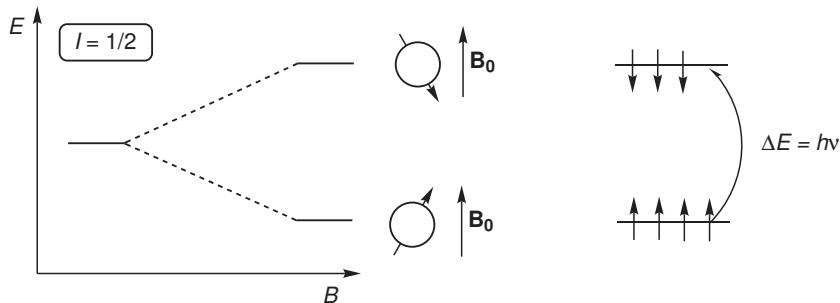


Nukleární magnetická rezonance

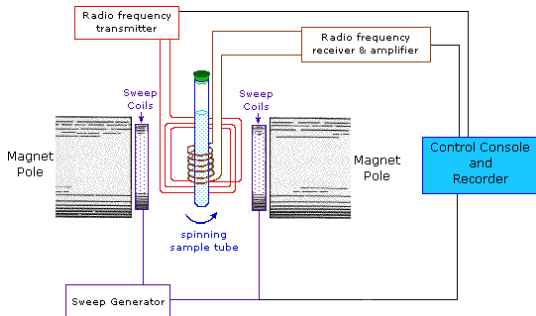


Jádra s **nenulovým jaderným spinem**, prakticky nejčastěji s $I = 1/2$.

Například:

^1H (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:

$$\nu = \frac{-\gamma B}{2\pi} = \frac{-\gamma(1-\sigma)B_0}{2\pi}$$

Chemický posun:

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

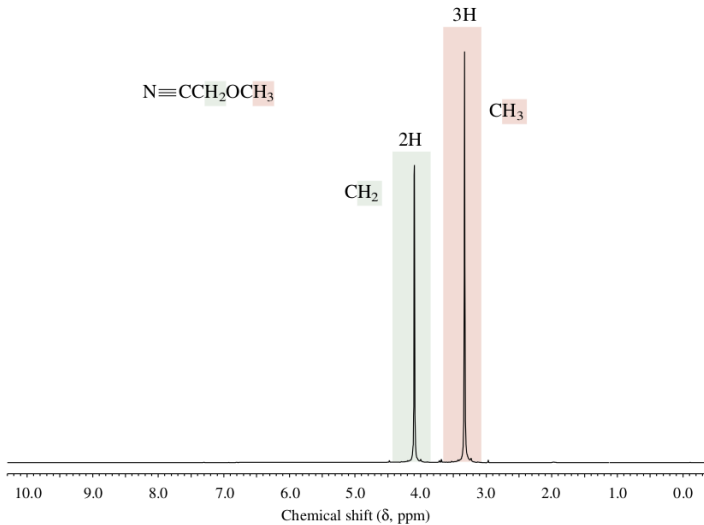
Nukleární magnetická rezonance



Nukleární magnetická rezonance

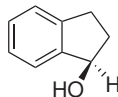
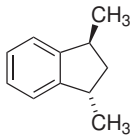
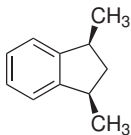
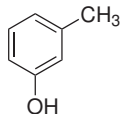
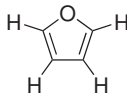
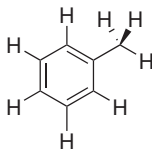
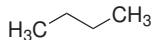
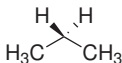
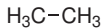


Nukleární magnetická rezonance

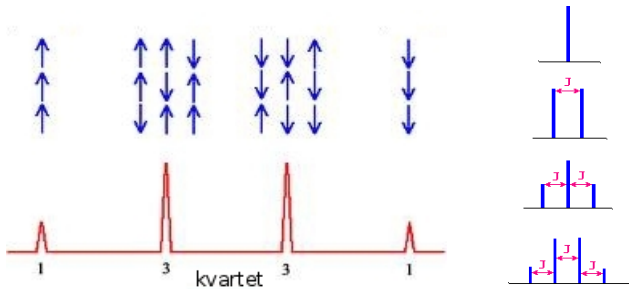
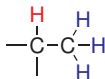


Nukleární magnetická rezonance

Počet chemicky neekvivalentních atomů vodíku?



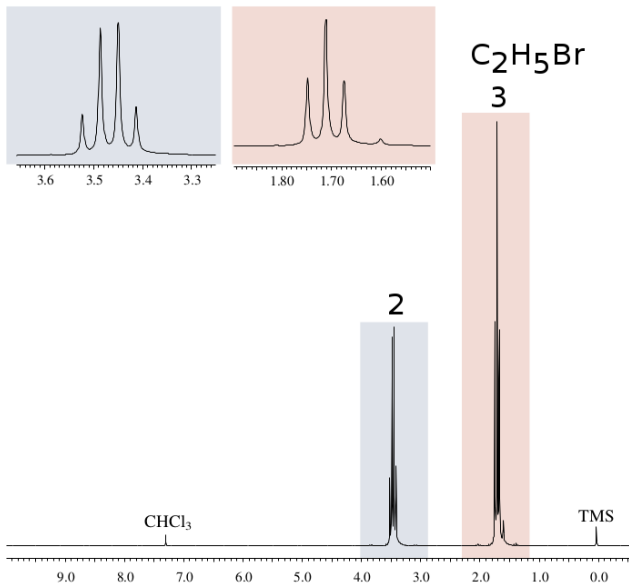
NMR – spin-spinová skalární interakce



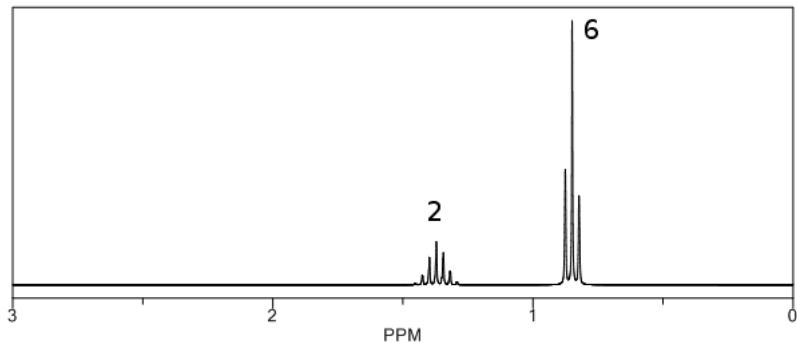
Polarizace **přenášena vazbami**. Obvykle pozorujeme přes **1 až 3 vazby**.
Počet linií:

$$N = 2nI + 1$$

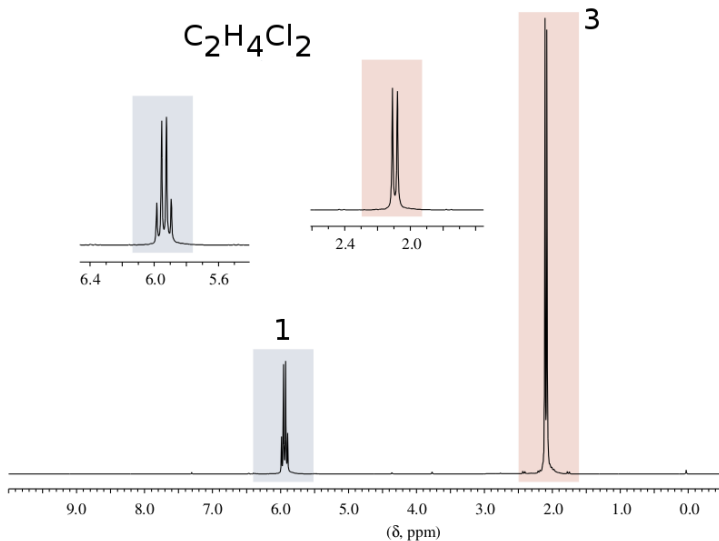
Nukleární magnetická rezonance



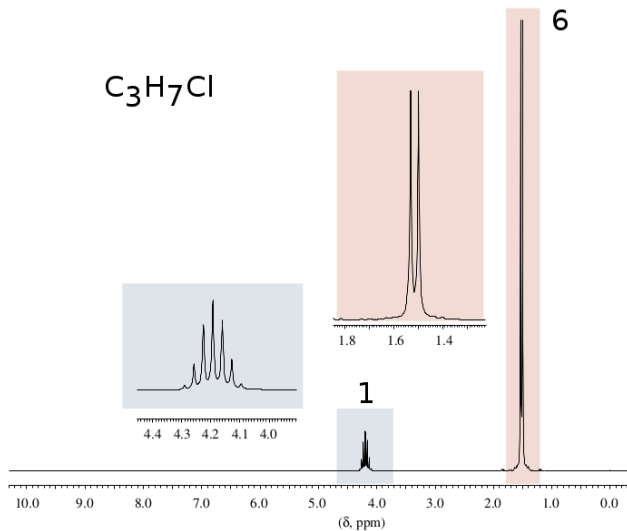
Nukleární magnetická rezonance



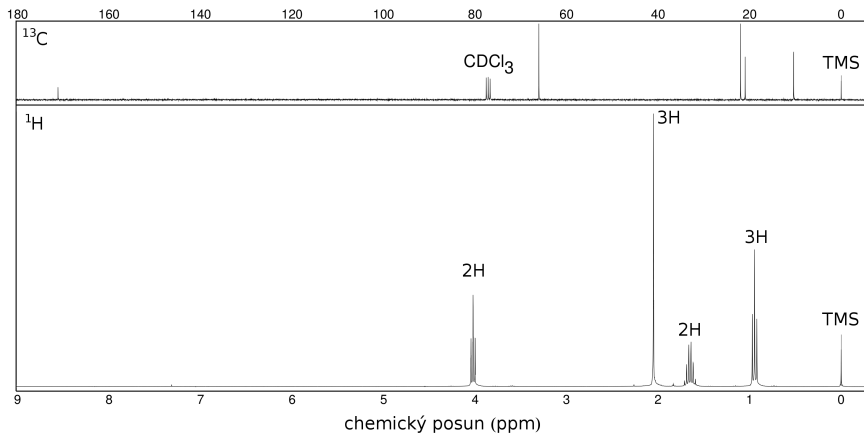
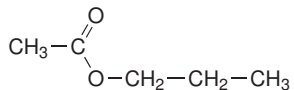
Nukleární magnetická rezonance



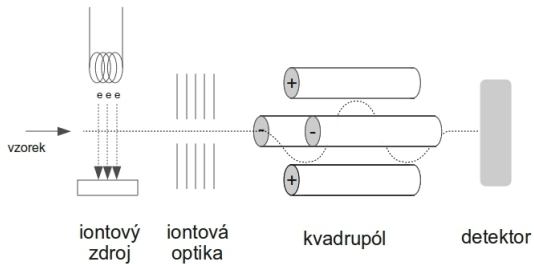
Nukleární magnetická rezonance



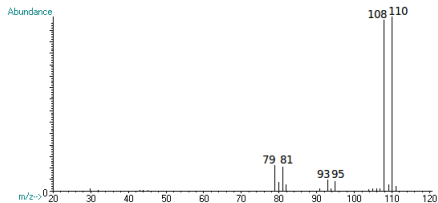
NMR – propyl-acetát



Hmotnostní spektroskopie



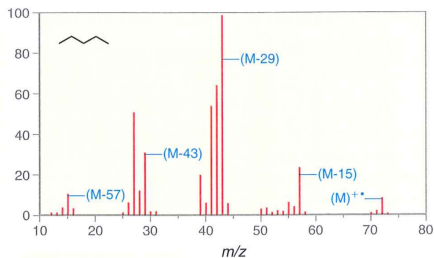
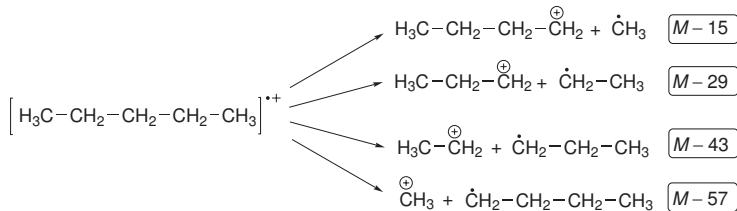
Bromethan:



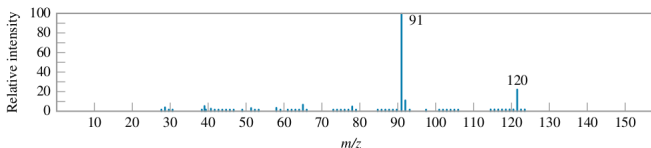
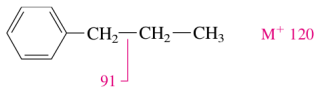
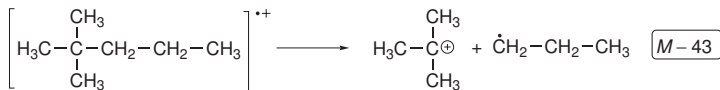
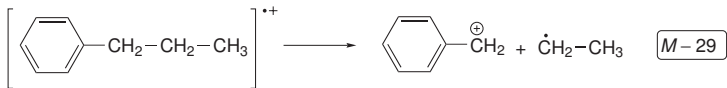
Typické fragmentační reakce po EI

Alkany

Pentan:



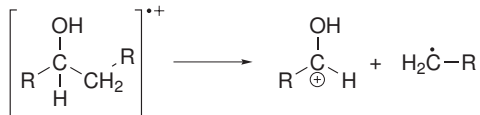
Typické fragmentační reakce po EI



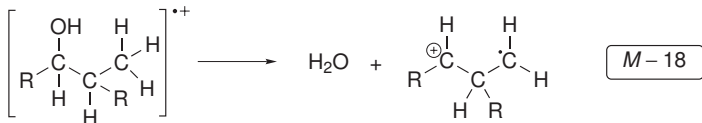
Typické fragmentační reakce po EI

Alkoholy

α -Štěpení:



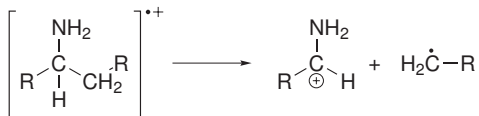
Eliminace vody:



Typické fragmentační reakce po EI

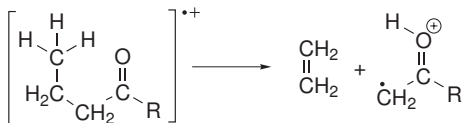
Aminy

α -Štěpení:



Ketony s atomem vodíku v γ -pozici

McLaffertyho přesmyk:

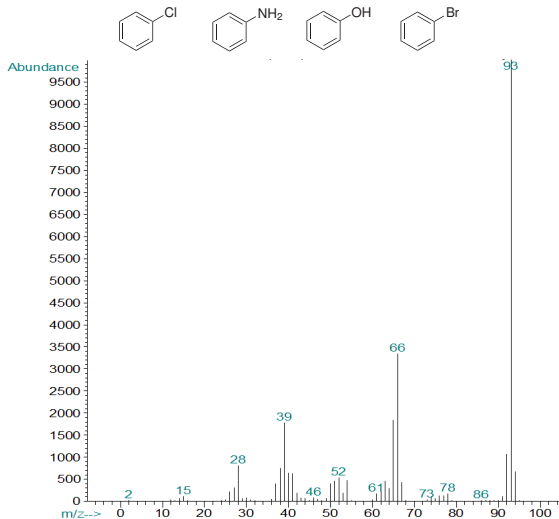


Zastoupení isotopů

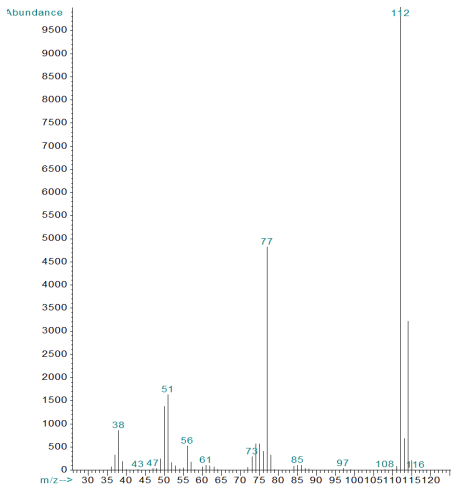
Prvek	Isotop	Relativní zastoupení	Isotop	Relativní zastoupení	Isotop	Relativní zastoupení
Uhlík	^{12}C	100	^{13}C	1,11		
Vodík	^1H	100	^2H	0,016		
Dusík	^{14}N	100	^{15}N	0,38		
Kyslík	^{16}O	100	^{17}O	0,04	^{18}O	0,2
Fluor	^{19}F	100				
Křemík	^{28}Si	100	^{29}Si	5,1	^{30}Si	3,35
Fosfor	^{31}P	100				
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

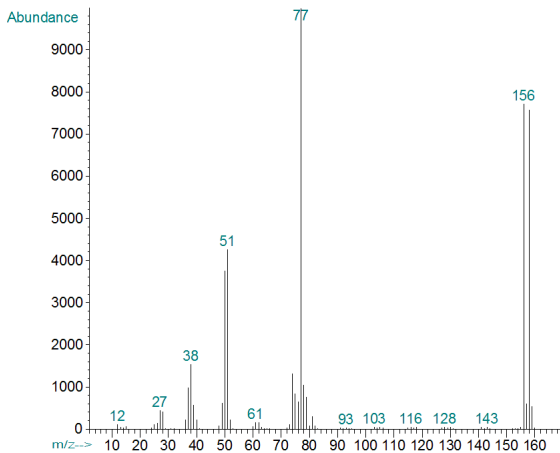
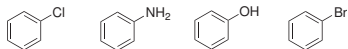
Hmotnostní spektroskopie



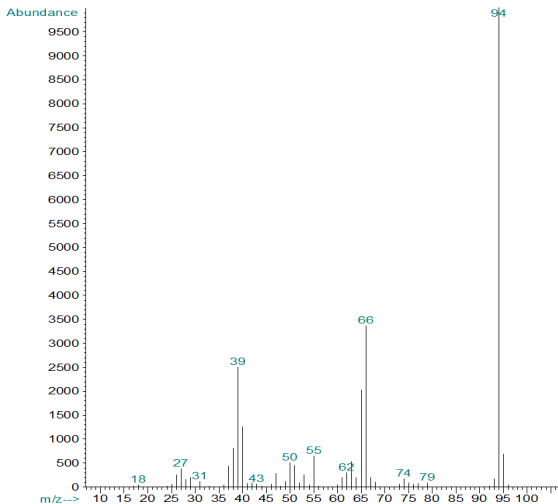
Hmotnostní spektroskopie



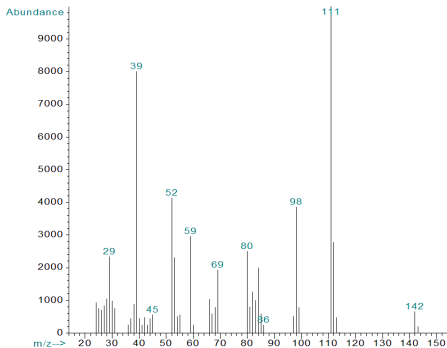
Hmotnostní spektroskopie



Hmotnostní spektroskopie



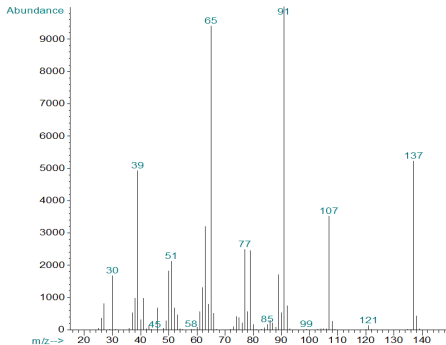
Určení molekulové hmotnosti



Intenzita iontů v oblasti molekulového iontu

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

















Určení molekulové hmotnosti



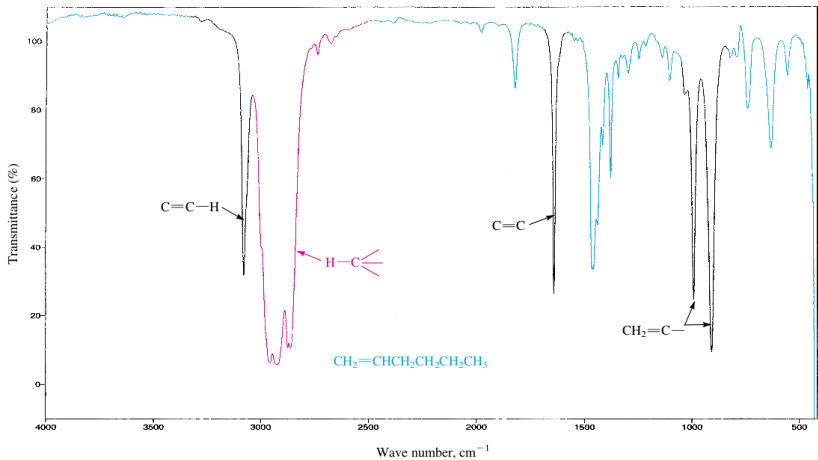
Intenzita iontů v oblasti molekulového iontu

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

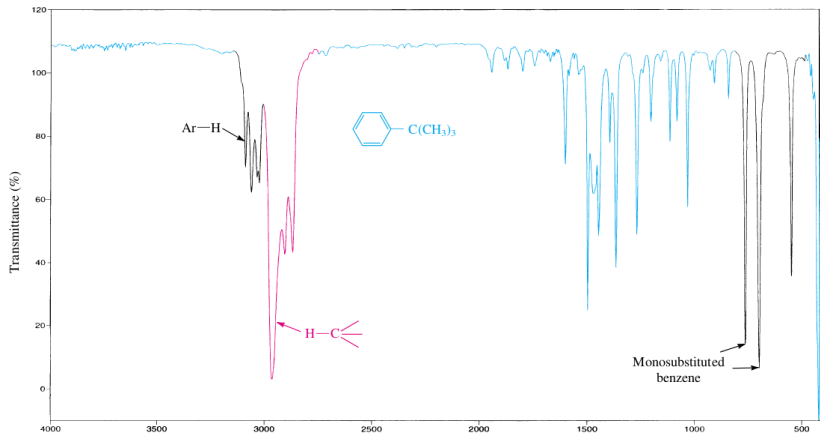
Infračervená spektroskopie

	3200-3600		1750-1850
	2200-3600		1700-1750
	3350-3500		1700-1750
	~3300		1680-1750
	3000-3100		1650-1700
	2850-3000		1600-1700
	2750-2850		1450-1600 1650-2000
	2100-2200		
	2200-2300		

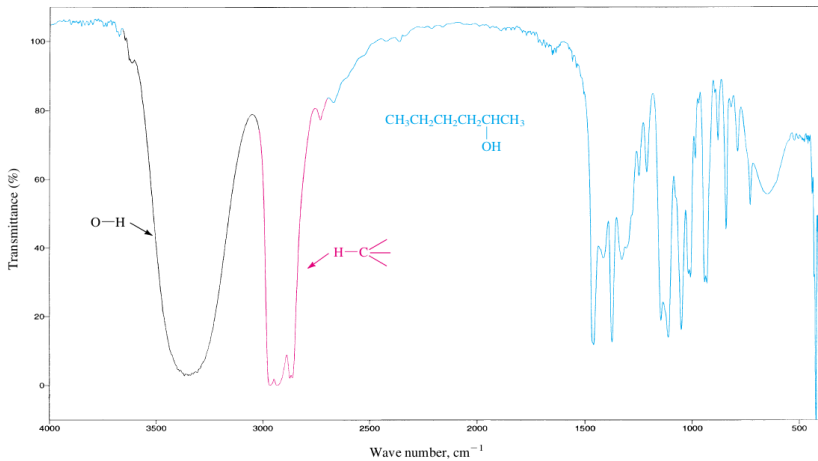
Infračervená spektroskopie



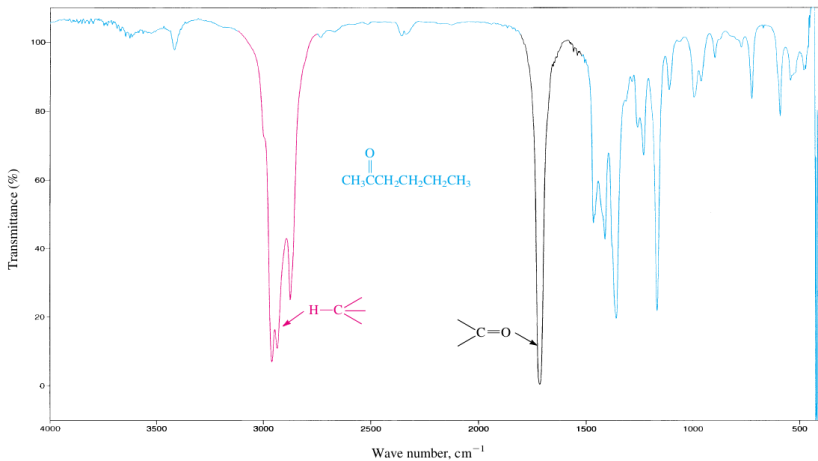
Infračervená spektroskopie



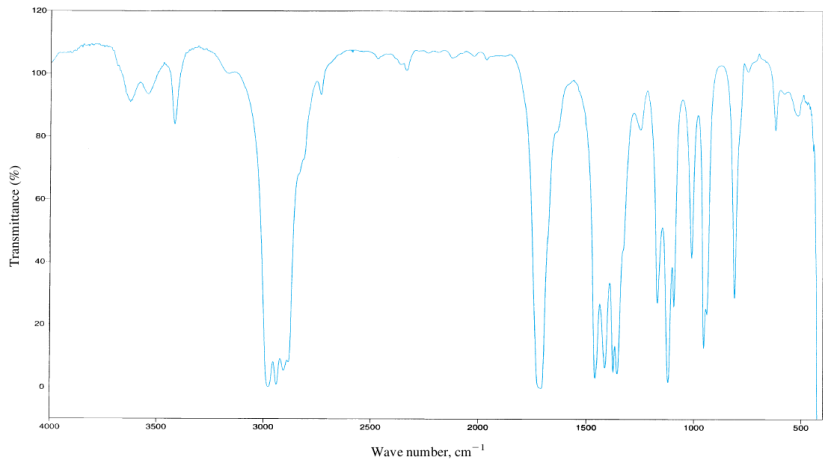
Infračervená spektroskopie



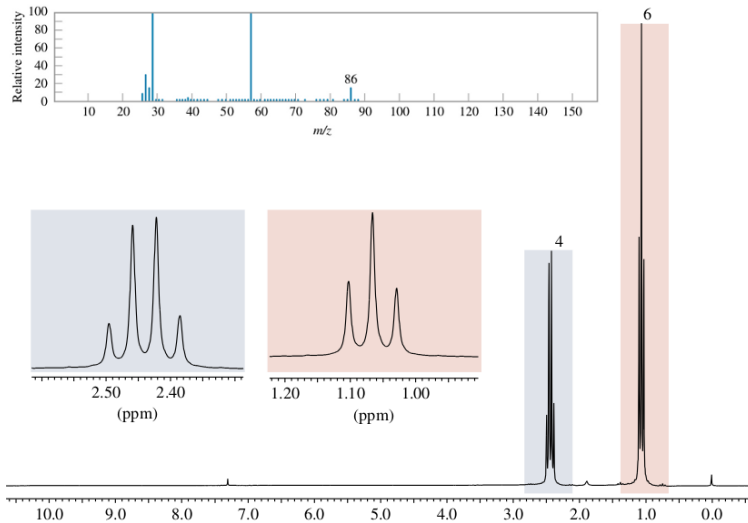
Infračervená spektroskopie



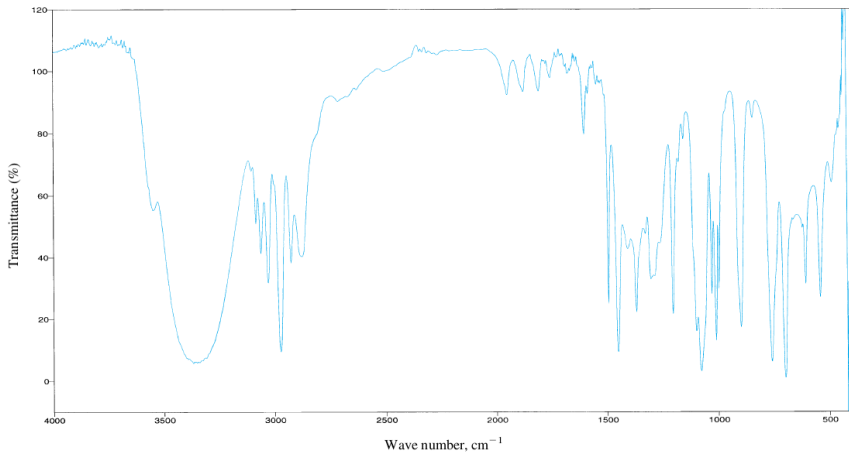
Příklad č. 1



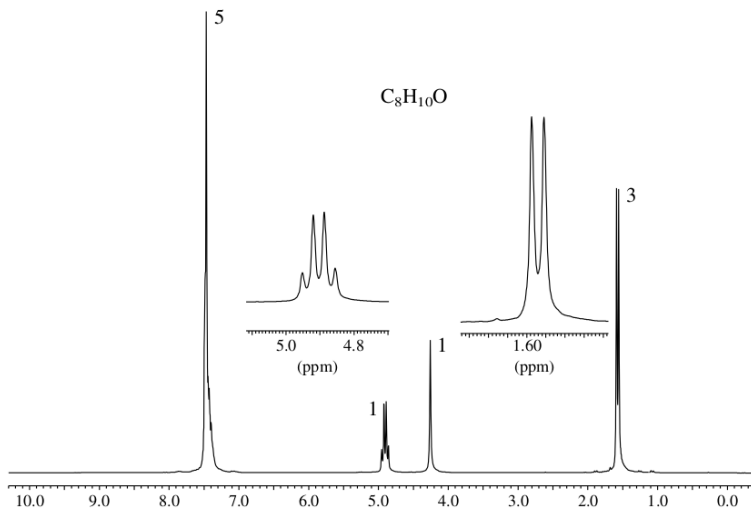
Příklad č. 1



Příklad č. 2



Příklad č. 2



Příklad č. 3

