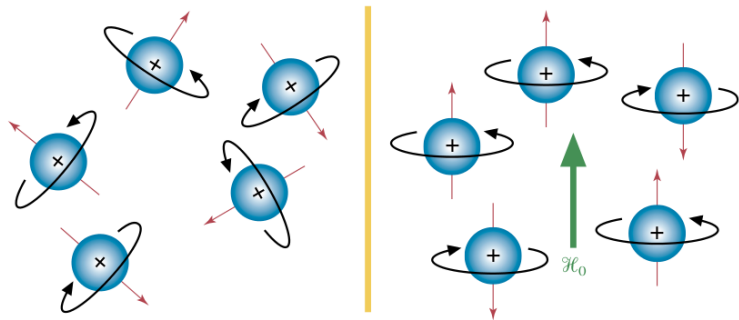


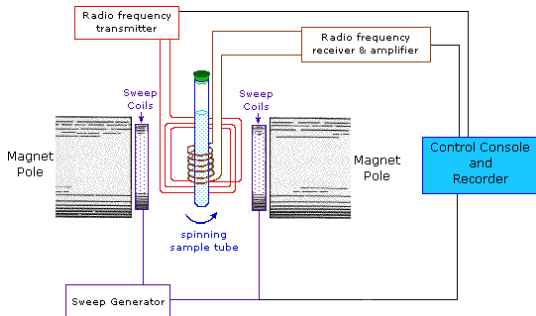
Nukleární magnetická rezonance



Jádra s $I = 1/2$, např.:

^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:

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

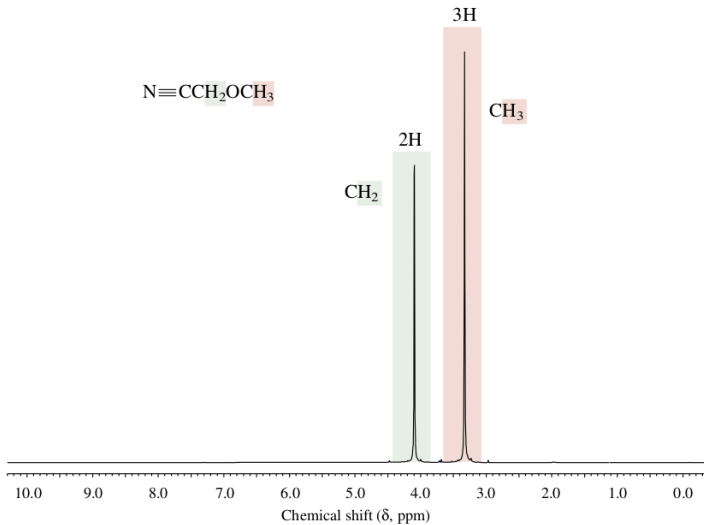
Chemický posun:

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

Nukleární magnetická rezonance

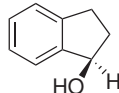
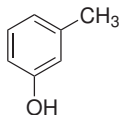
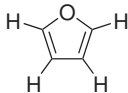
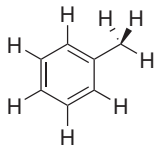
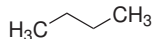
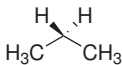
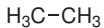


Nukleární magnetická rezonance

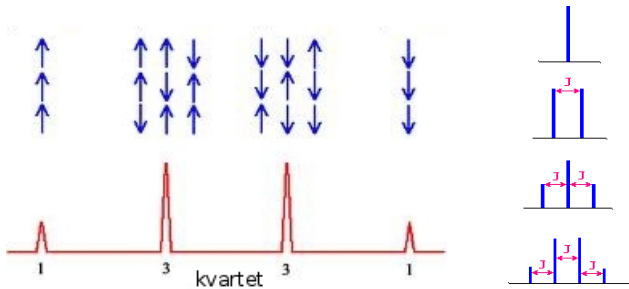
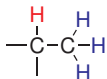


Nukleární magnetická rezonance

Počet chemicky neekvivalentních atomů vodíku?



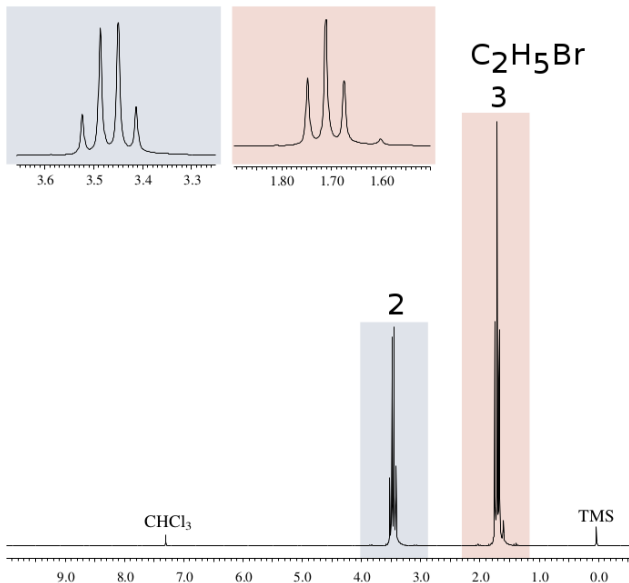
NMR – spin-spinová skalární interakce



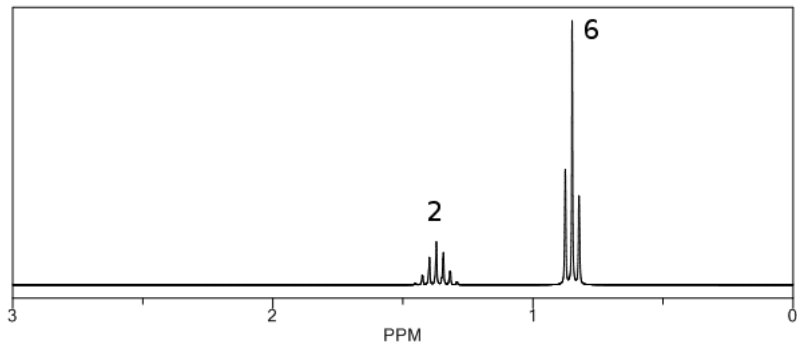
Polarizace **přenášena vazbami**. Obvykle pozorujeme přes **1 až 3 vazby**.
Počet linií:

$$N = 2nI + 1$$

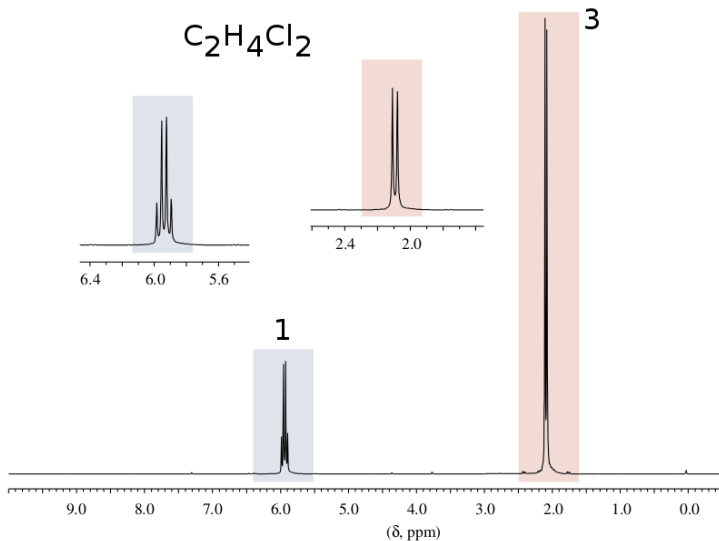
Nukleární magnetická rezonance



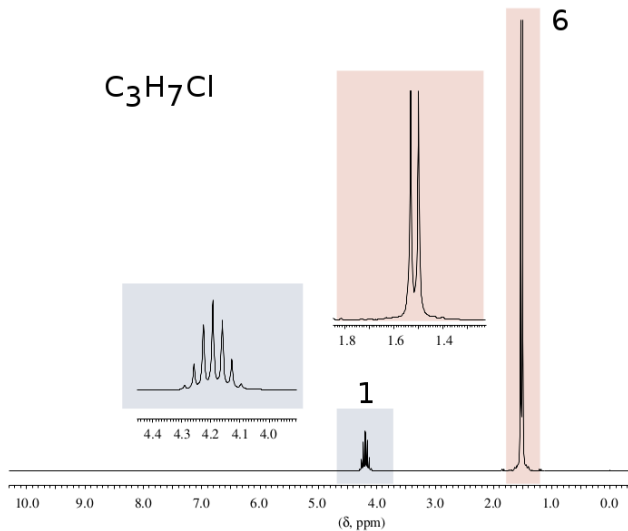
Nukleární magnetická rezonance



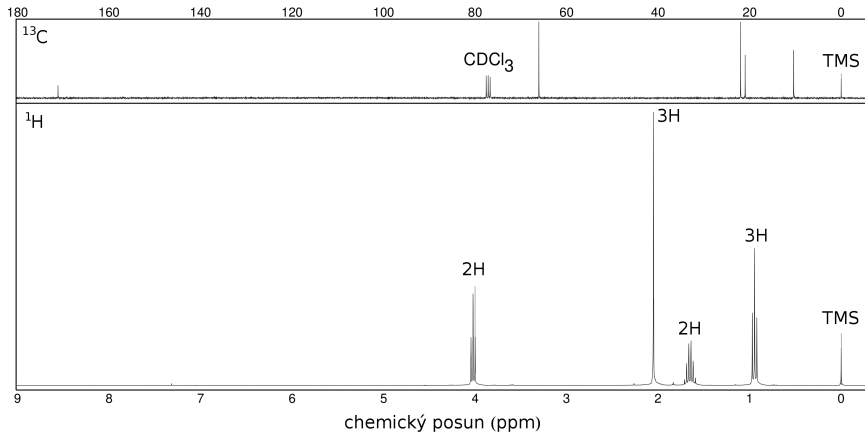
Nukleární magnetická rezonance



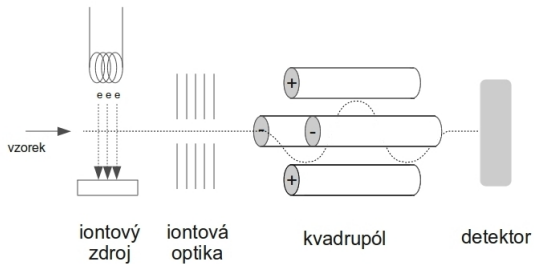
Nukleární magnetická rezonance



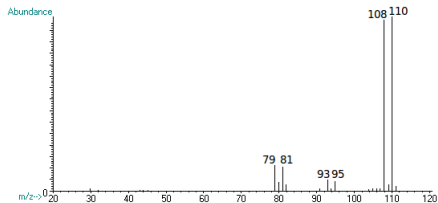
^{13}C NMR – propyl-acetát



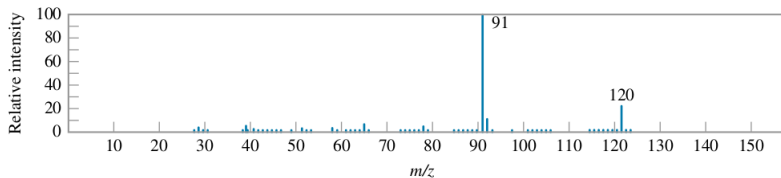
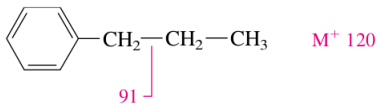
Hmotnostní spektroskopie



Bromethan:



Hmotnostní spektroskopie

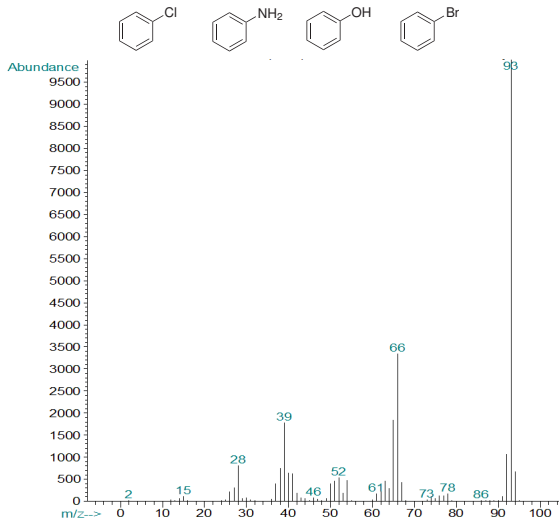


Zastoupení isotopů

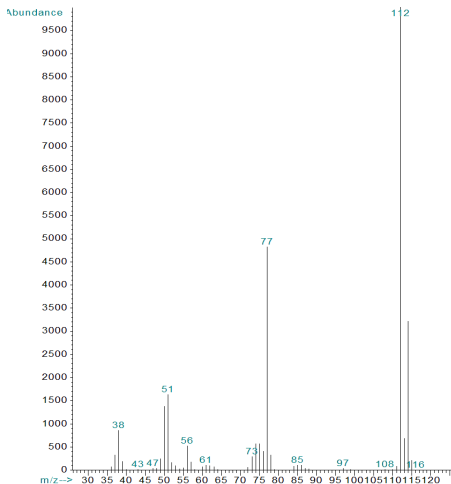
Prvek	Isotop	Relativní zastoupení	Isotop	Relativní zastoupení	Isotop	Relativní zastoupení
Uhlík	^{12}C	100	^{13}C	1,11		
Vodík	^1H	100	^2H	0,016		
Dusík	^{14}N	100	^{15}N	0,38		
Kyslík	^{16}O	100	^{17}O	0,04	^{18}O	0,2
Fluor	^{19}F	100				
Křemík	^{28}Si	100	^{29}Si	5,1	^{30}Si	3,35
Fosfor	^{31}P	100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

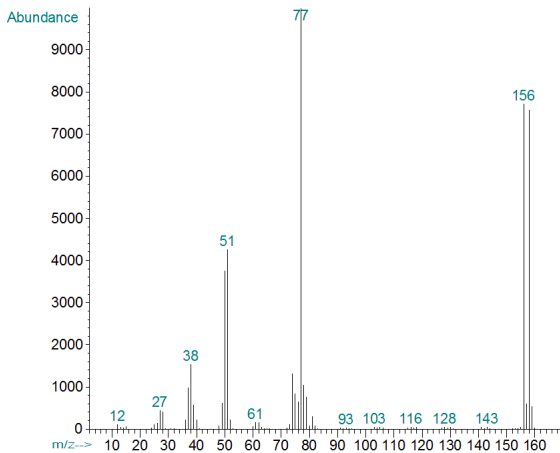
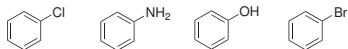
Hmotnostní spektroskopie



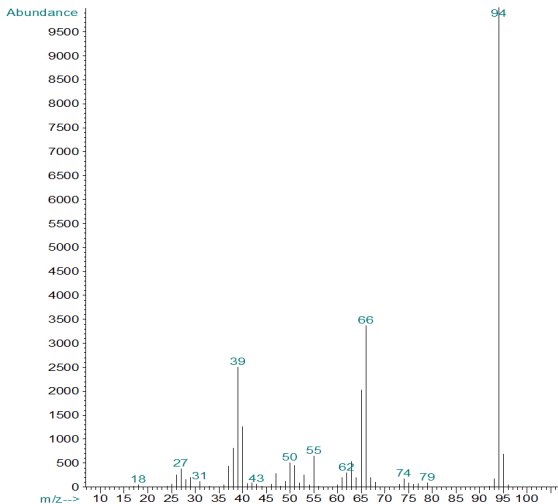
Hmotnostní spektroskopie



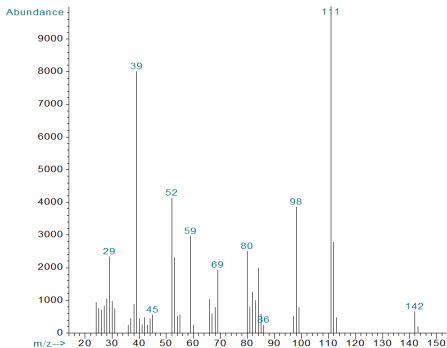
Hmotnostní spektroskopie



Hmotnostní spektroskopie



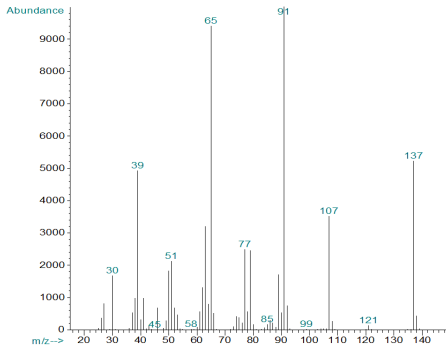
Určení molekulové hmotnosti



Intenzita iontů v oblasti molekulového iontu

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

Určení molekulové hmotnosti

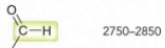
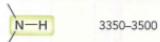


Intenzita iontů v oblasti molekulového iontu

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

Infračervená spektroskopie

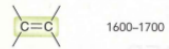
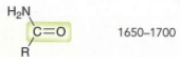
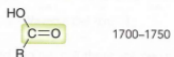
Single Bonds (X—H)



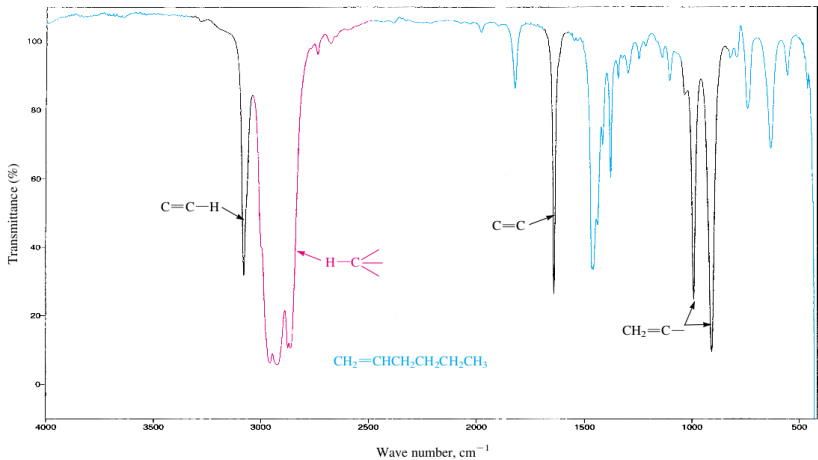
Triple Bonds



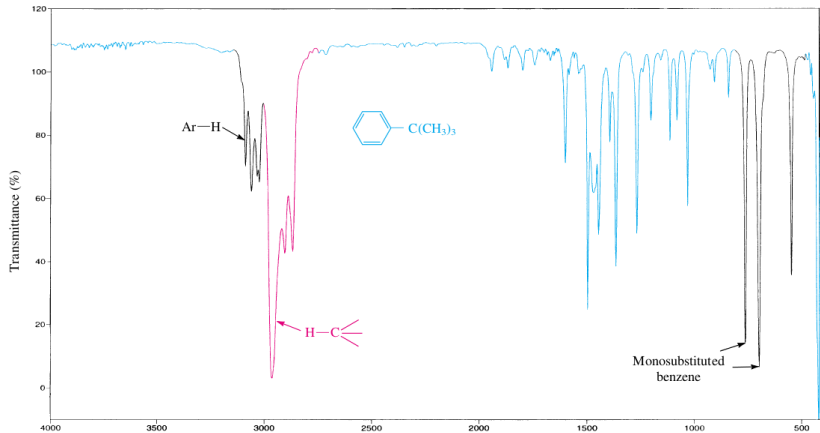
Double Bonds



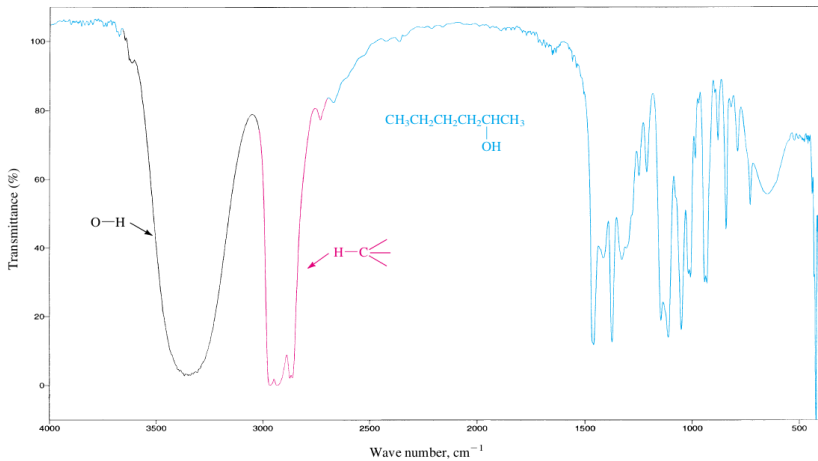
Infračervená spektroskopie



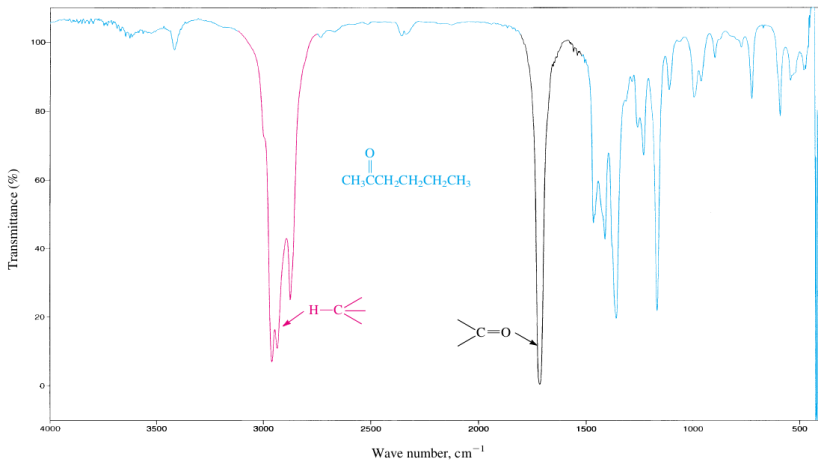
Infračervená spektroskopie



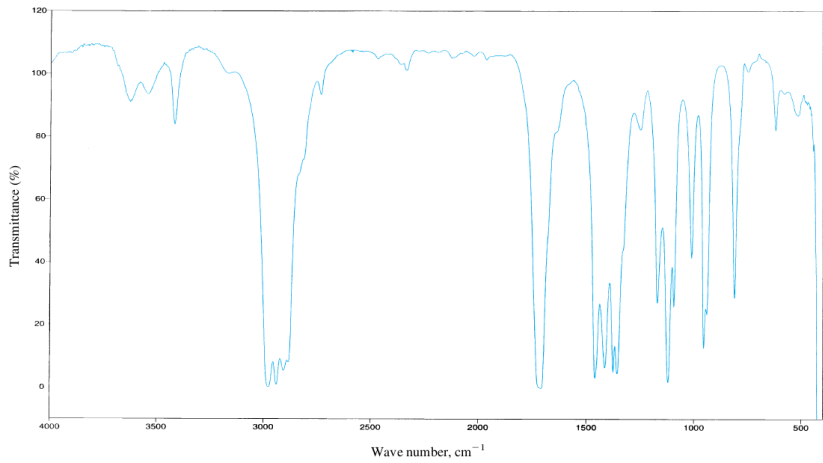
Infračervená spektroskopie



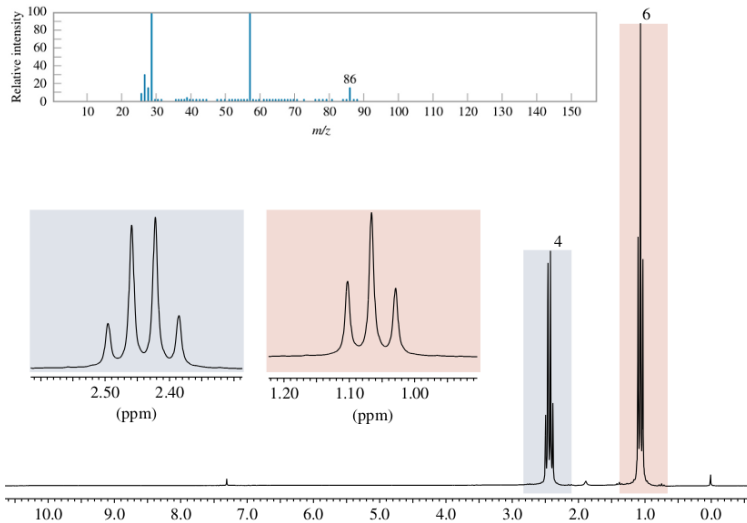
Infračervená spektroskopie



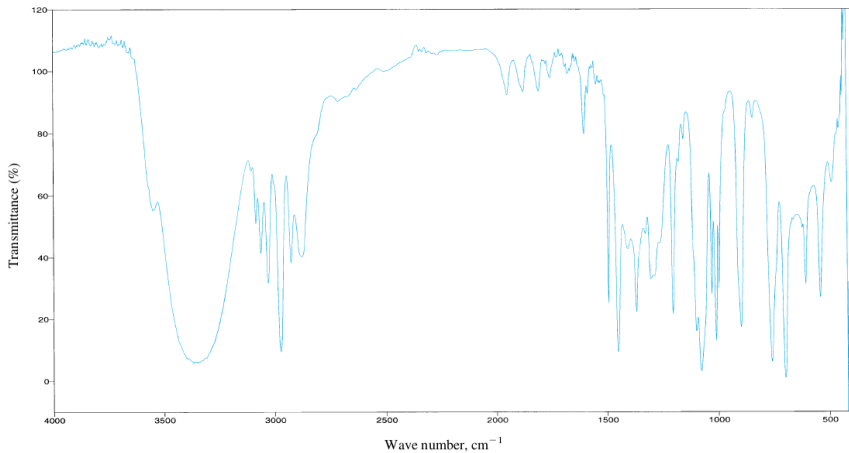
Příklad č. 1



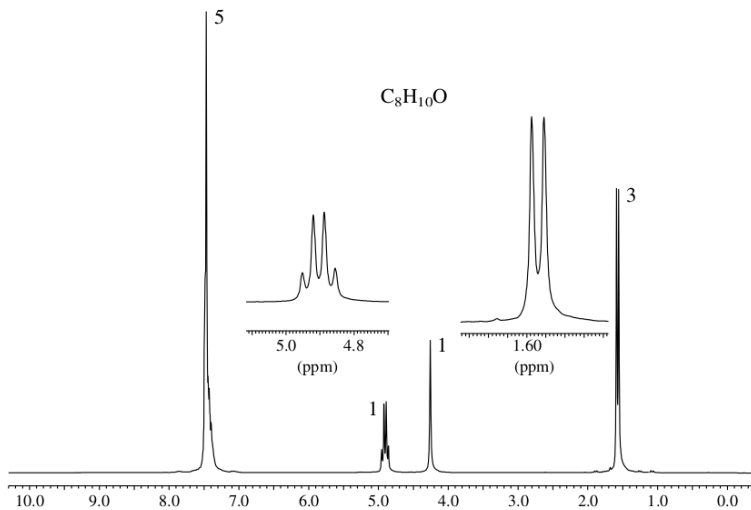
Příklad č. 1



Příklad č. 2



Příklad č. 2



Příklad č. 3

