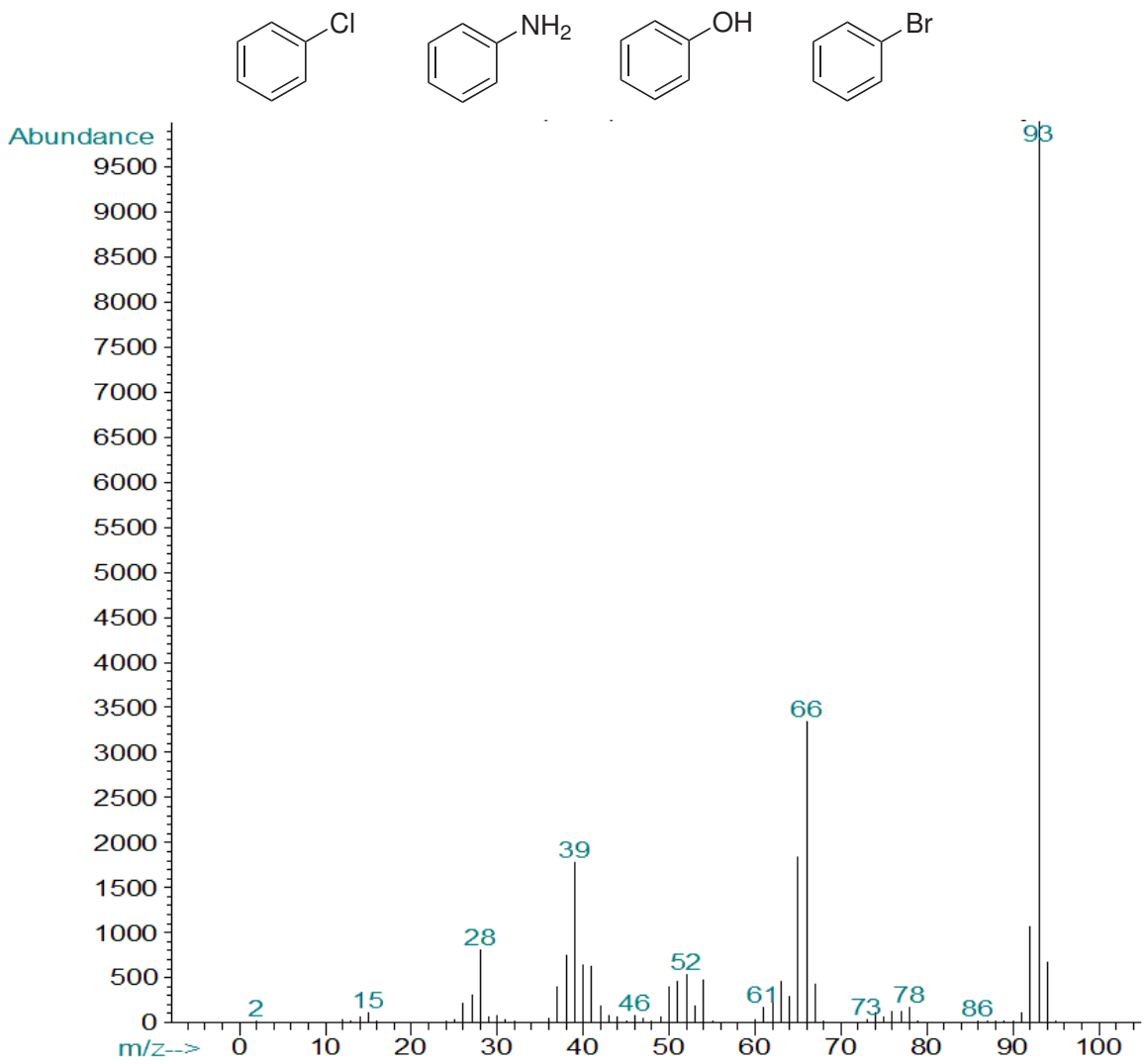


Zastoupení isotopů

Prvek	Isotop	Relativní zastoupení	Isotop	Relativní zastoupení	Isotop	Relativní zastoupení
Uhlík	^{12}C	100	^{13}C	1,11		
Vodík	^{1}H	100	^{2}H	0,016		
Dusík	^{14}N	100	^{15}N	0,38		
Kyslík	^{16}O	100	^{17}O	0,04	^{18}O	0,2
Fluor	^{19}F	100				
Křemík	^{28}Si	100	^{29}Si	5,1	^{30}Si	3,35
Fosfor	^{28}P	100				
Síra	^{32}S	100	^{33}S	0,78	^{34}S	4,4
Chlor	^{35}Cl	100			^{37}Cl	32,5
Brom	^{79}Br	100			^{81}Br	98
Jod	^{127}I	100				

Dusíkové pravidlo

Hmotnostní spektroskopie



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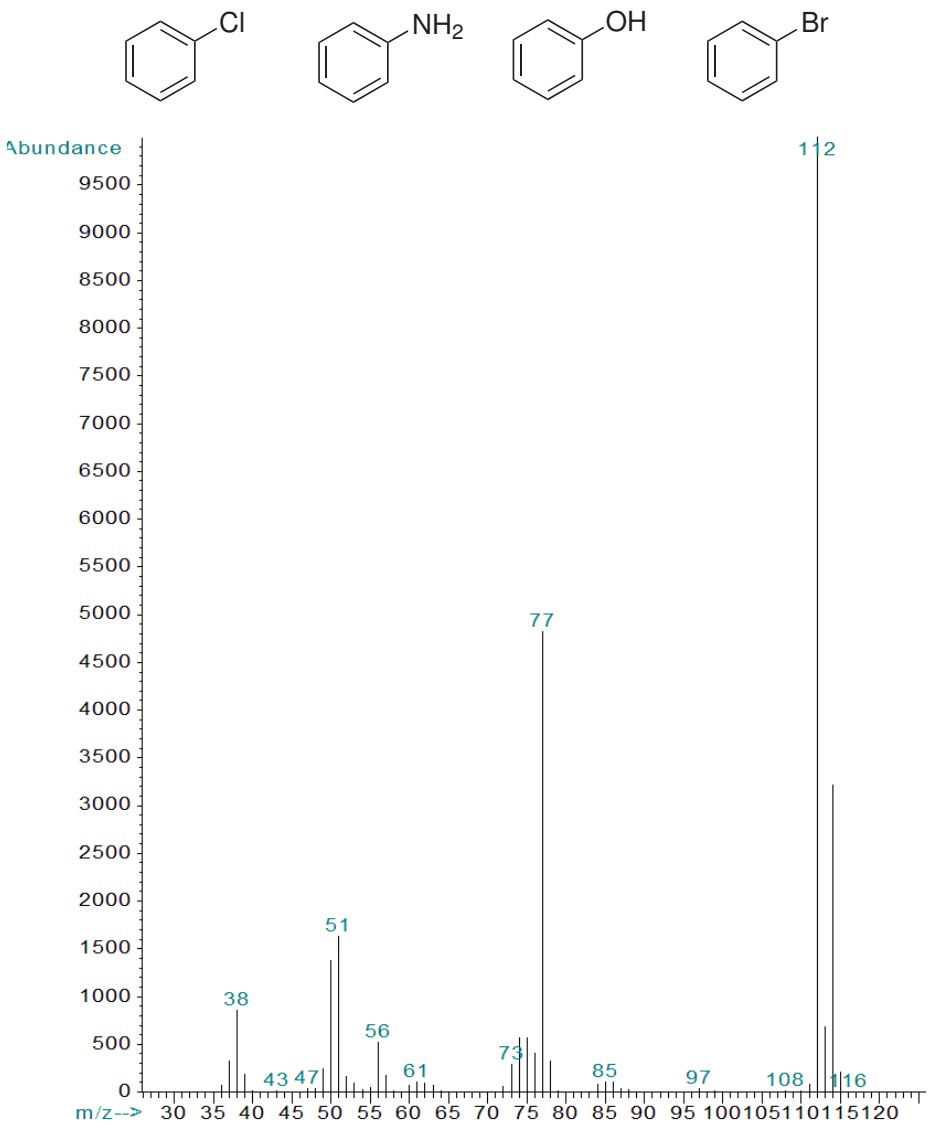

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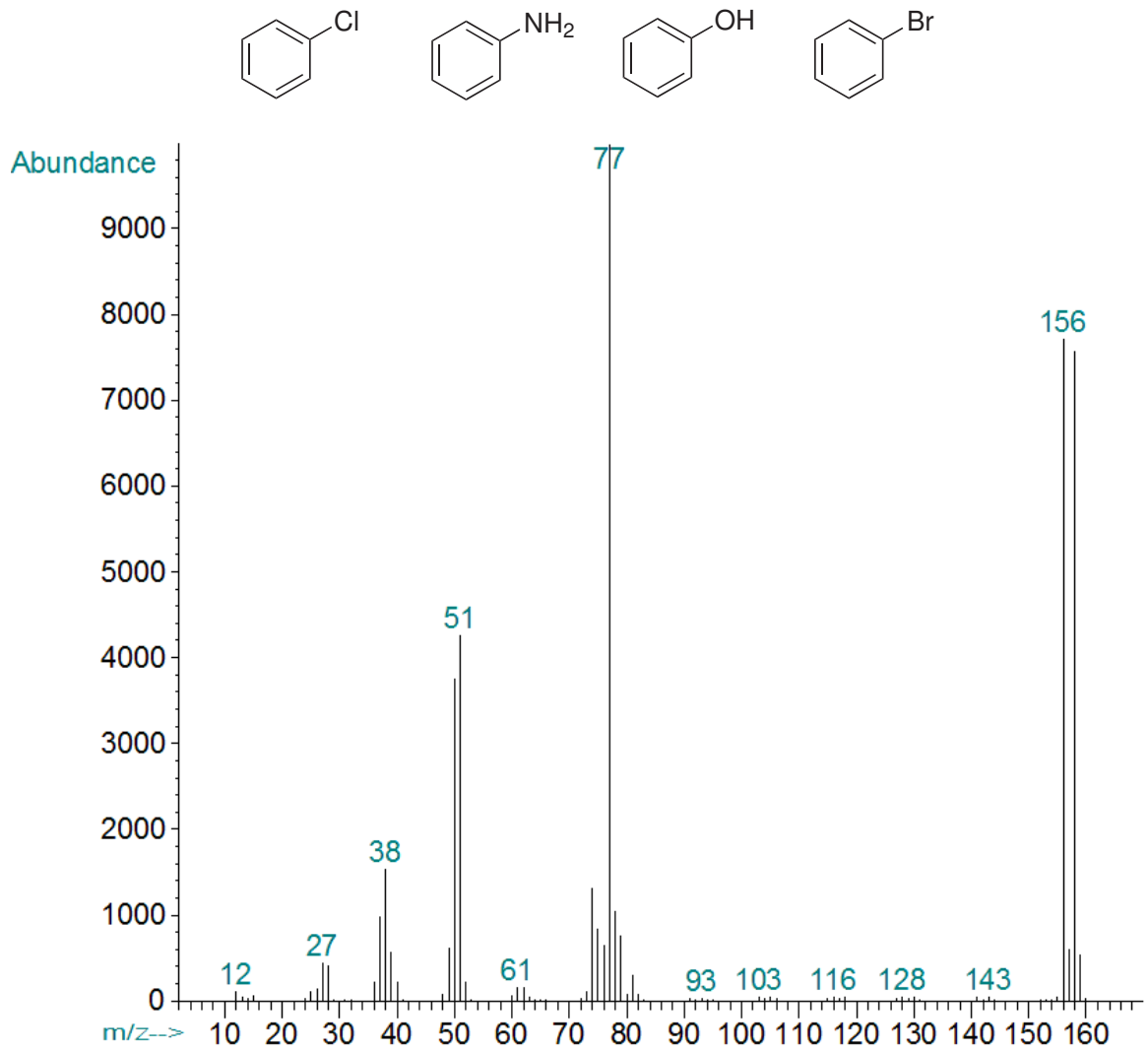
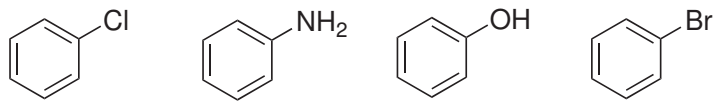
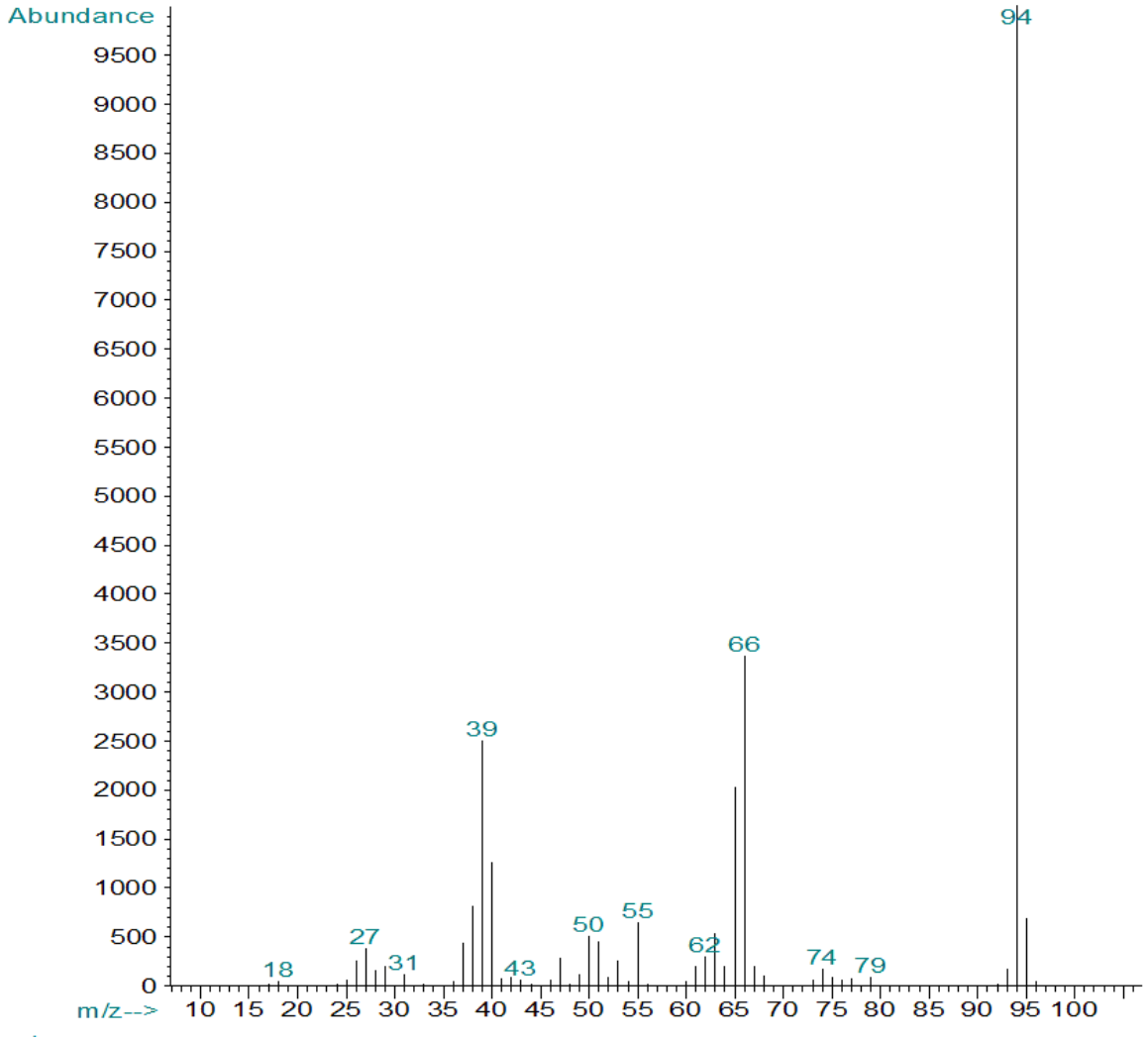
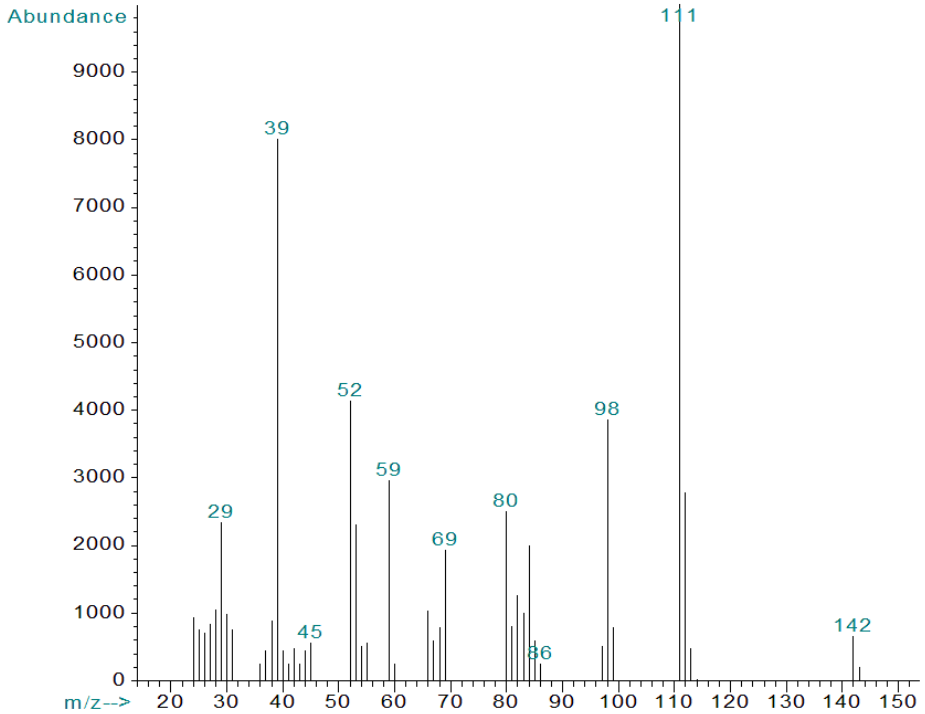


Hmotnostní spektroskopie





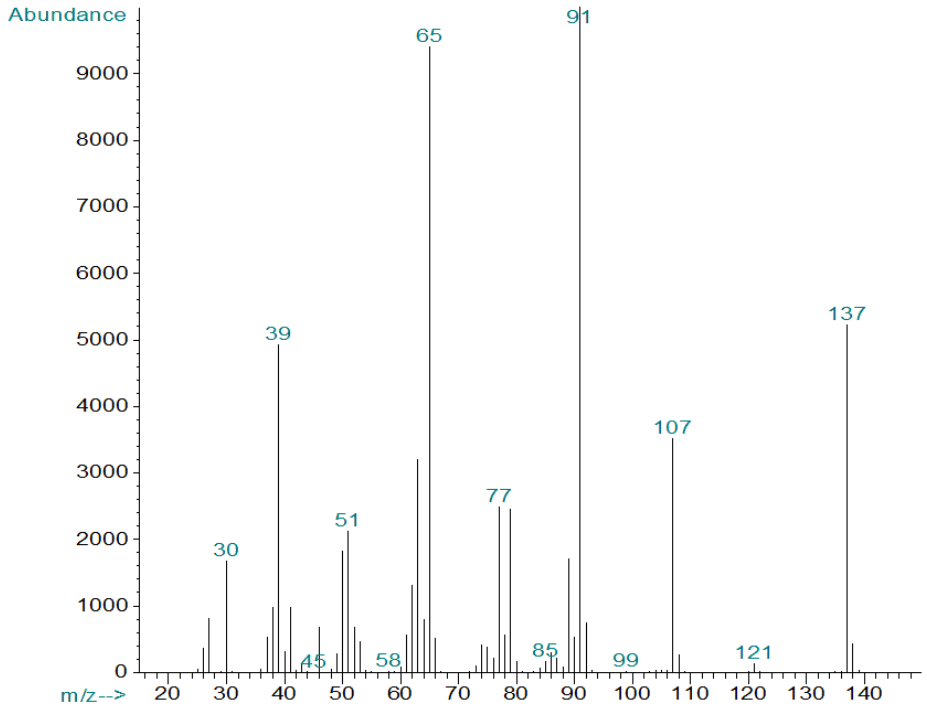
Určení molekulové hmotnosti



Intenzita iontů v oblasti molekulového iontu

m/z	Intenzita
142	100,0 %
143	7,0 %
144	1,0 %

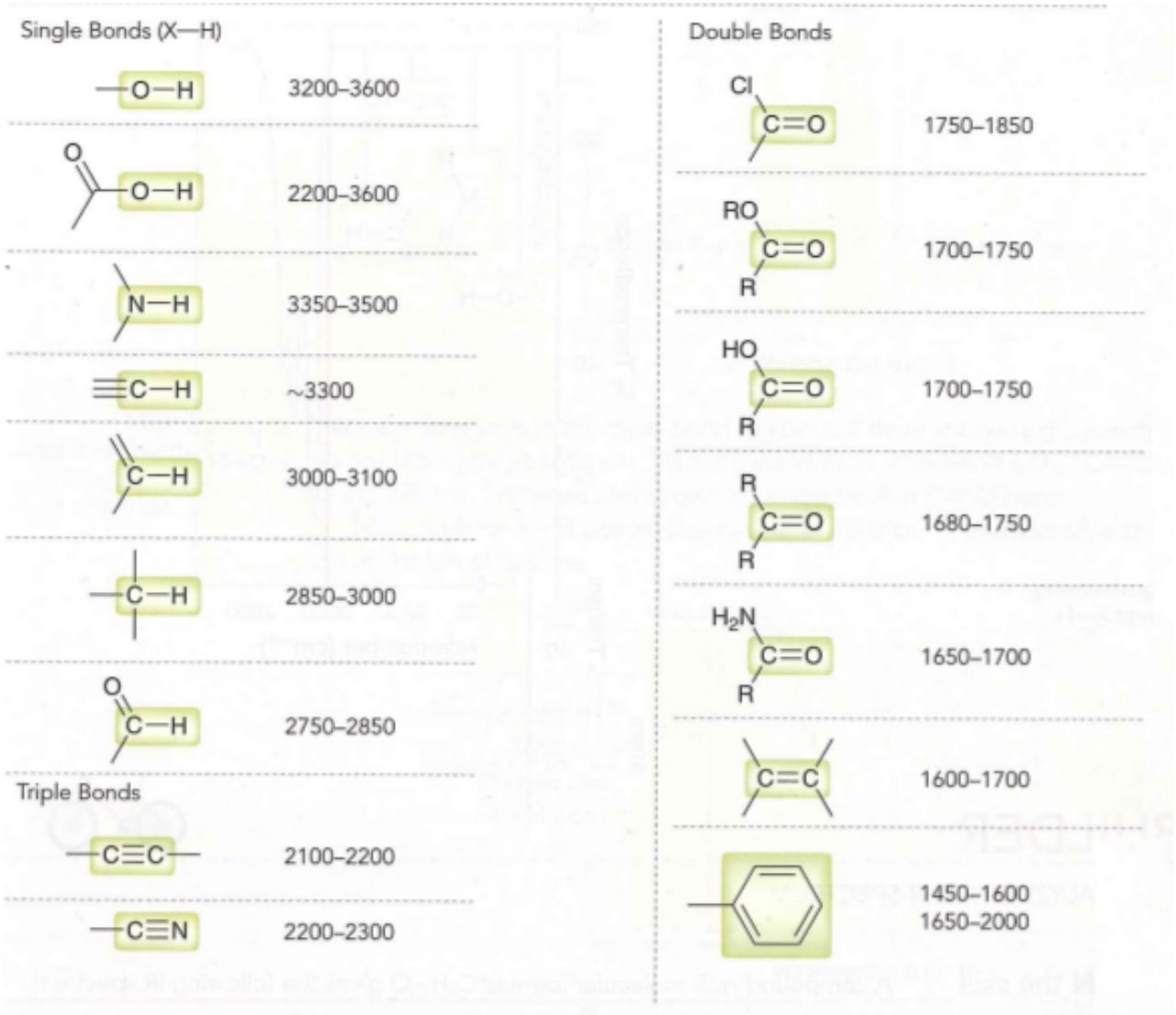
Určení molekulové hmotnosti



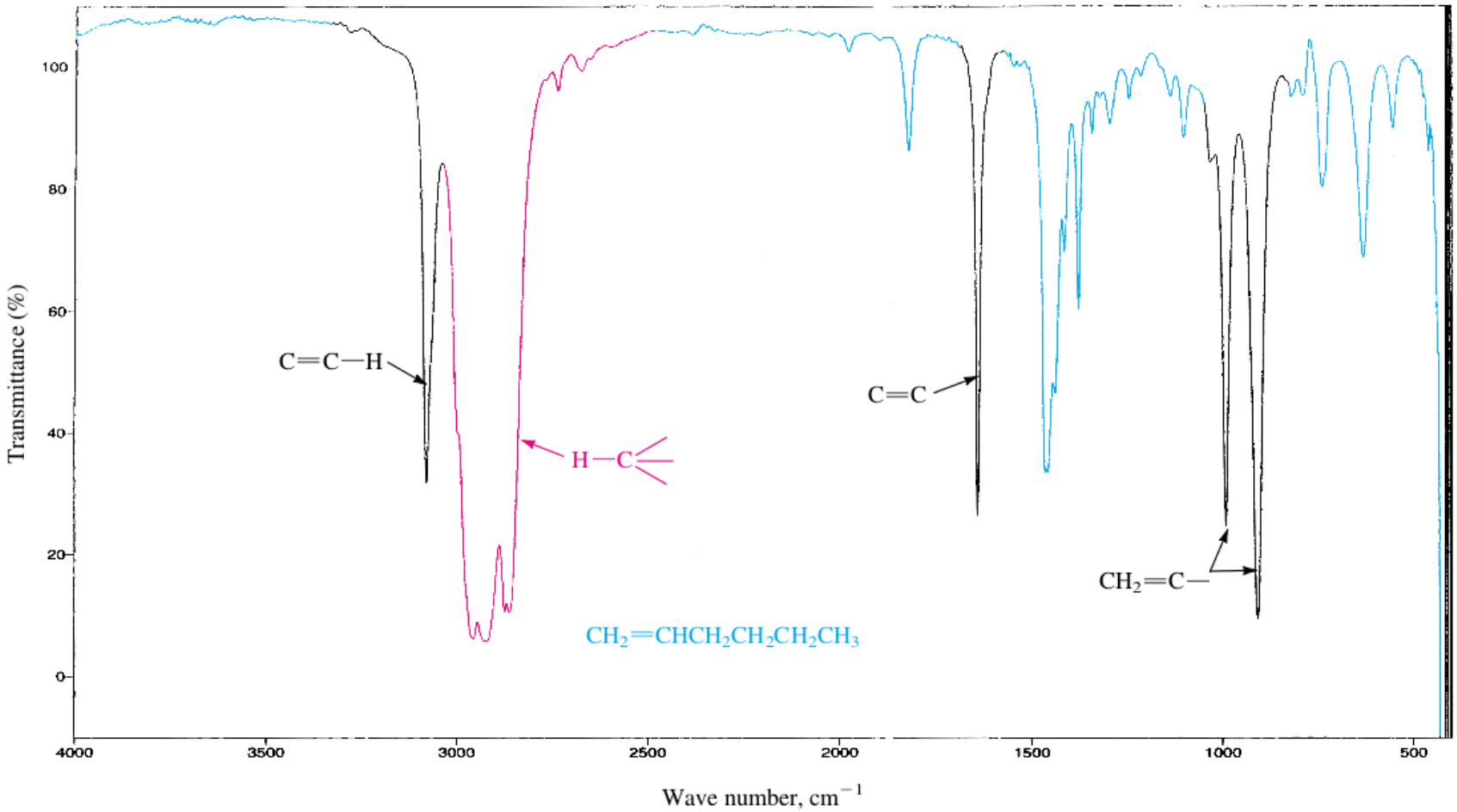
Intenzita iontů v oblasti molekulového iontu

m/z	Intenzita
137	100,0 %
138	8,4 %
139	0,7 %

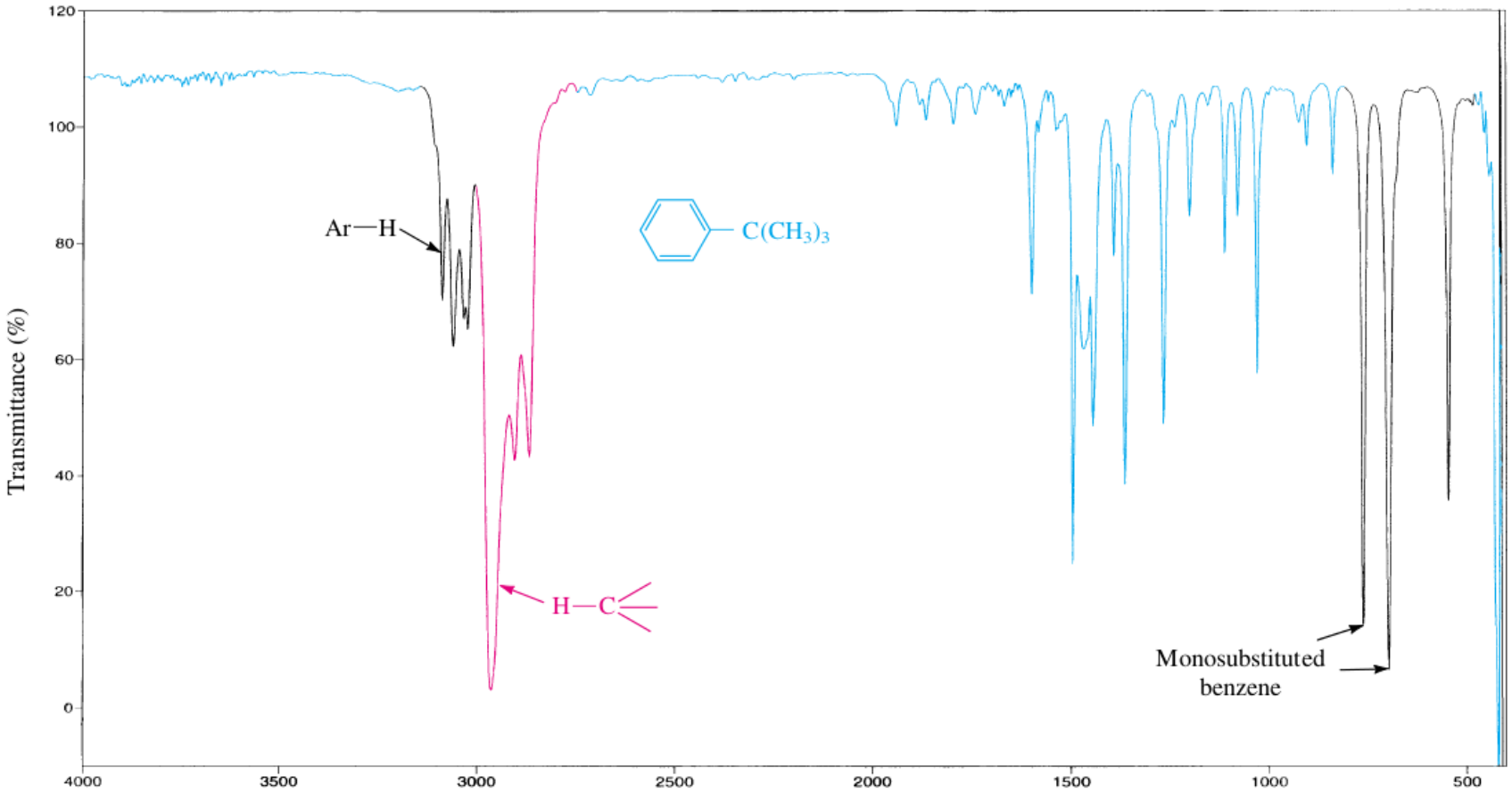
Infračervená spektroskopie



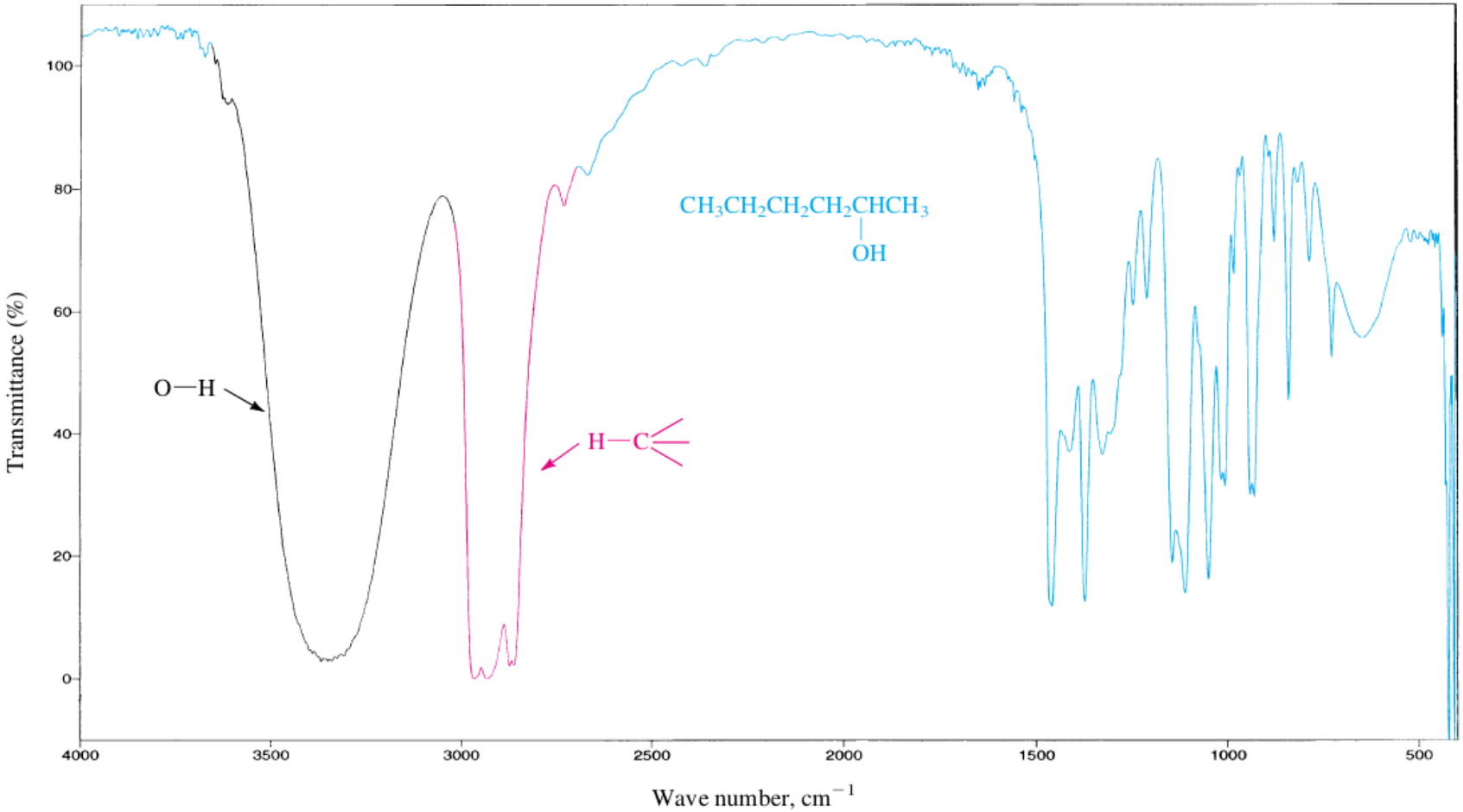
Infračervená spektroskopie



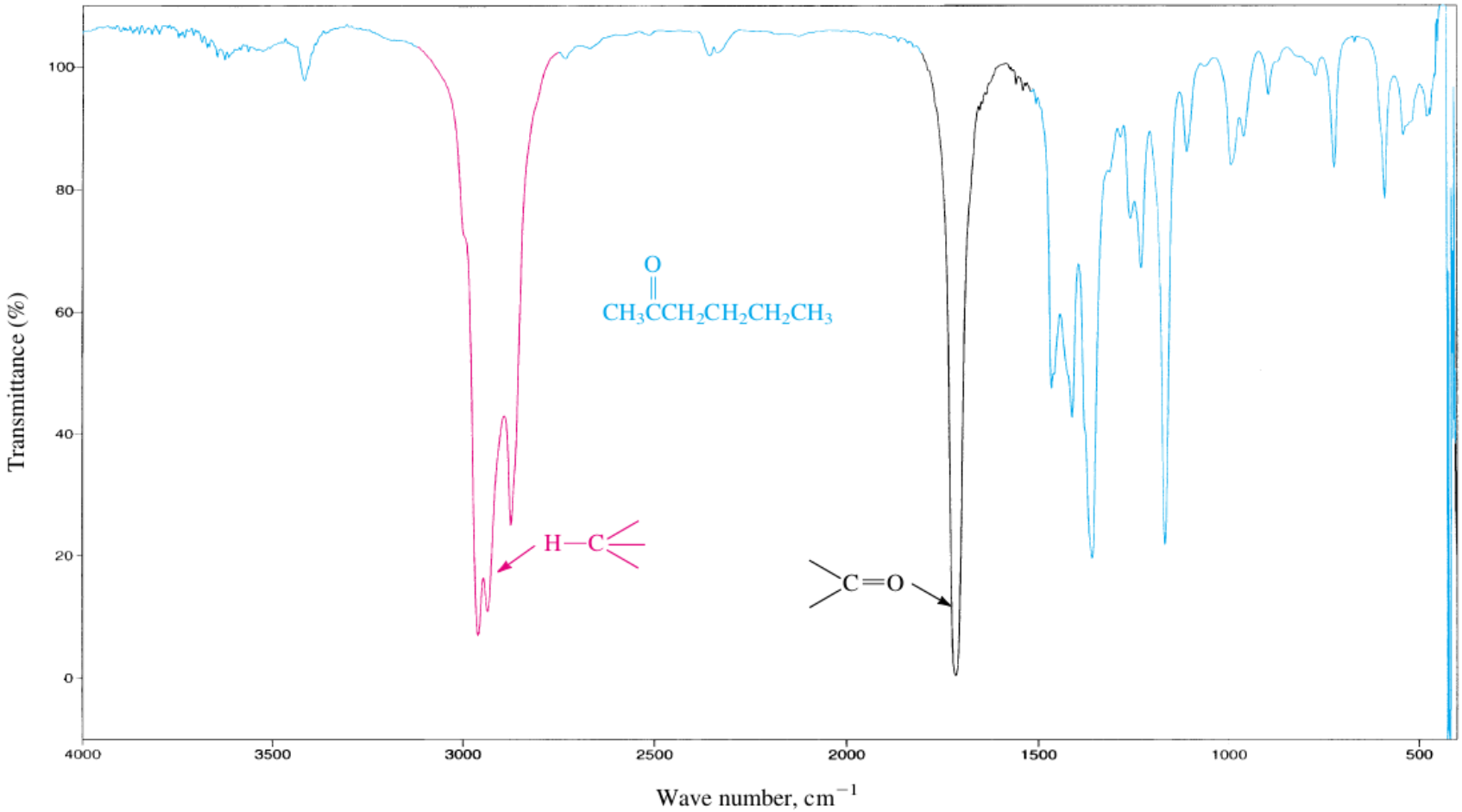
Infračervená spektroskopie



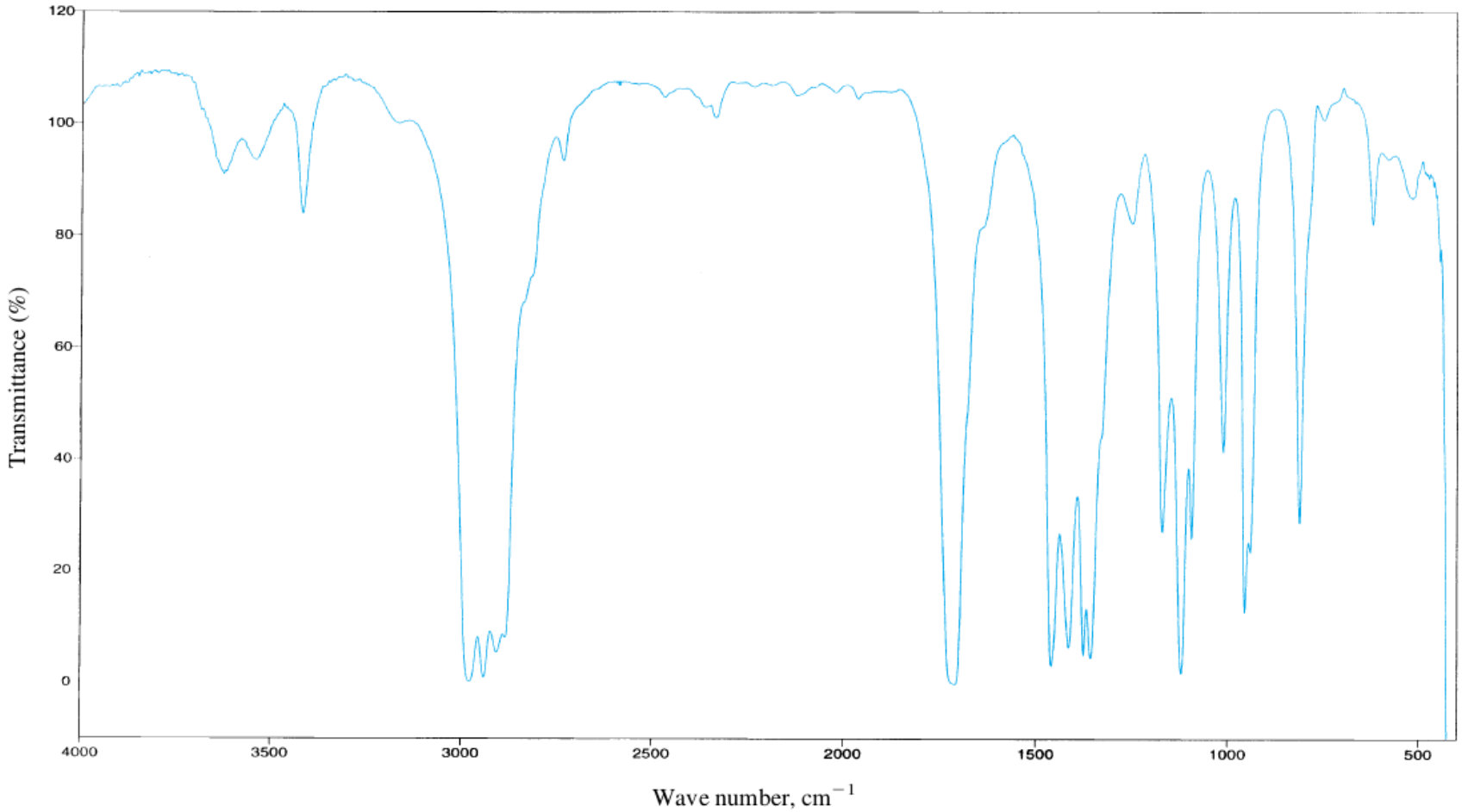
Infračervená spektroskopie



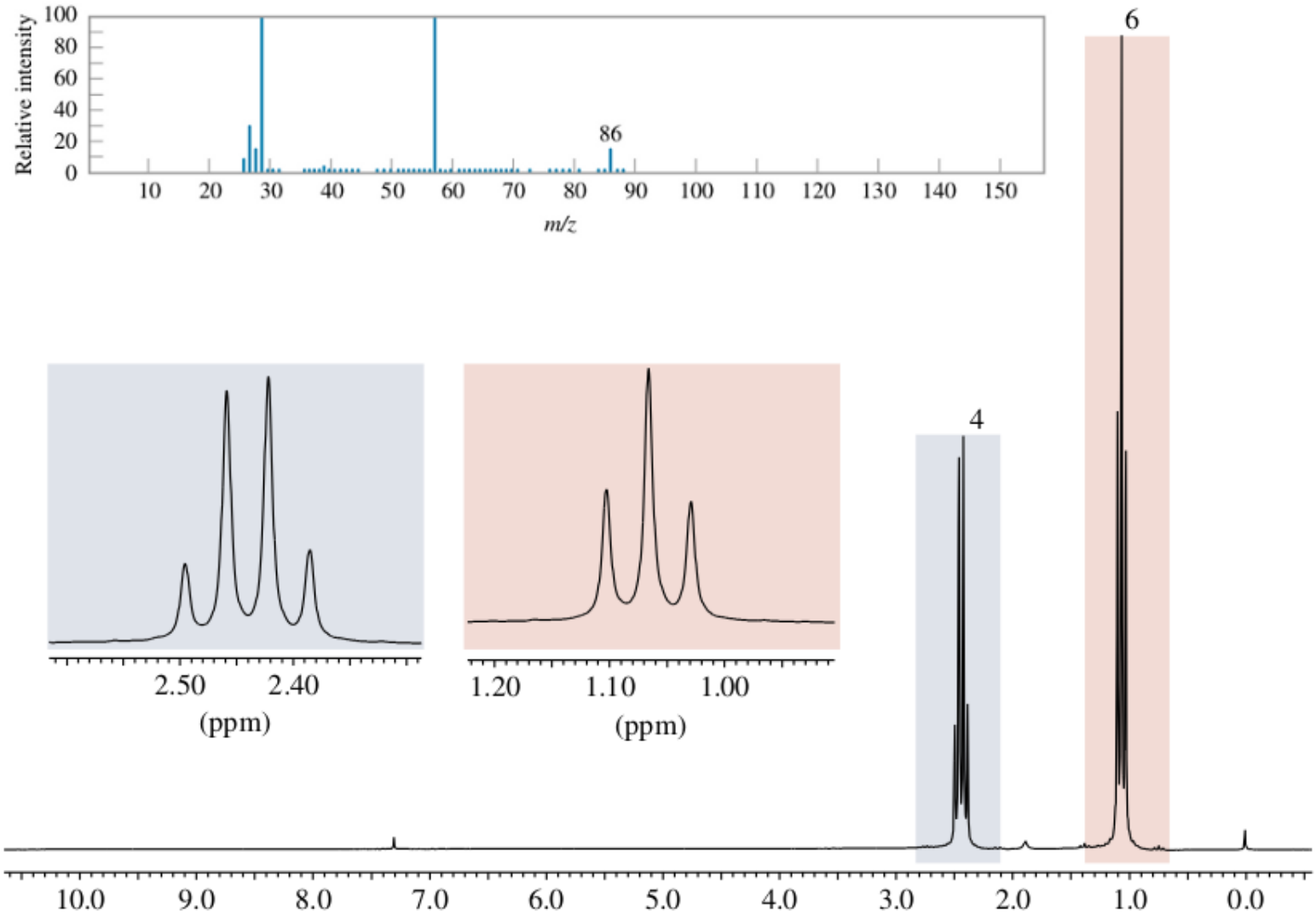
Infračervená spektroskopie



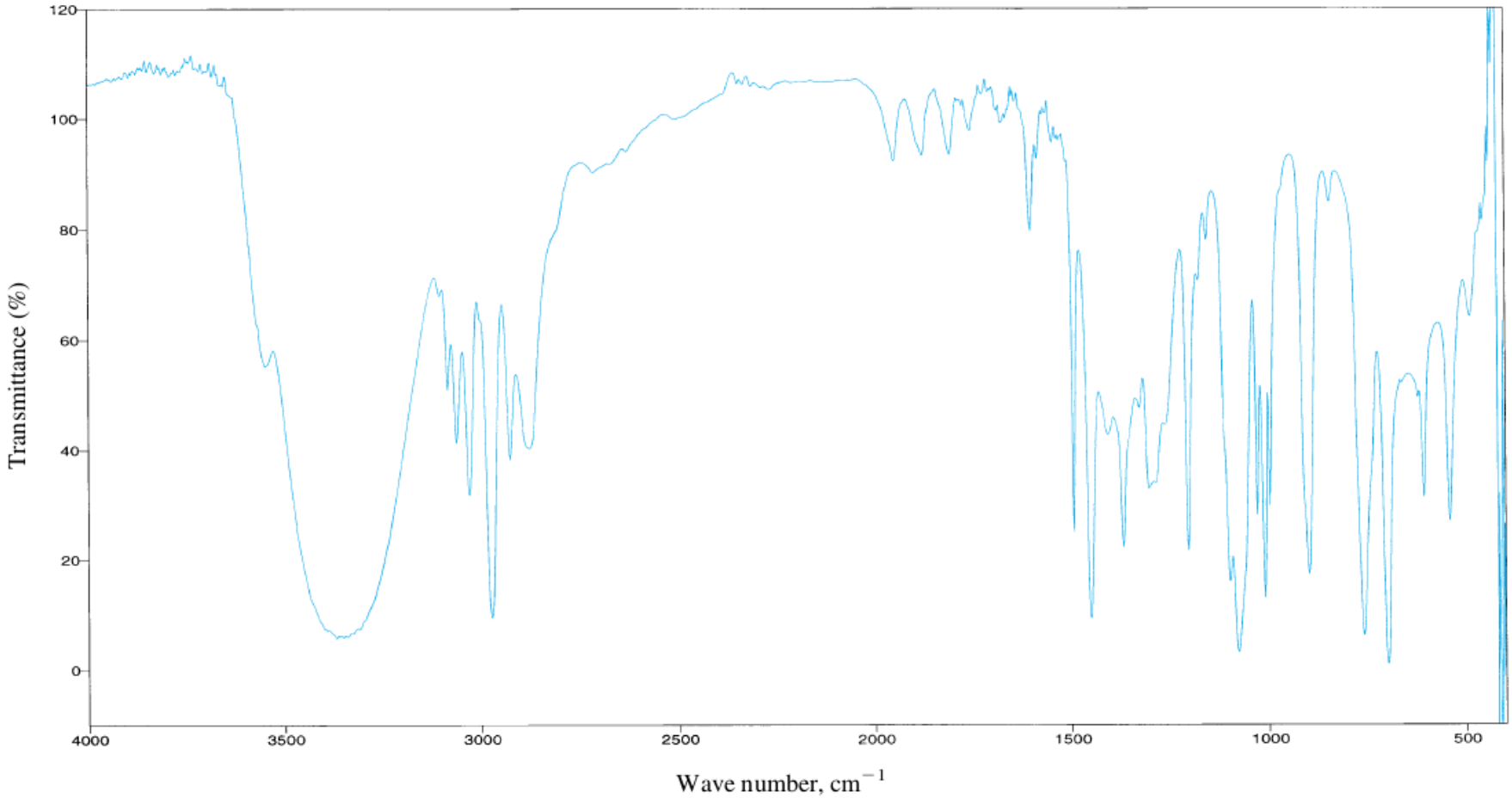
Příklad č. 1


120
100
80
60
40
20
0
Transmittance (%)
4000
3500
3000
2500
2000
1500
1000
500
Wave number, cm⁻¹

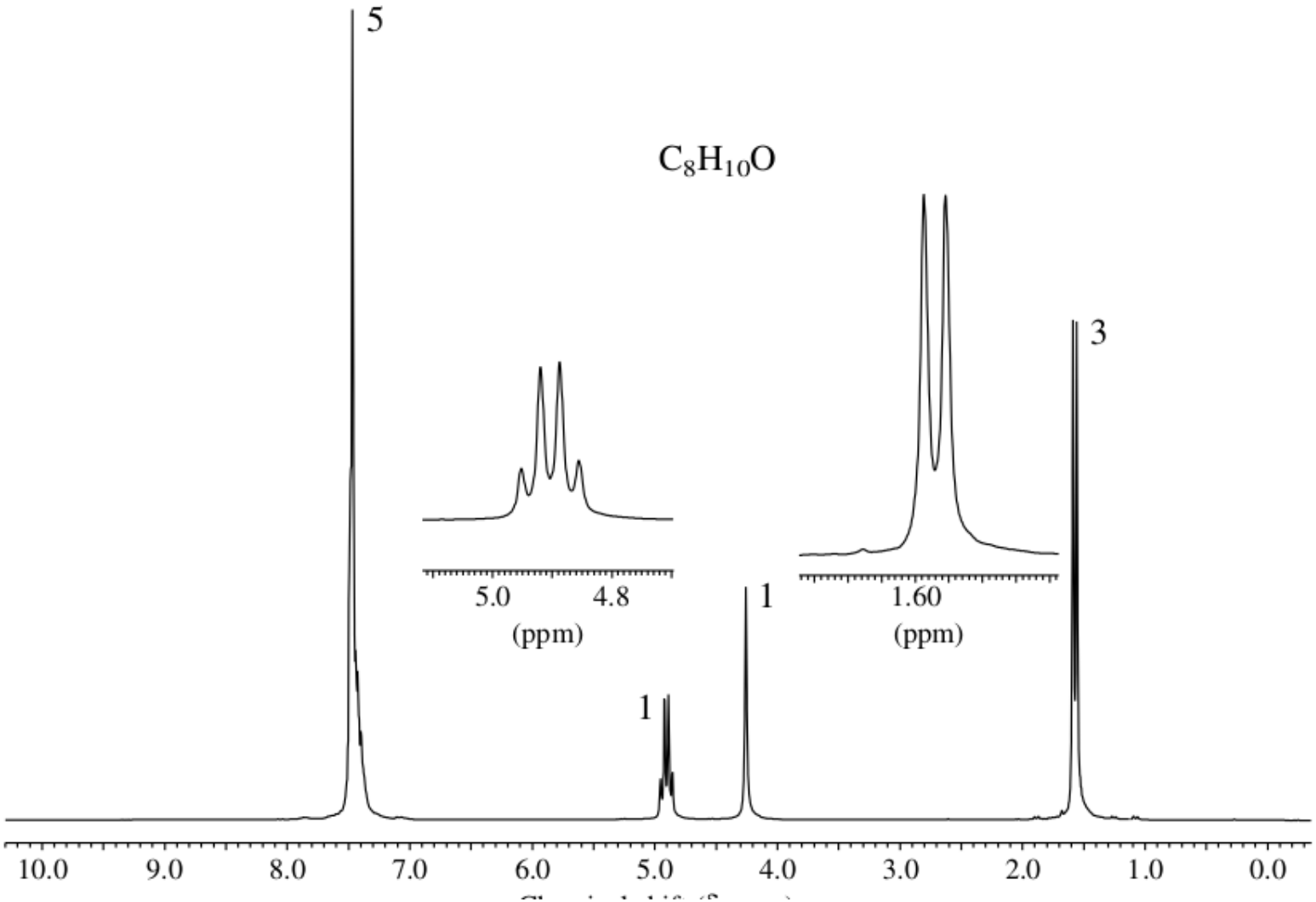
Příklad č. 1


Relative intensity
100
80
60
40
20
0
10 20 30 40 50 60 70 80 90 100 110 120 130 140 150
m/z
86
6
4
2.50 2.40
(ppm)
1.20 1.10 1.00
(ppm)
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0

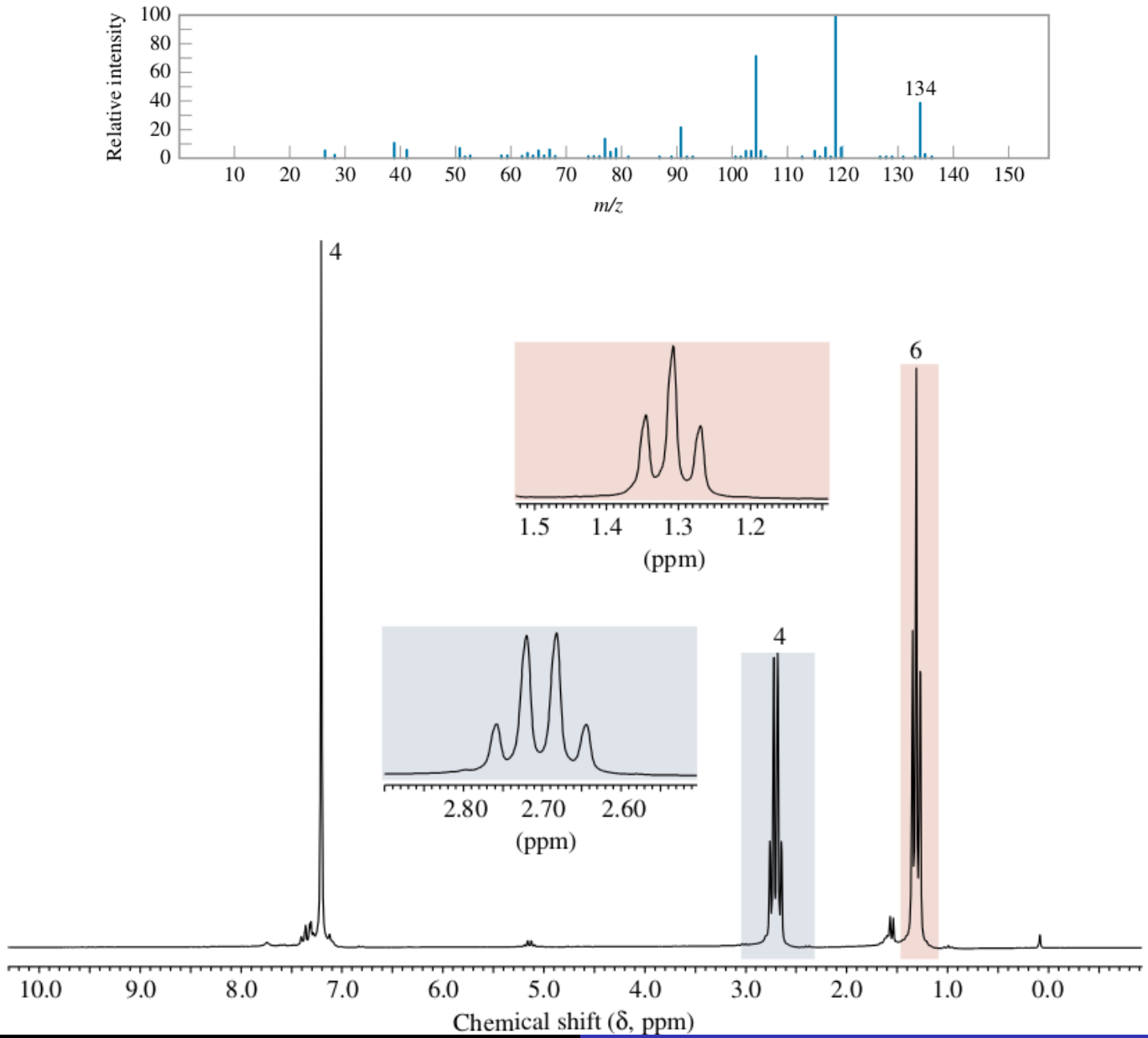
Příklad č. 2


120
100
80
60
40
20
0
Transmittance (%)
4000
3500
3000
2500
2000
1500
1000
500
Wave number, cm^{-1}

Příklad č. 2



Příklad č. 3


Relative intensity
100
80
60
40
20
0
10 20 30 40 50 60 70 80 90 100 110 120 130 140 150
m/z
134
4
6
1.5 1.4 1.3 1.2
(ppm)
4
2.80 2.70 2.60
(ppm)
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
Chemical shift (δ, ppm)