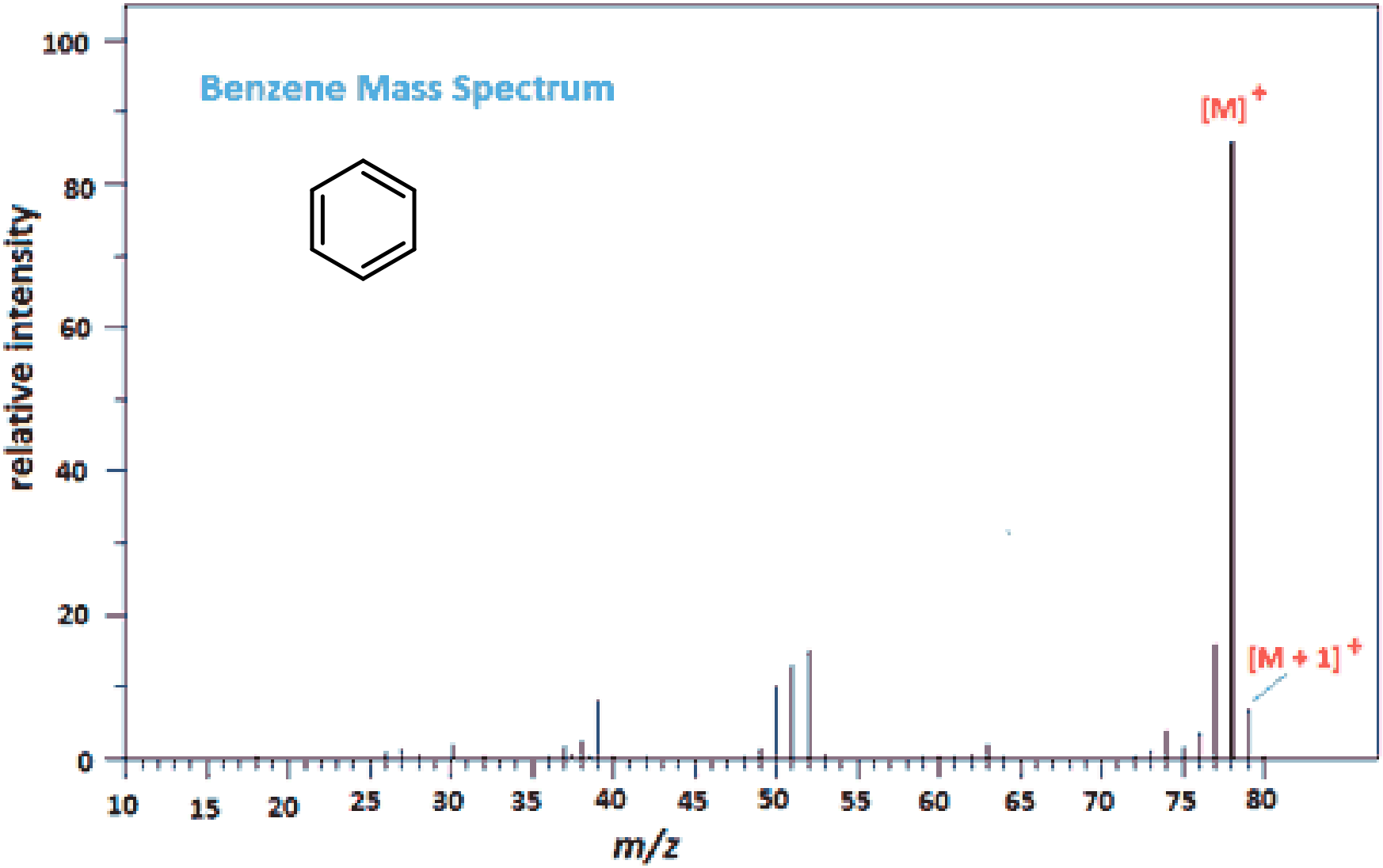
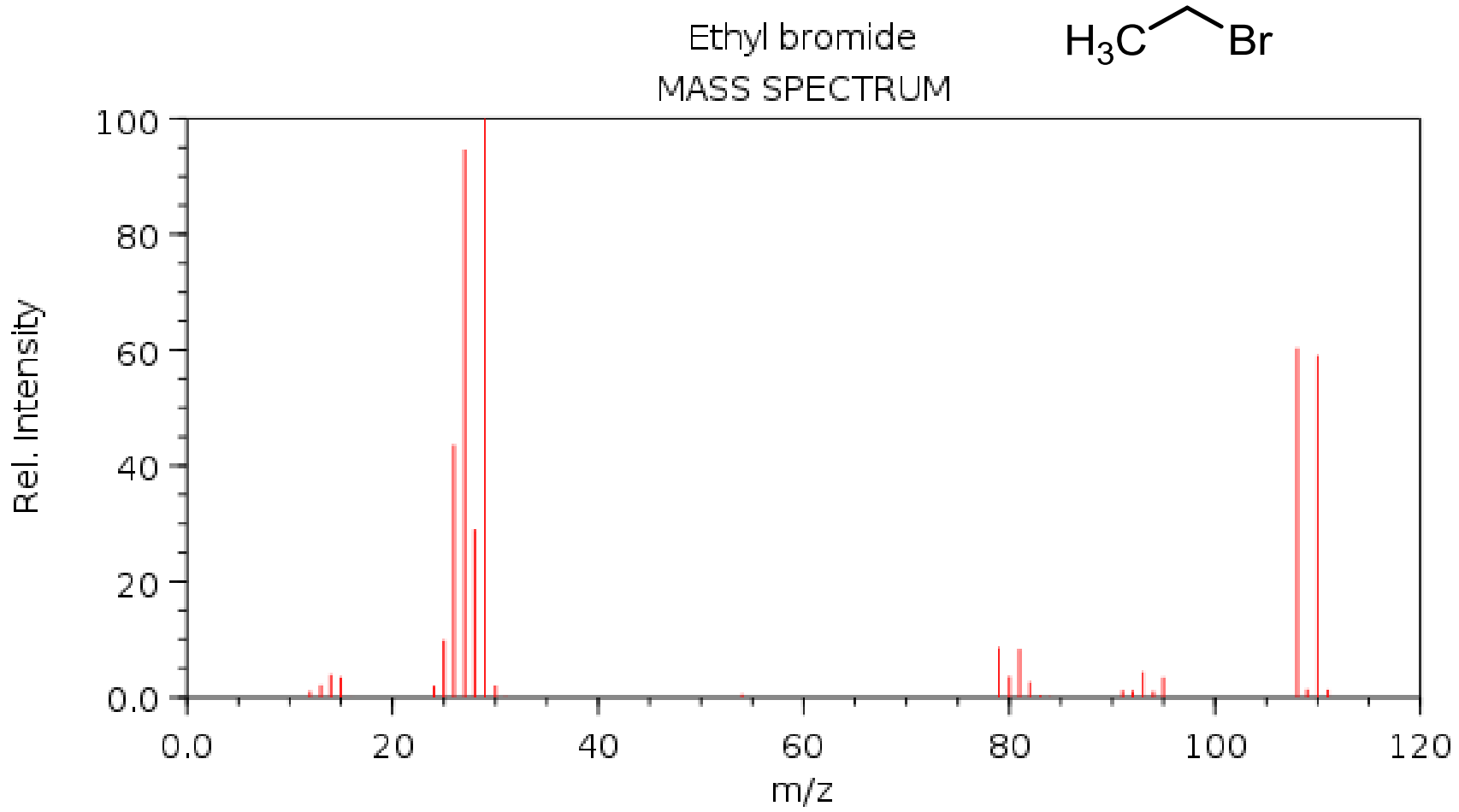
Strukturní analýza

MS, IČ, NMR

Hmotnostní spektrometrie

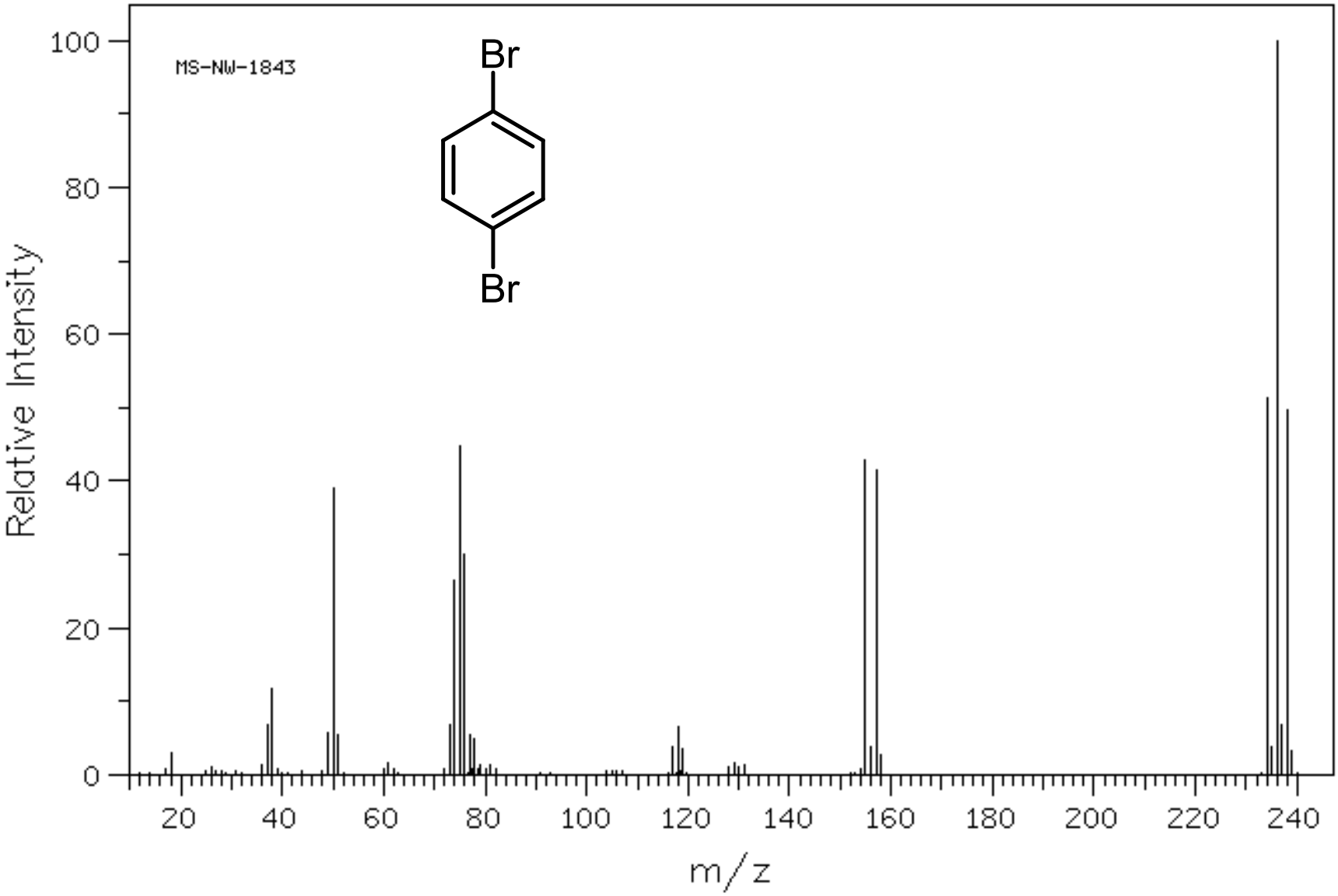


Hmotnostní spektrometrie

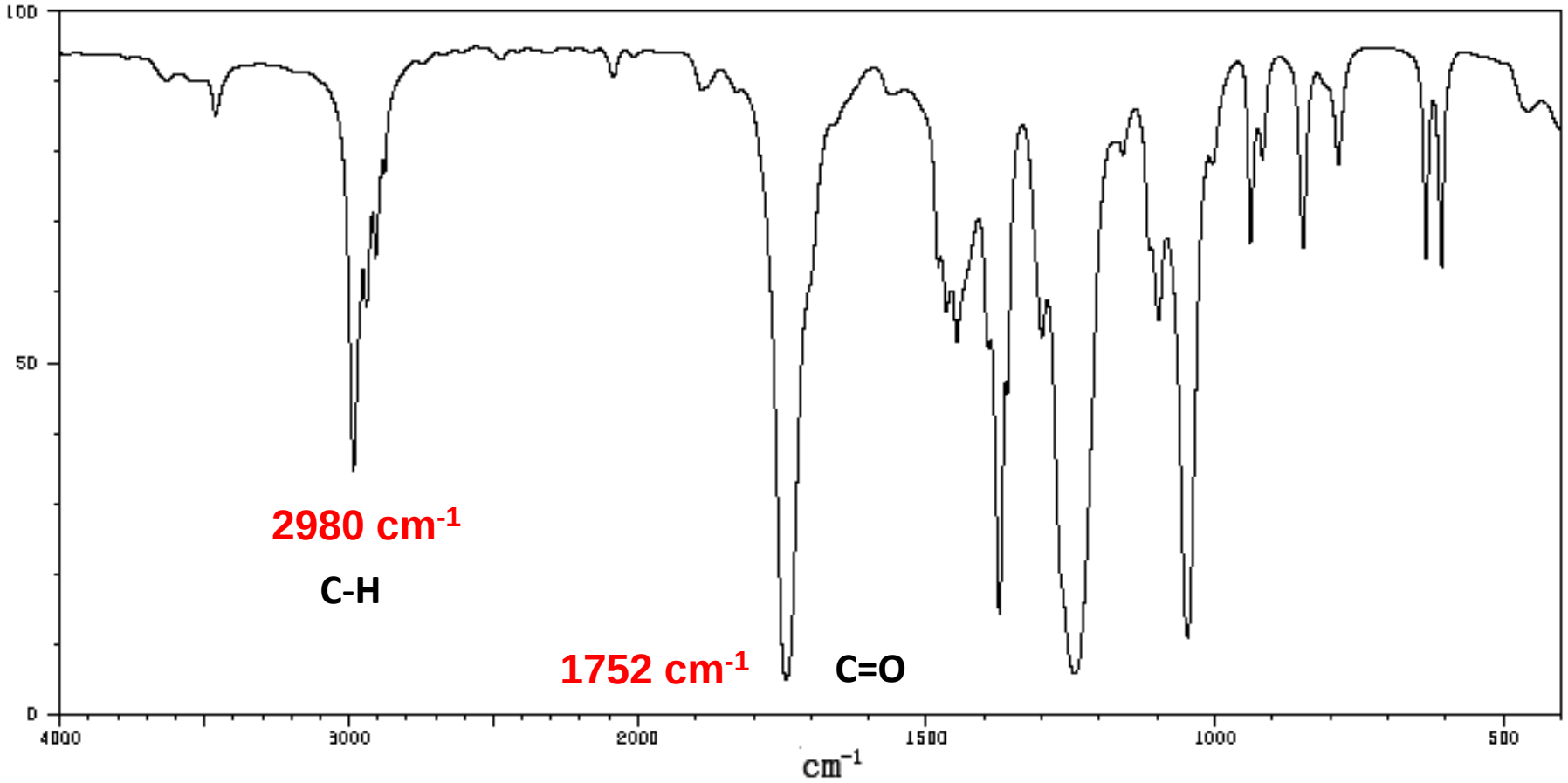


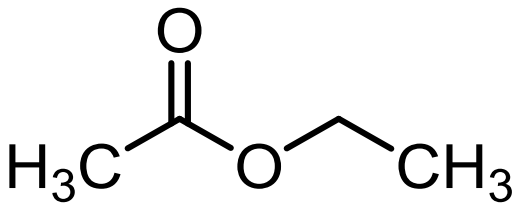
NIST Chemistry WebBook (http://webbook.nist.gov/chemistry)

Hmotnostní spektrometrie

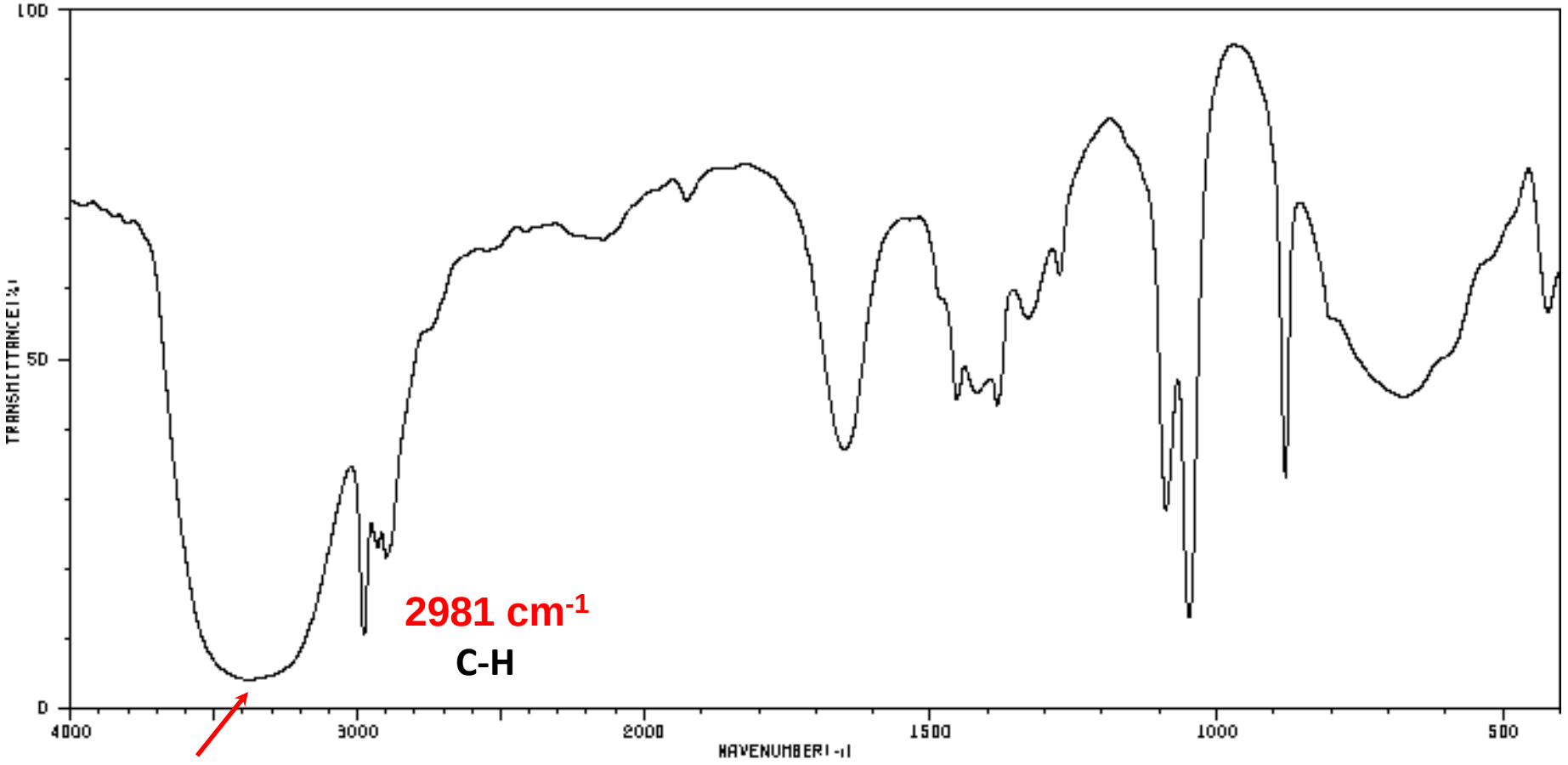


IČ/IR spektroskopie





IČ/IR spektroskopie

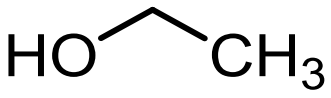


2981 cm^{-1}

C-H

3400 cm^{-1}

O-H



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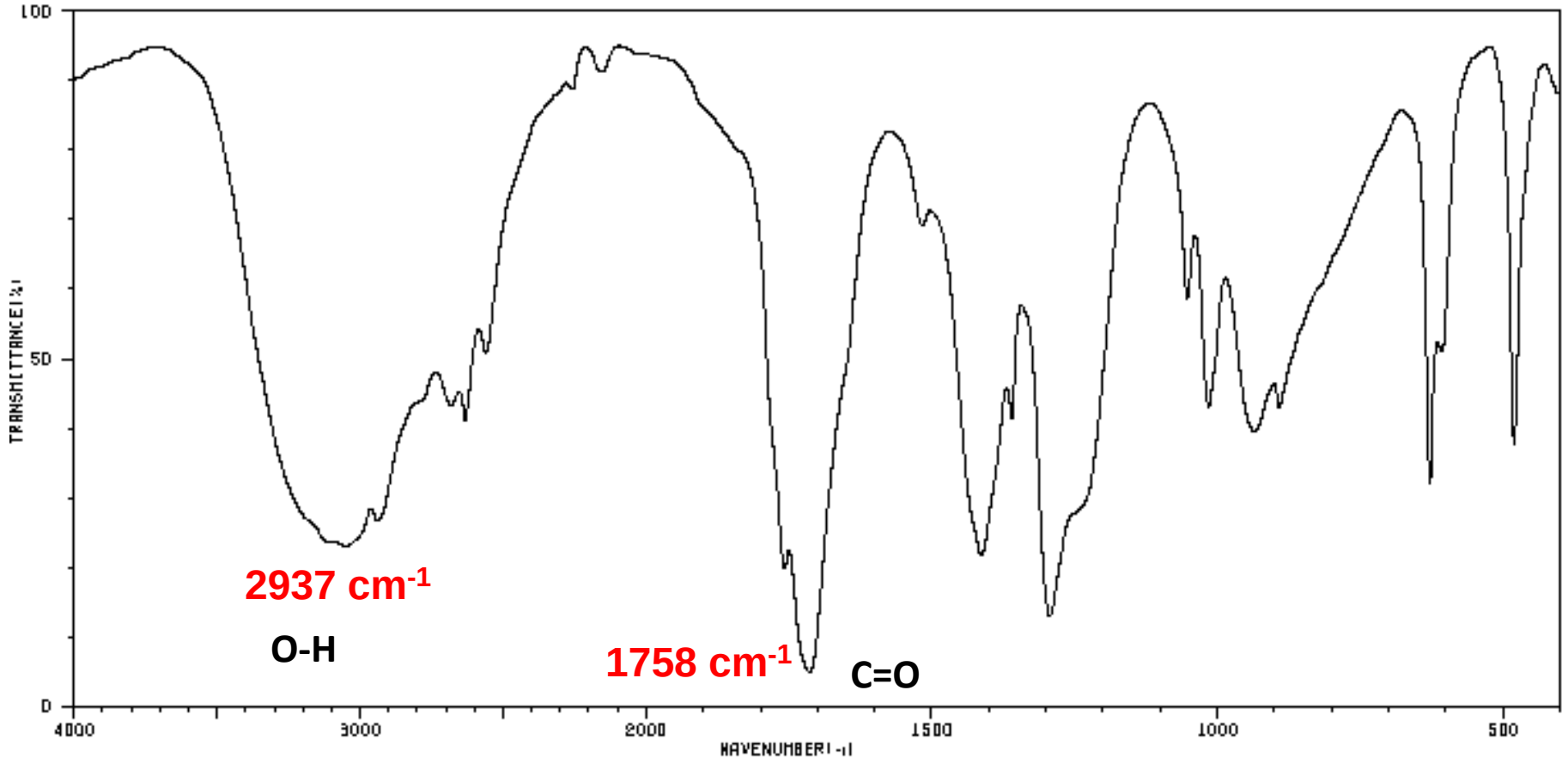

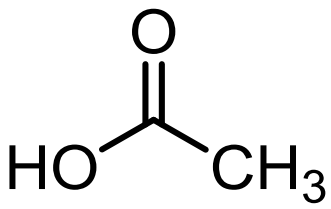

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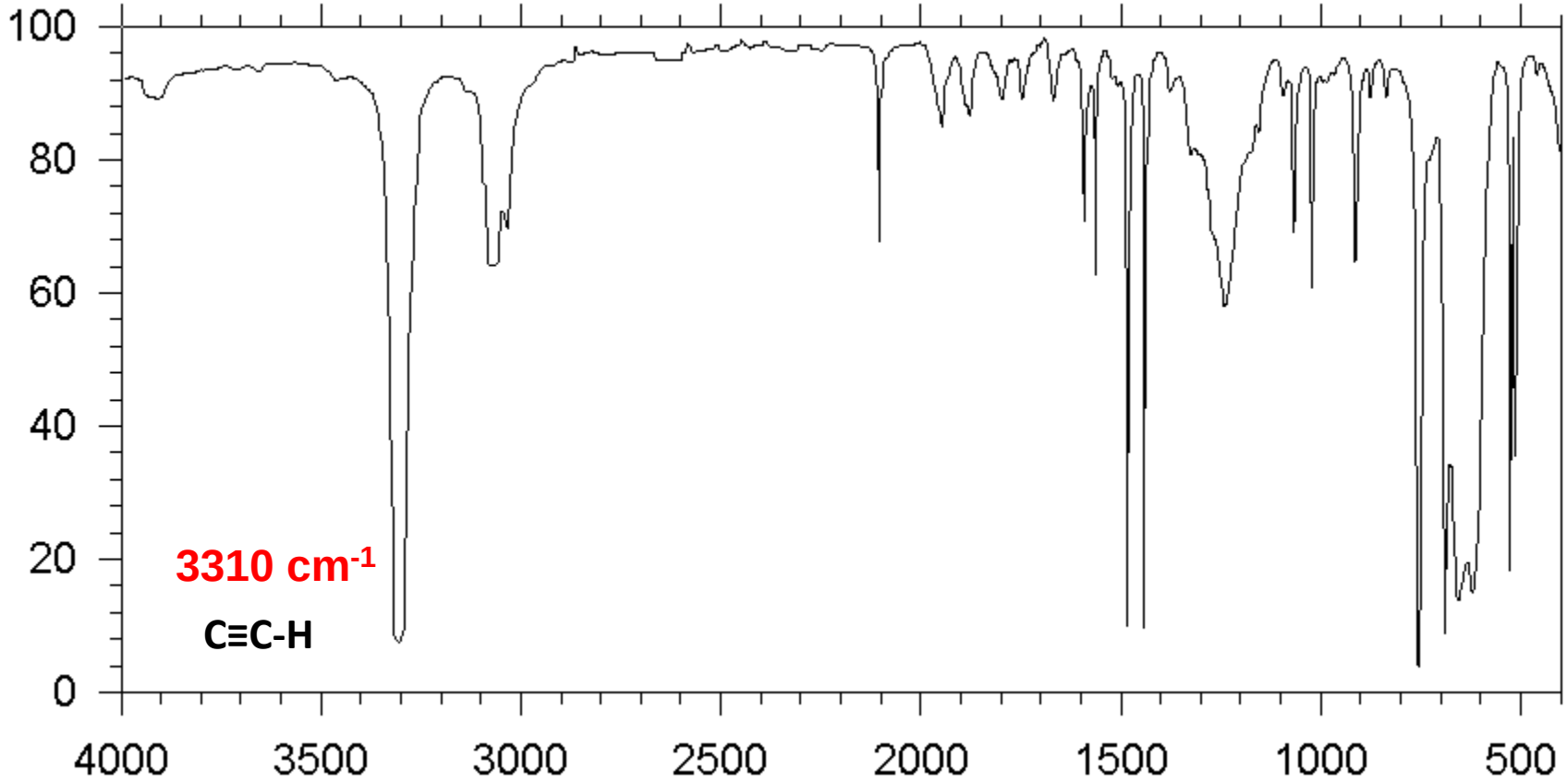
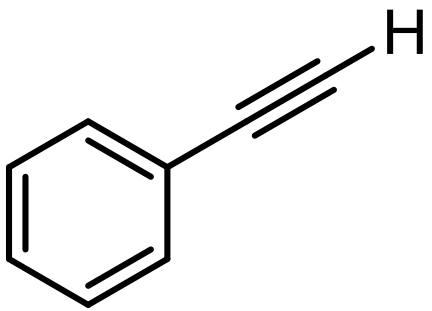
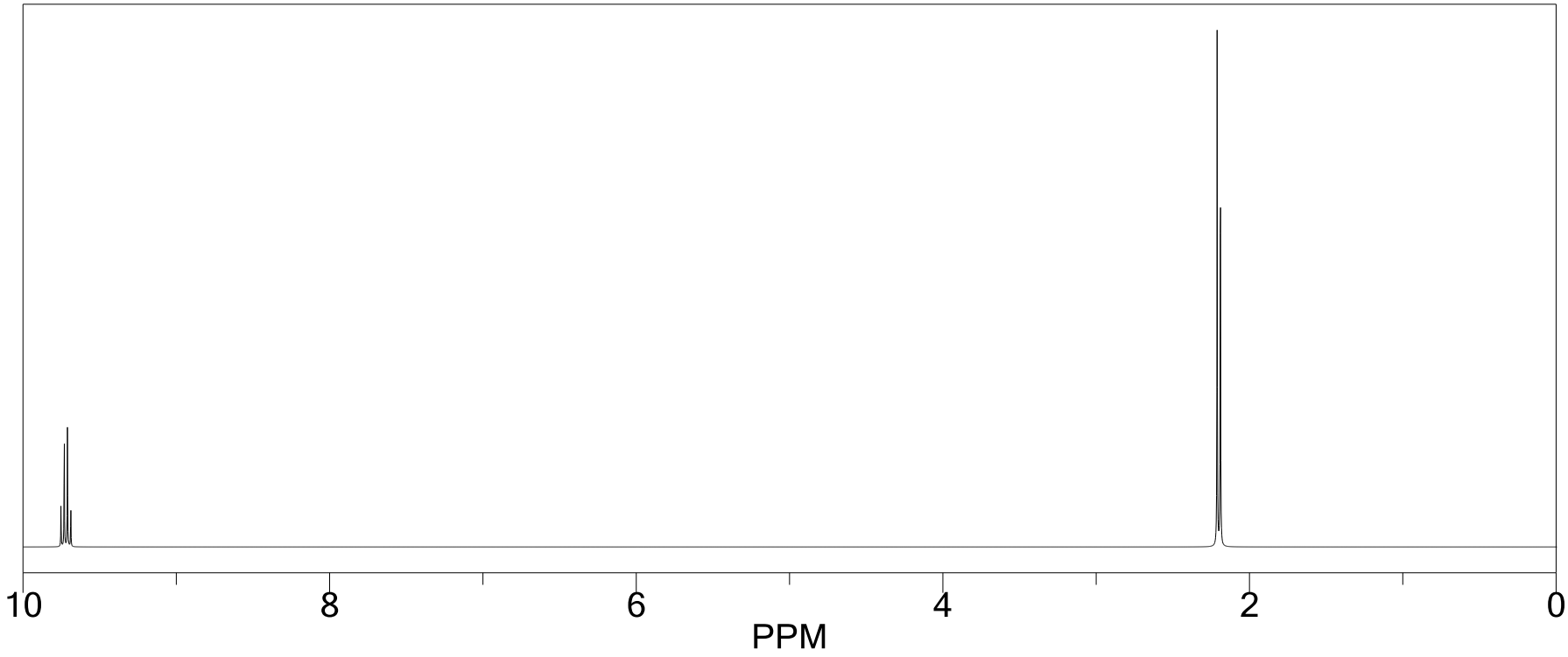




Nukleární magnetická rezonance ^{1}H

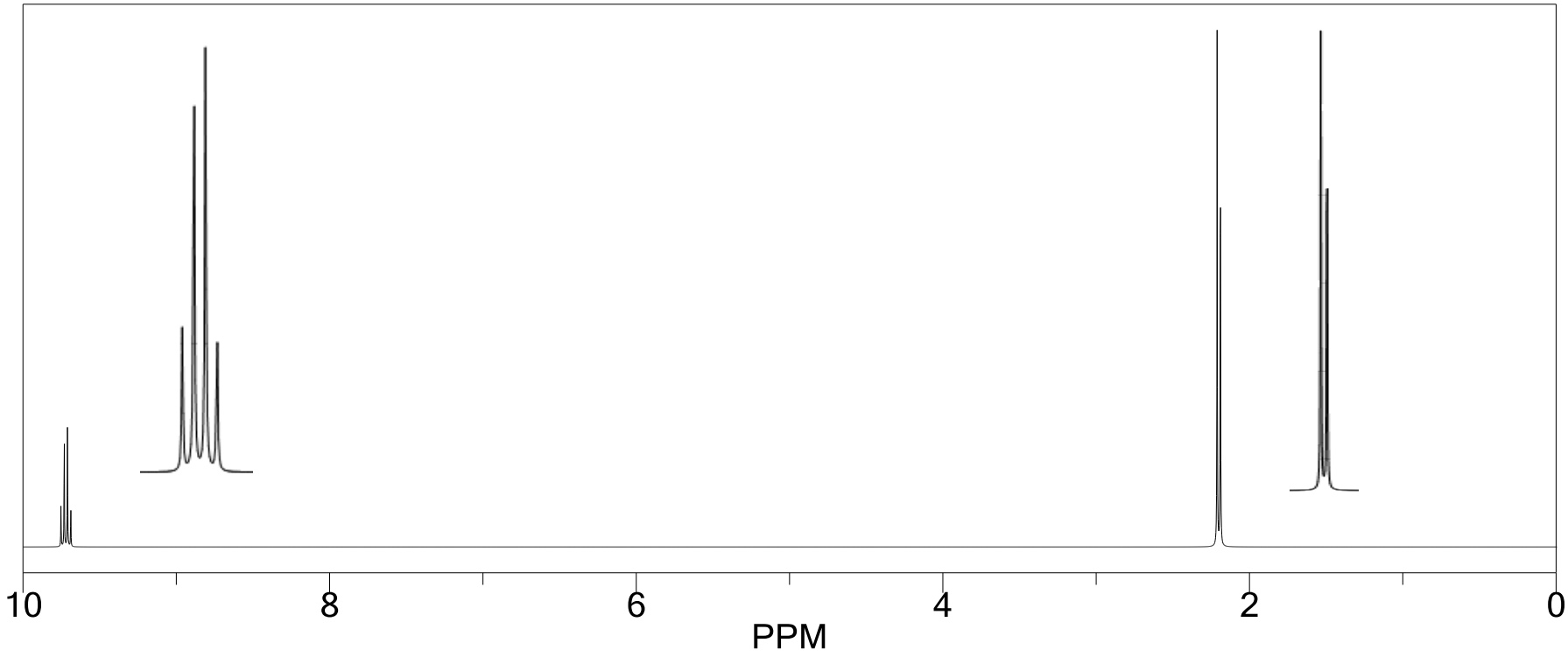


CHEMICKÝ POSUN: KVALITATIVNÍ CHARAKTERISTIKA

INTEGRÁLNÍ INTENZITA: KVANTITATIVNÍ CHARAKTERISTIKA

ŠTĚPĚNÍ/MULTIPLICITA: CHARAKTERISTIKA OKOLÍ

Nukleární magnetická rezonance ^{1}H

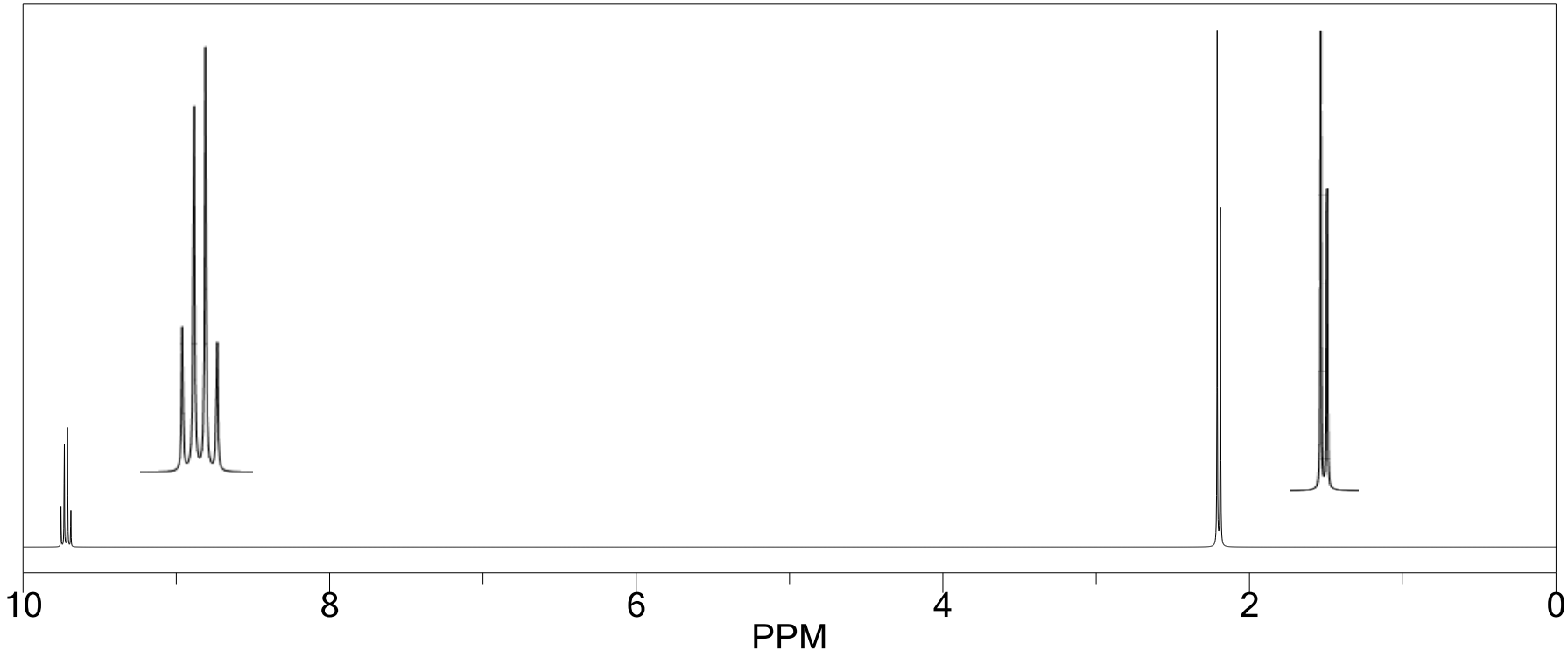


CHEMICKÝ POSUN: δ 2.20 ppm, 9.72 ppm

INTEGRÁLNÍ INTENZITA: 2.20 (3H), 9.72 (1H)

ŠTĚPĚNÍ/MULTIPLICITA: 2.20 (d, 3H), 9.72 (q, 1 H)

Nukleární magnetická rezonance ^{1}H



CHEMICKÝ POSUN: δ 2.20 ppm, 9.72 ppm

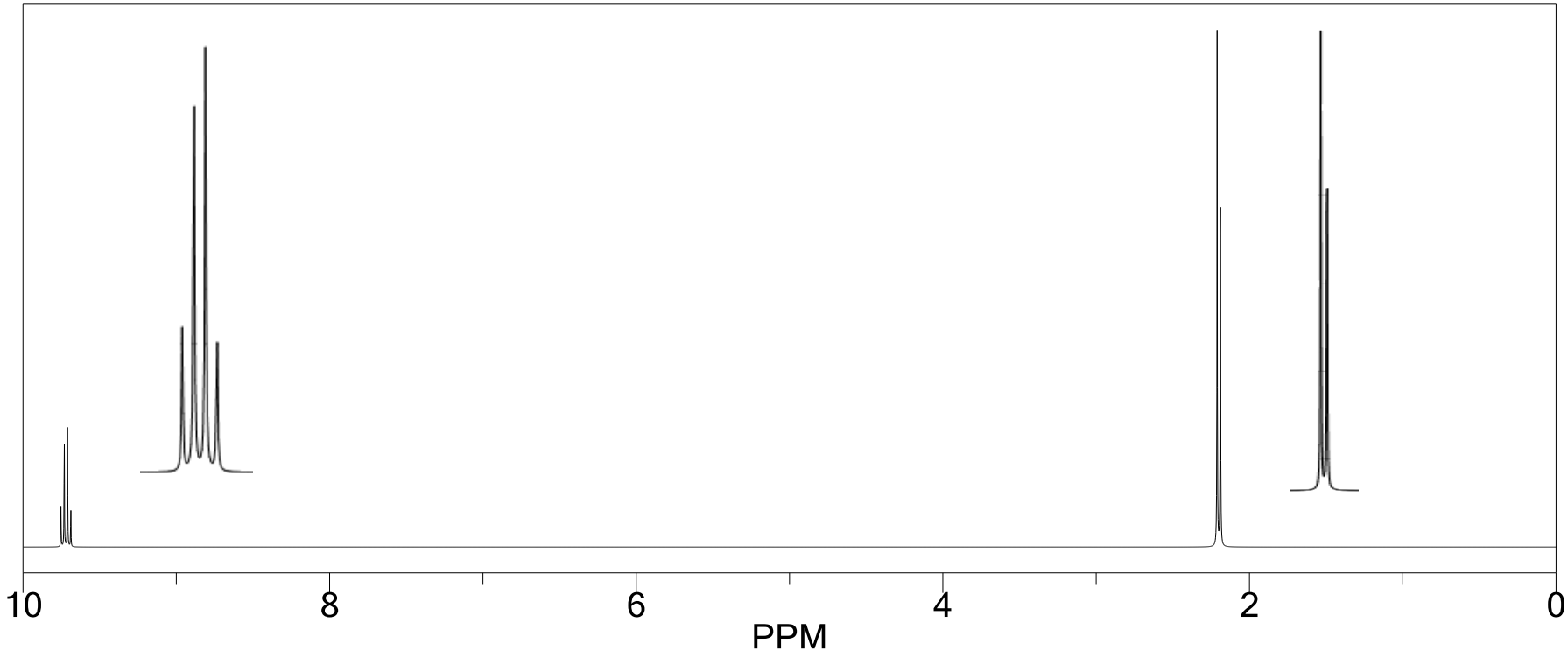
INTEGRÁLNÍ INTENZITA: 2.20 (3H), 9.72 (1H)

ŠTĚPĚNÍ/MULTIPLICITA: dublet (1:1), kvartet (1:3:3:1)

Pravidlo (n+1)

1
1 1
1 2 1
1 3 3 1
1 4 6 4 1
1 5 10 10 5 1

Nukleární magnetická rezonance ^{1}H



CHEMICKÝ POSUN: δ 2.20 ppm, 9.72 ppm

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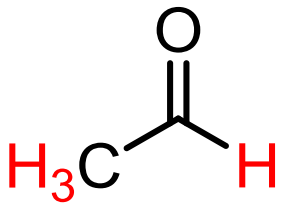
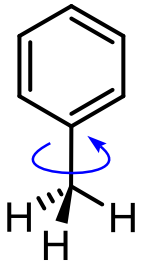
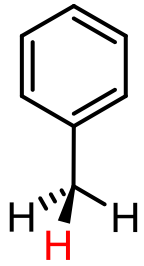


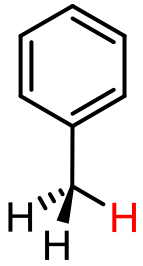
ŠTĚPĚNÍ/MULTIPLICITA: dublet (1:1), kvartet (1:3:3:1)

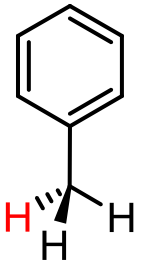
Pravidlo (n+1)

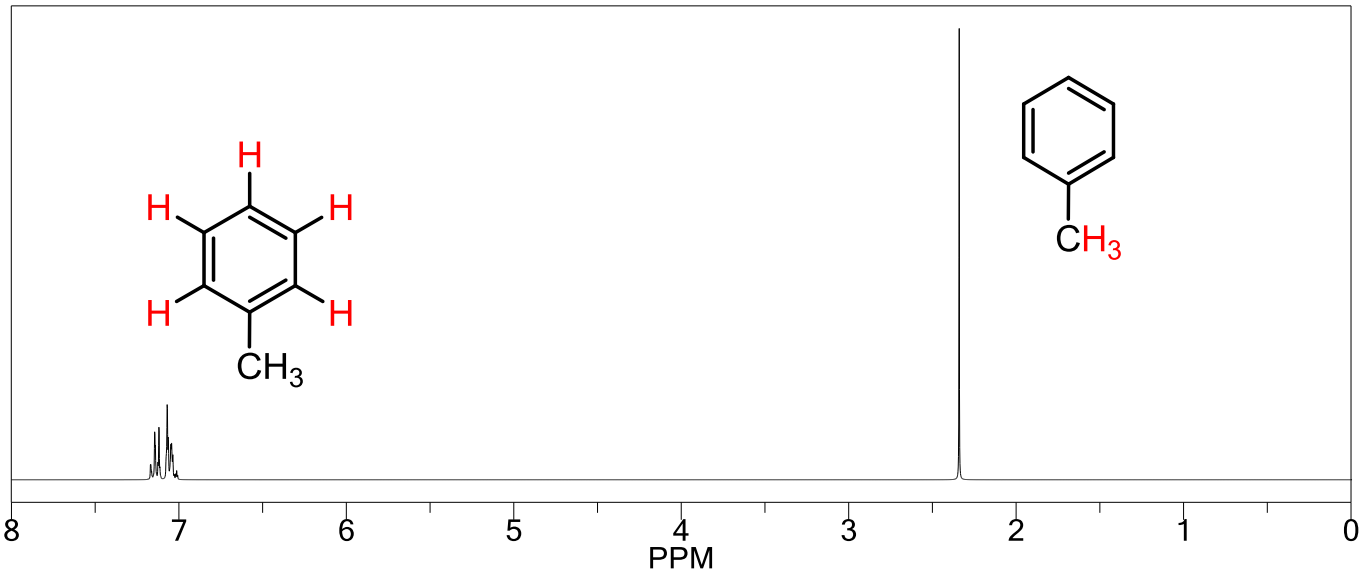
Nukleární magnetická rezonance ^{1}H – rotace kolem jednoduché vazby: methyl



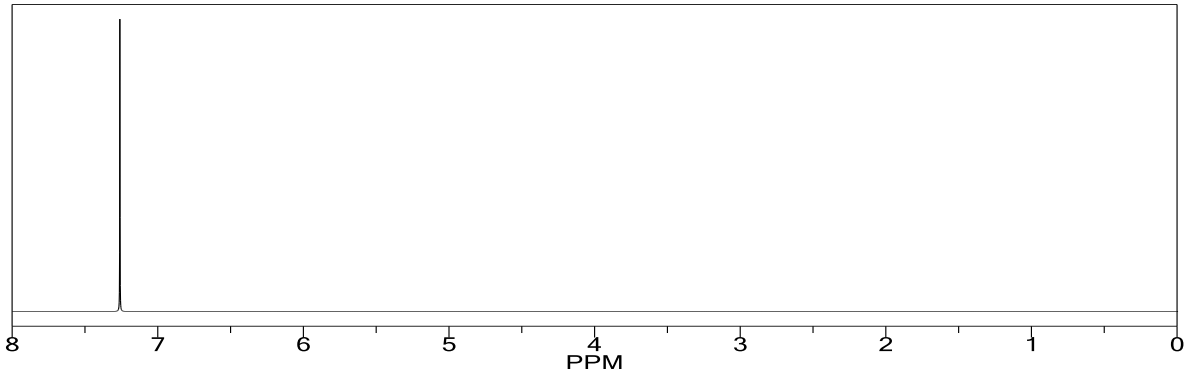


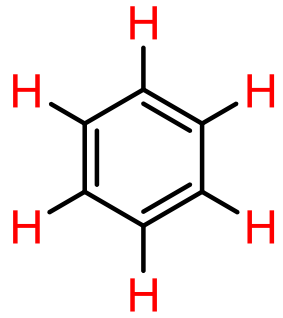






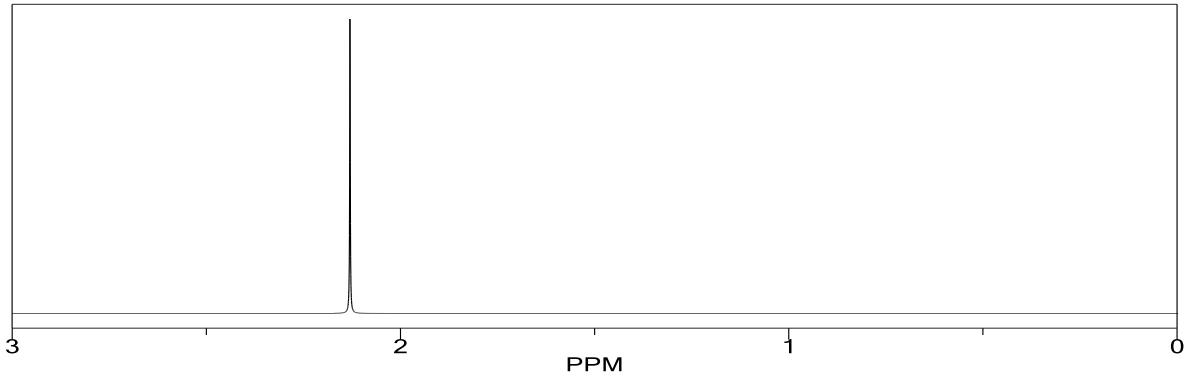
Nukleární magnetická rezonance ^1H - operace symetrie

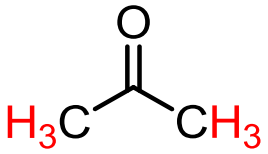




7.26 ppm (s)

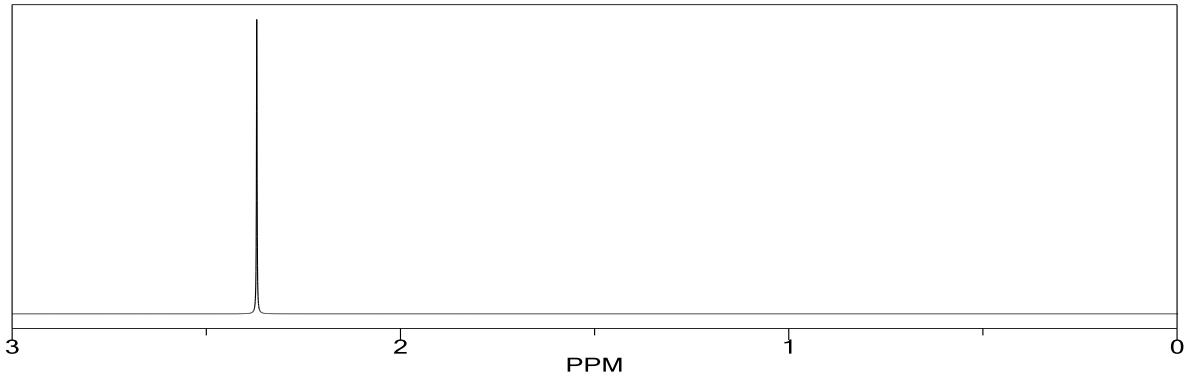
rotace: šestičetná osa
zrcadlení

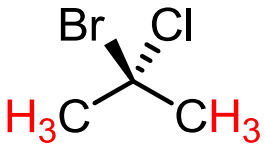




2.13 ppm (s)

rotace: dvojčetná osa
zrcadlení

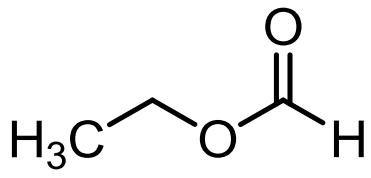


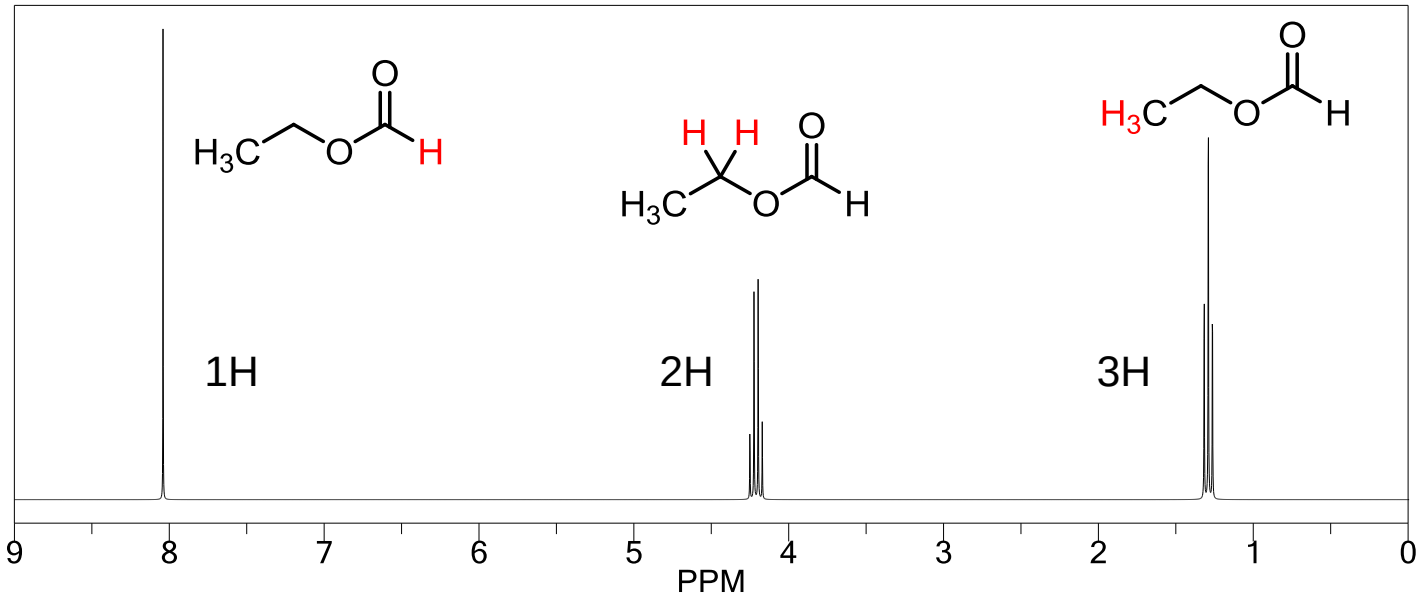


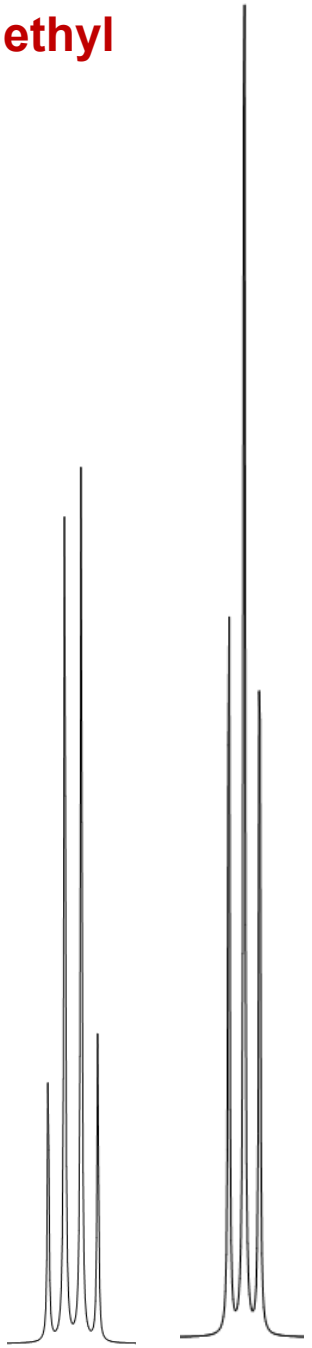
2.37 ppm (s)

zrcadlení: rovina Br-C-Cl

Nukleární magnetická rezonance ^1H – typické signály: ethyl

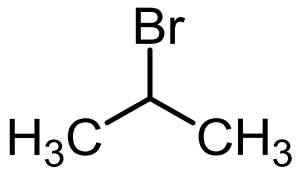


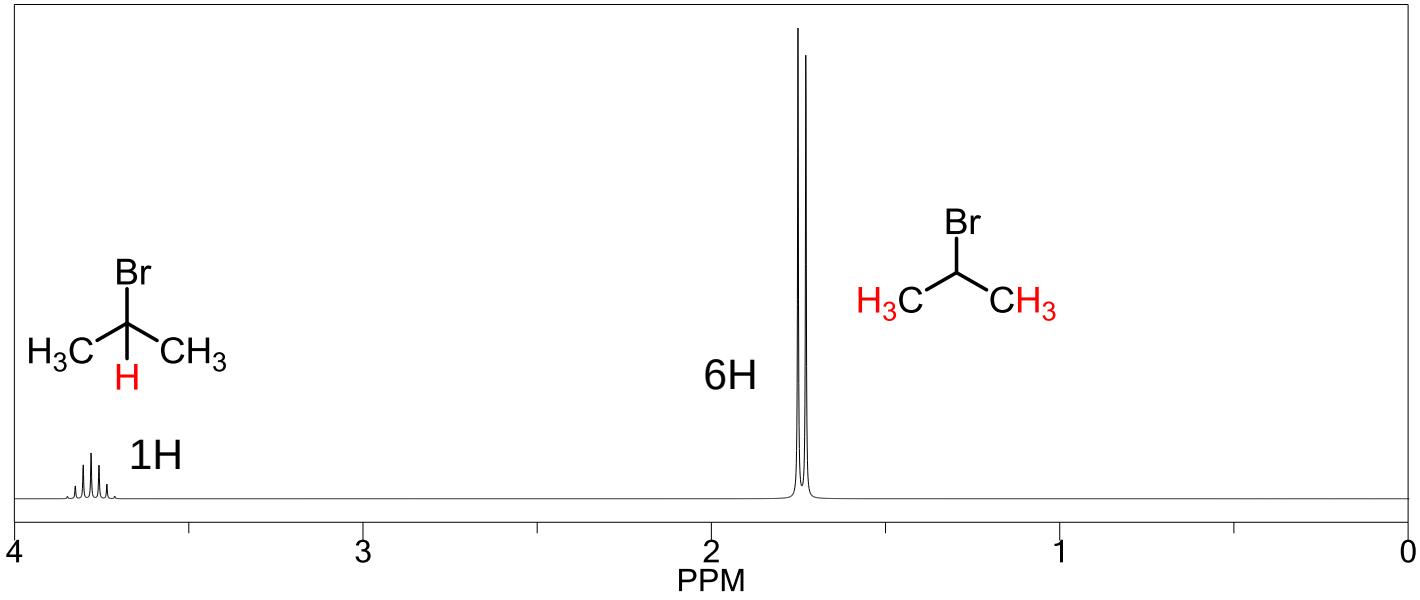




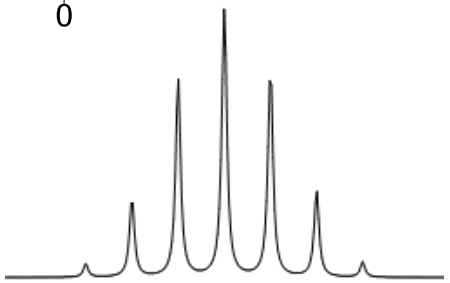
triplet a kvartet v poměru 3:2 bývá často ethyl

Nukleární magnetická rezonance ^1H – typické signály: isopropyl

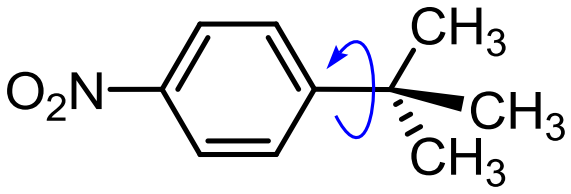


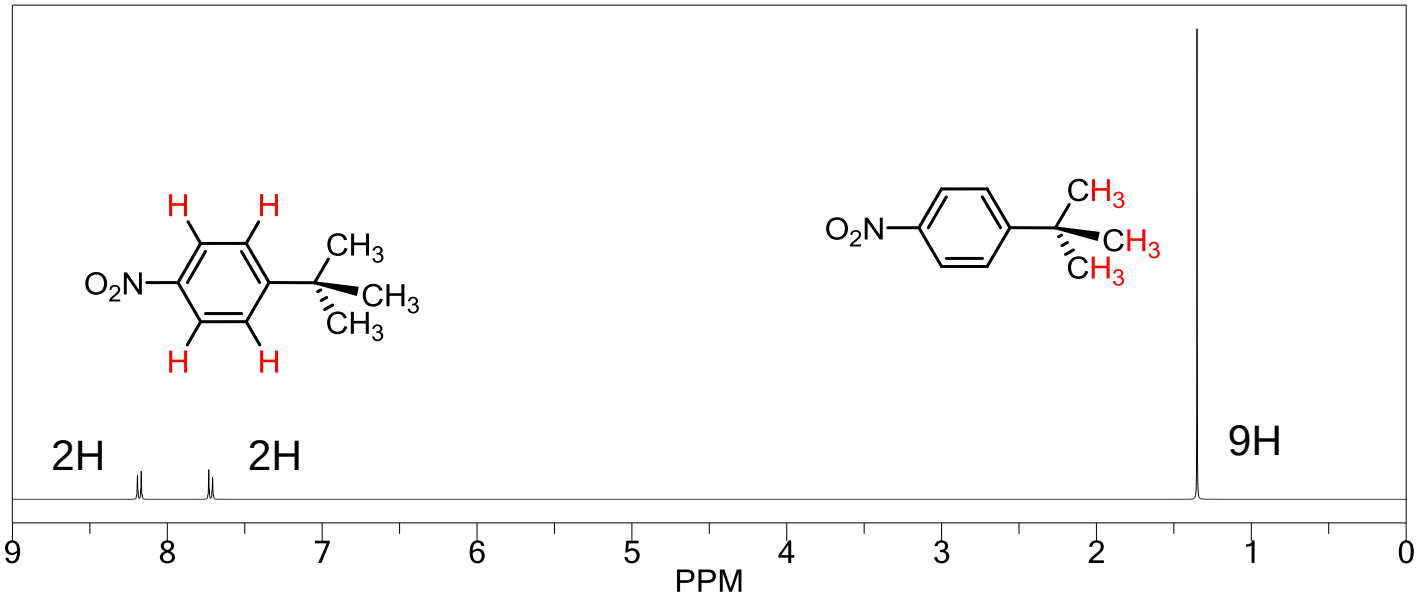


dublet a septet v poměru 6:1 bývá často isopropyl



Nukleární magnetická rezonance ^{1}H – typické signály: *terc*-butyl

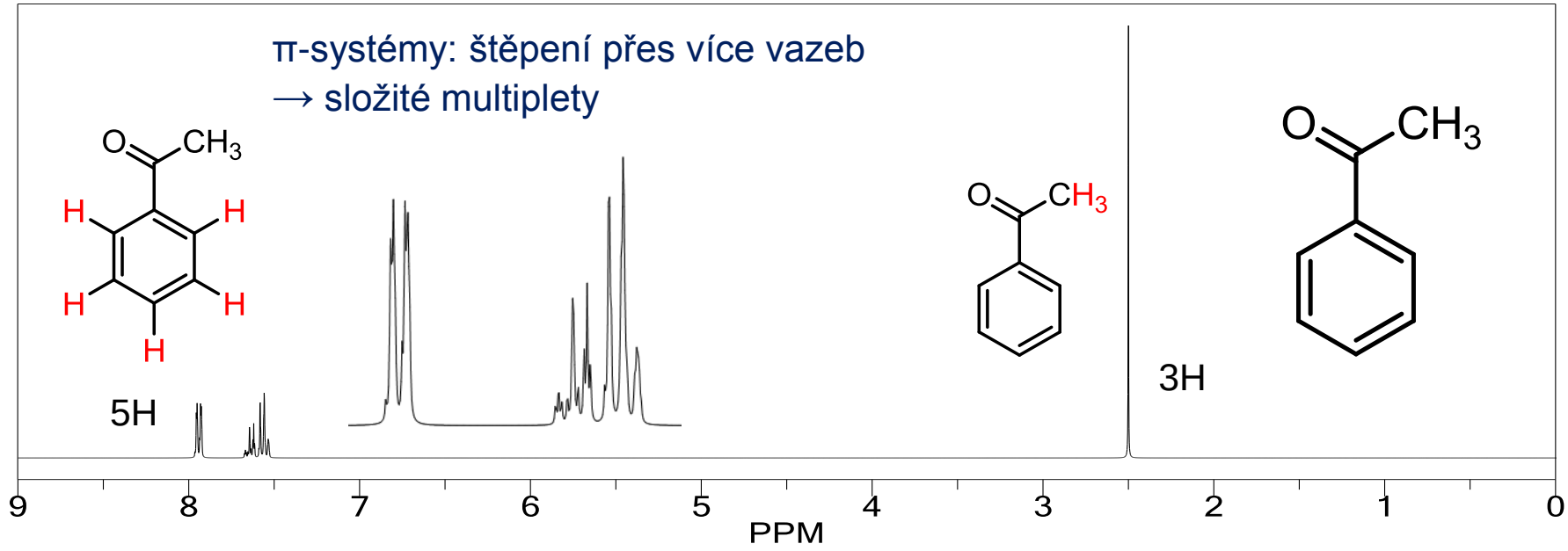


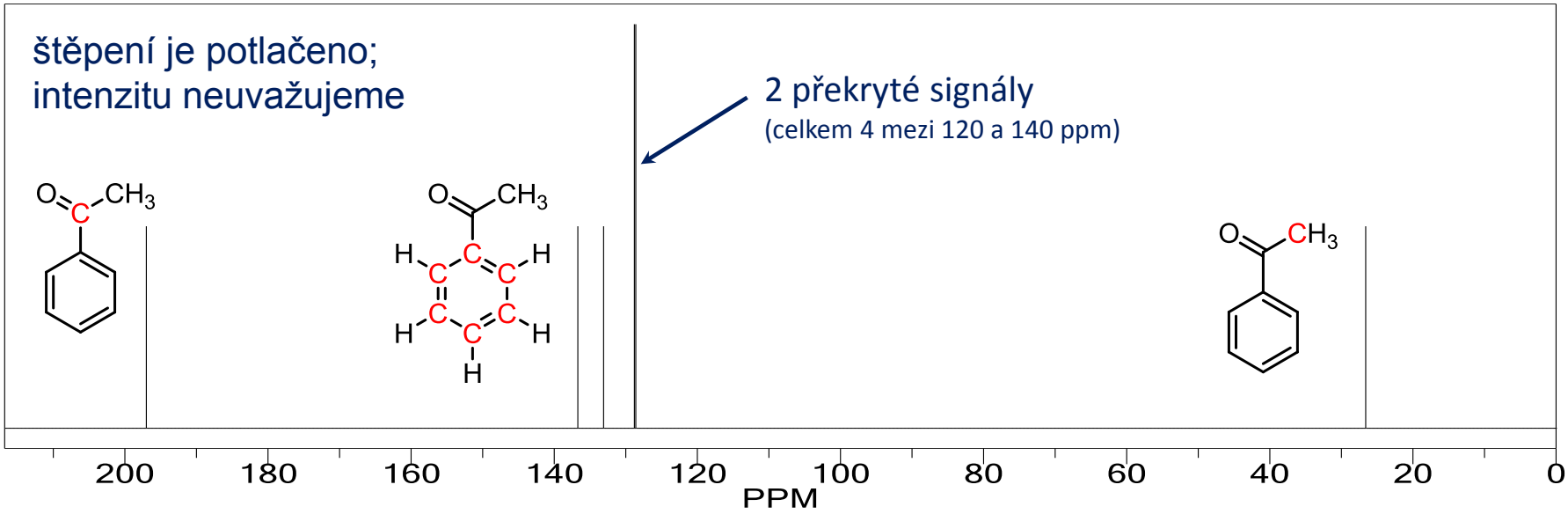


singlet odpovídající 9 vodíkům může být *terc*-butyl

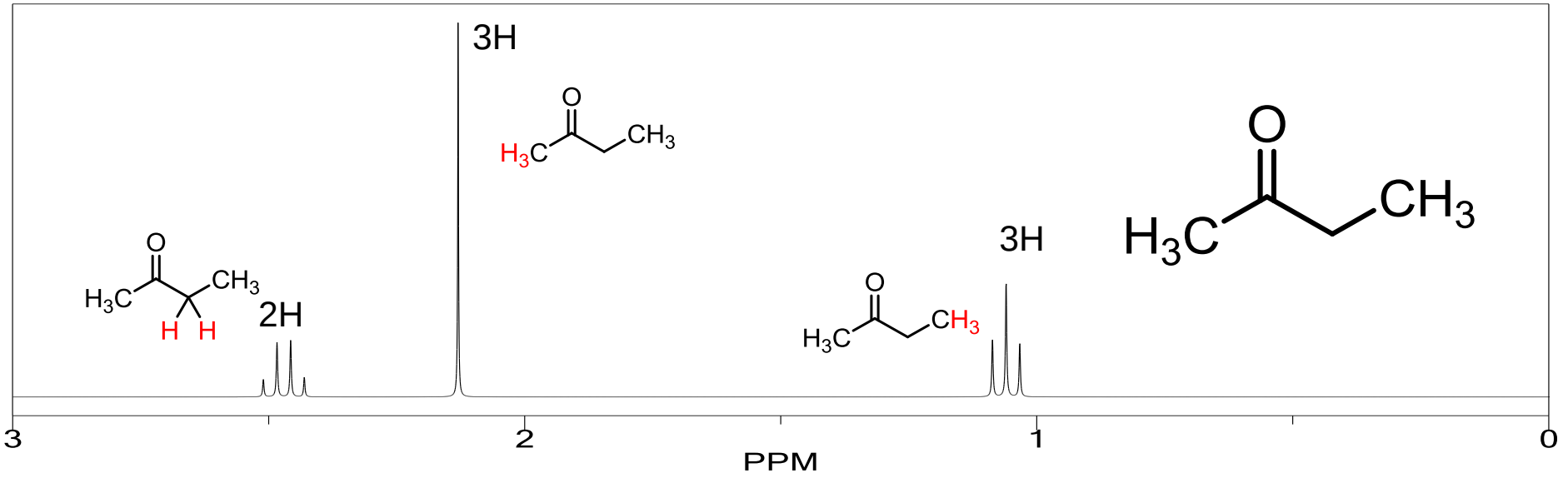
(rotace kolem jednoduchých vazeb způsobí, že je všech 9 vodíků ekvivalentních)

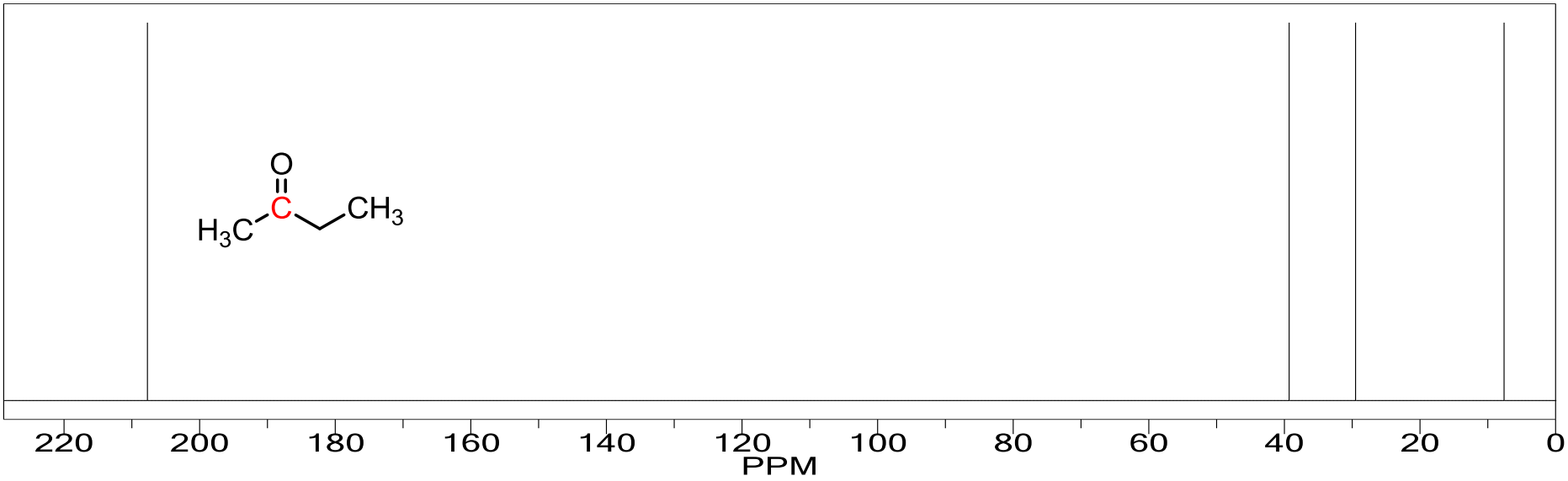
Nukleární magnetická rezonance ^{1}H, ^{13}C



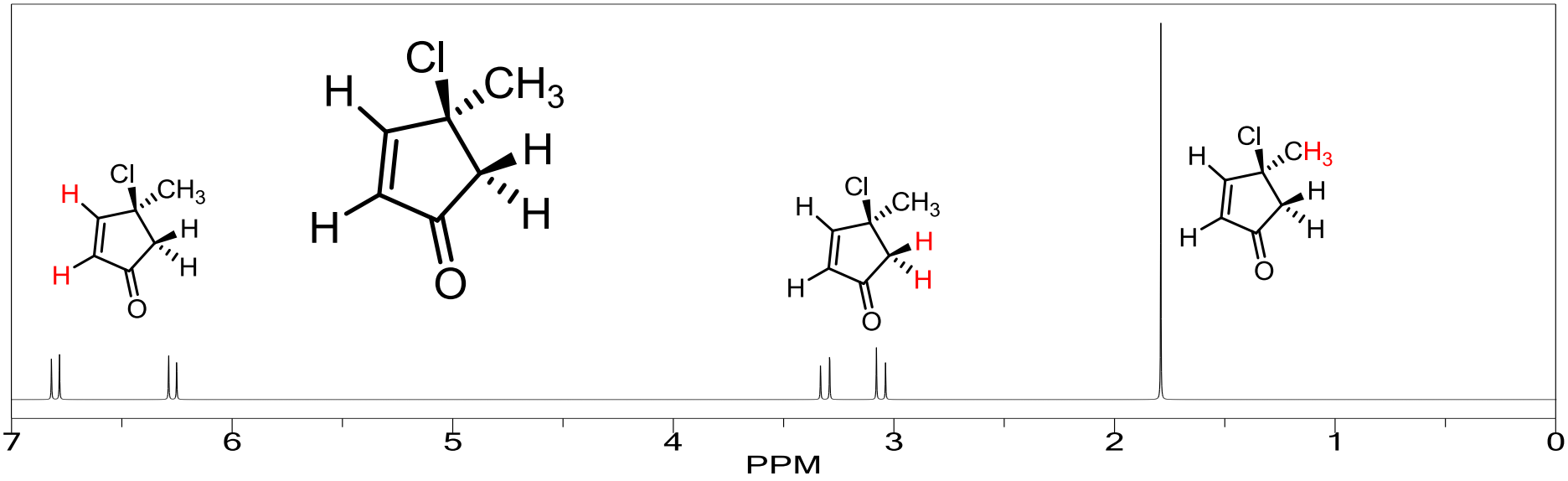


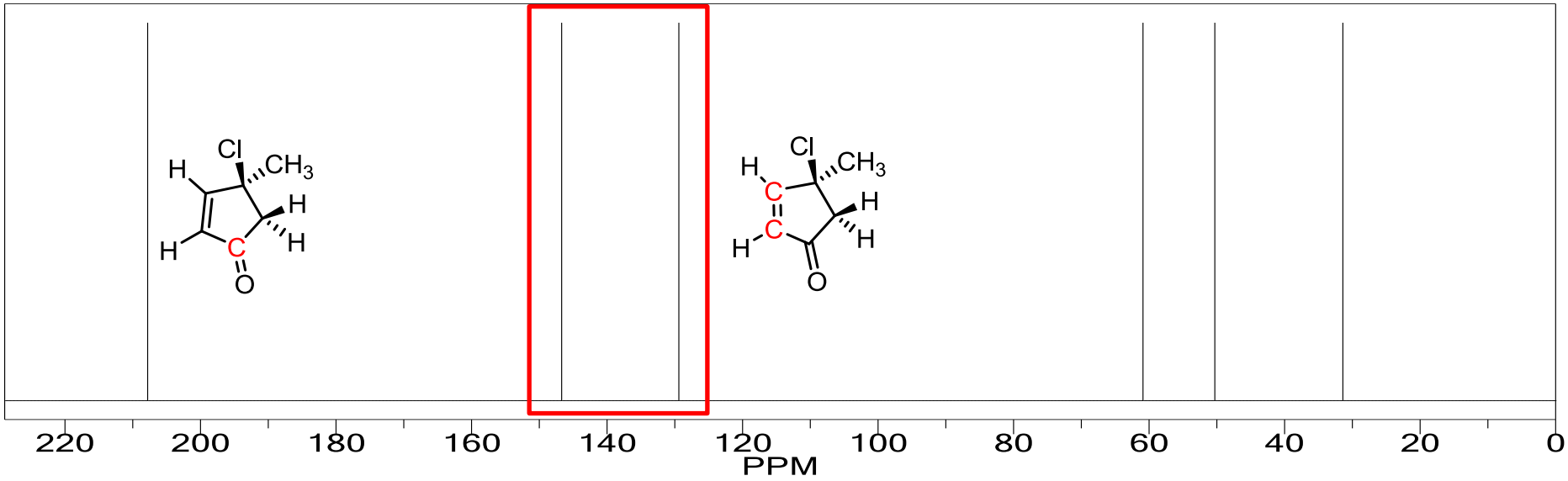
Nukleární magnetická rezonance ^{1}H, ^{13}C





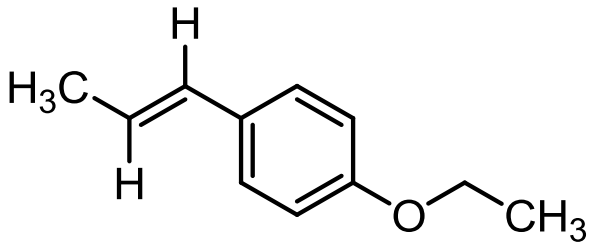
Nukleární magnetická rezonance ^{1}H, ^{13}C

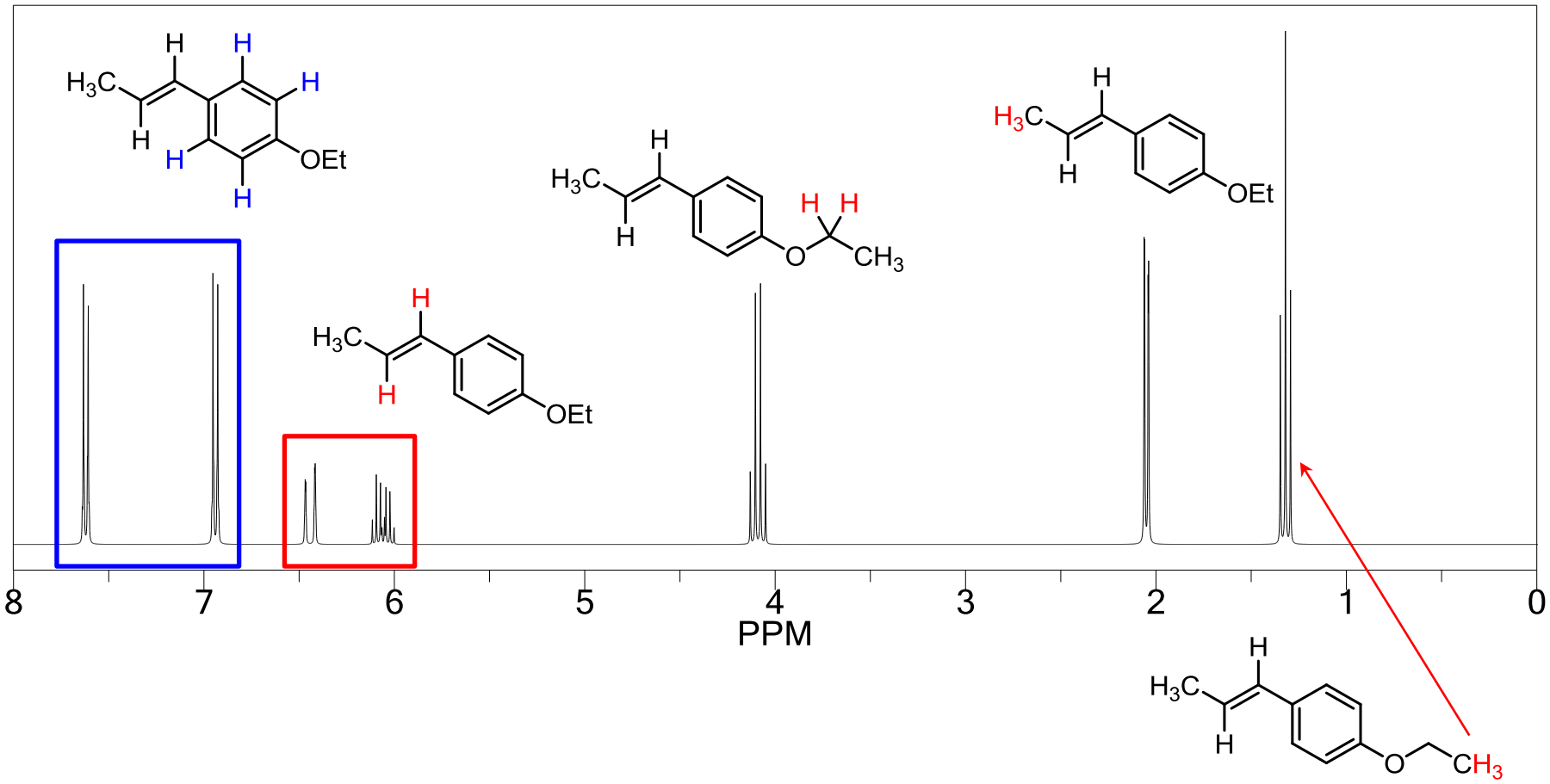




Nukleární magnetická rezonance ^{1}H, ^{13}C

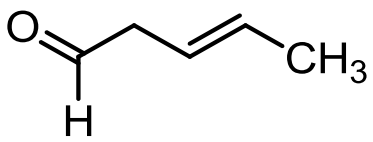
Odhadněte chemické posuny ve vodíkovém spektru

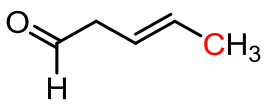


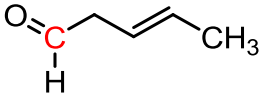


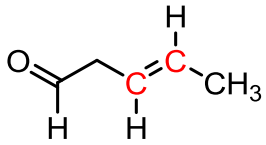
Nukleární magnetická rezonance ^{1}H, ^{13}C

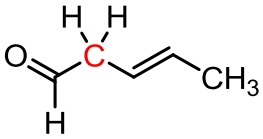
Odhadněte chemické posuny v uhlíkovém spektru





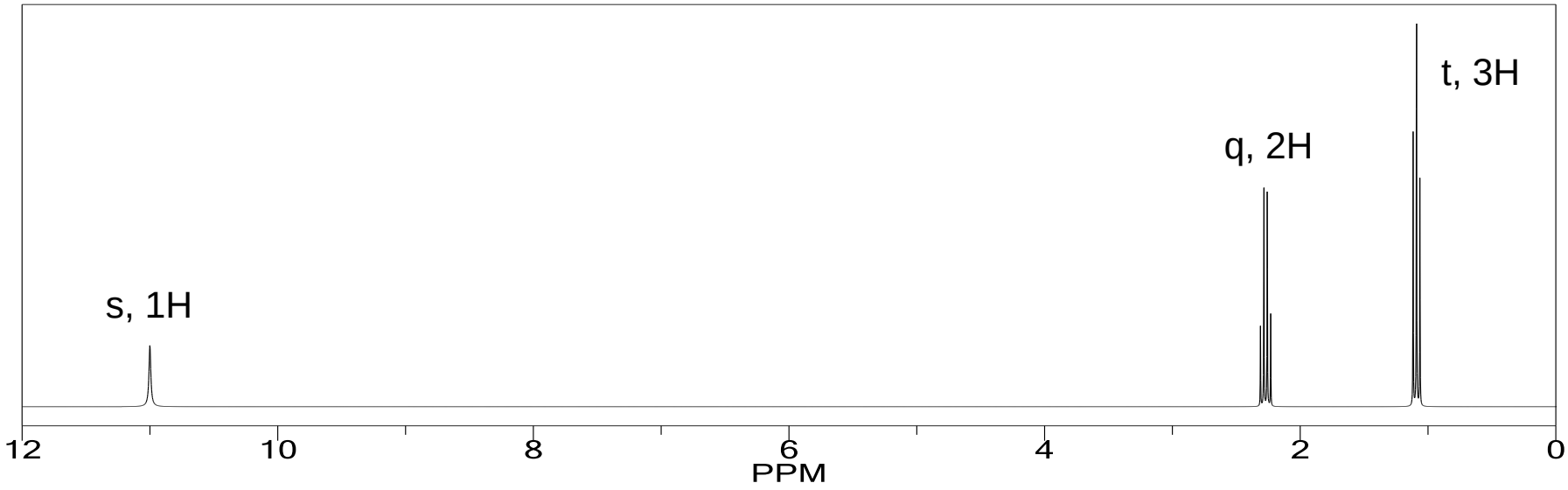


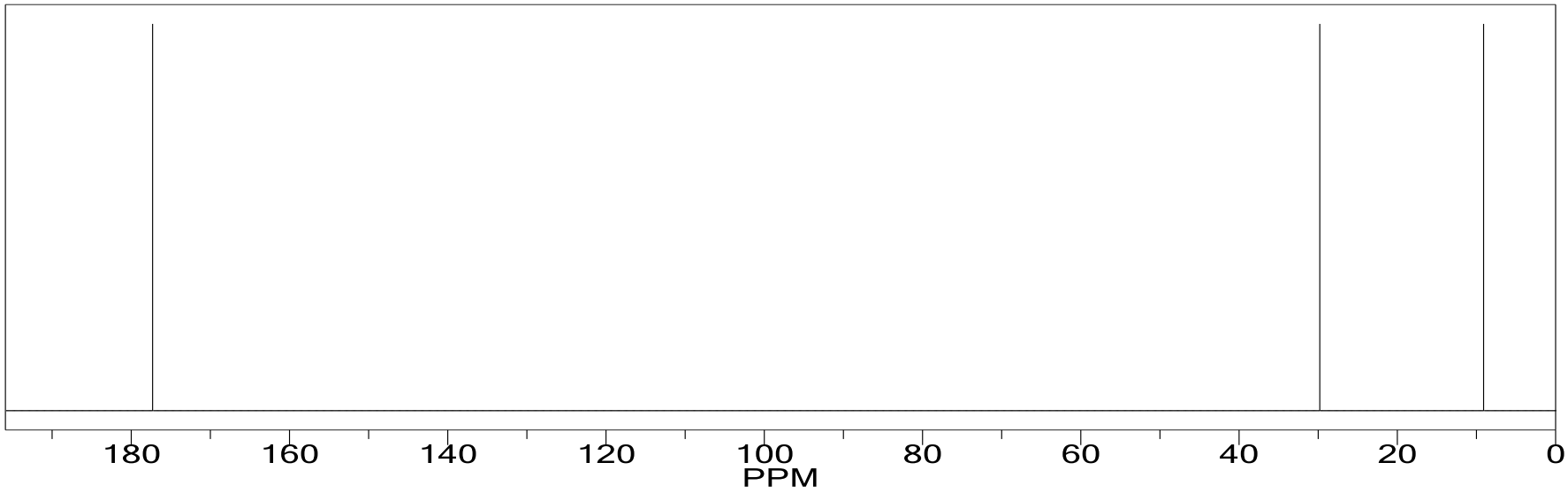




Nukleární magnetická rezonance ^{1}H, ^{13}C, IČ, MS

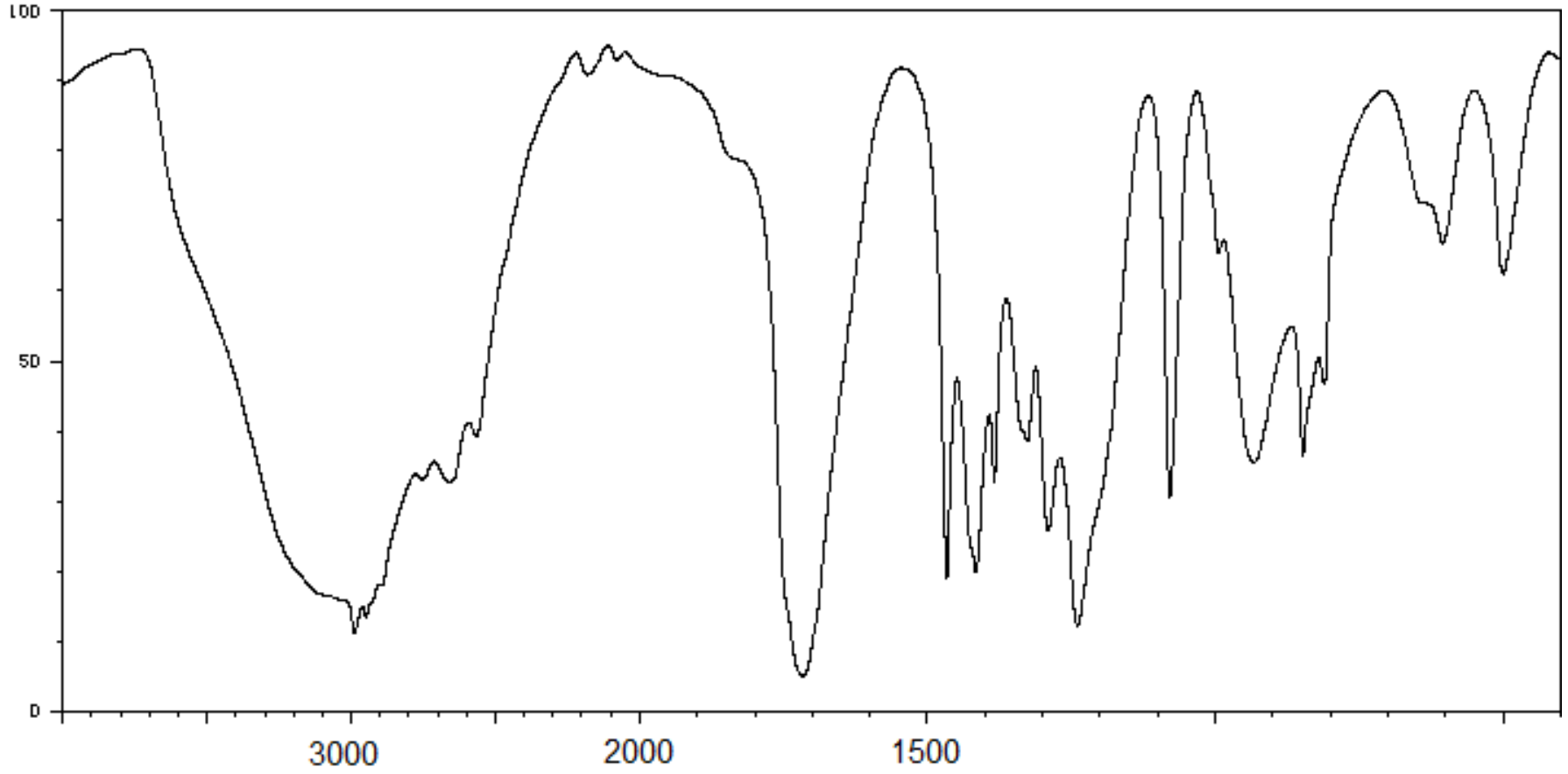
Navrhněte strukturu:



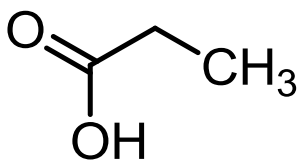


Nukleární magnetická rezonance ^{1}H, ^{13}C, IČ, MS

Navrhněte strukturu:

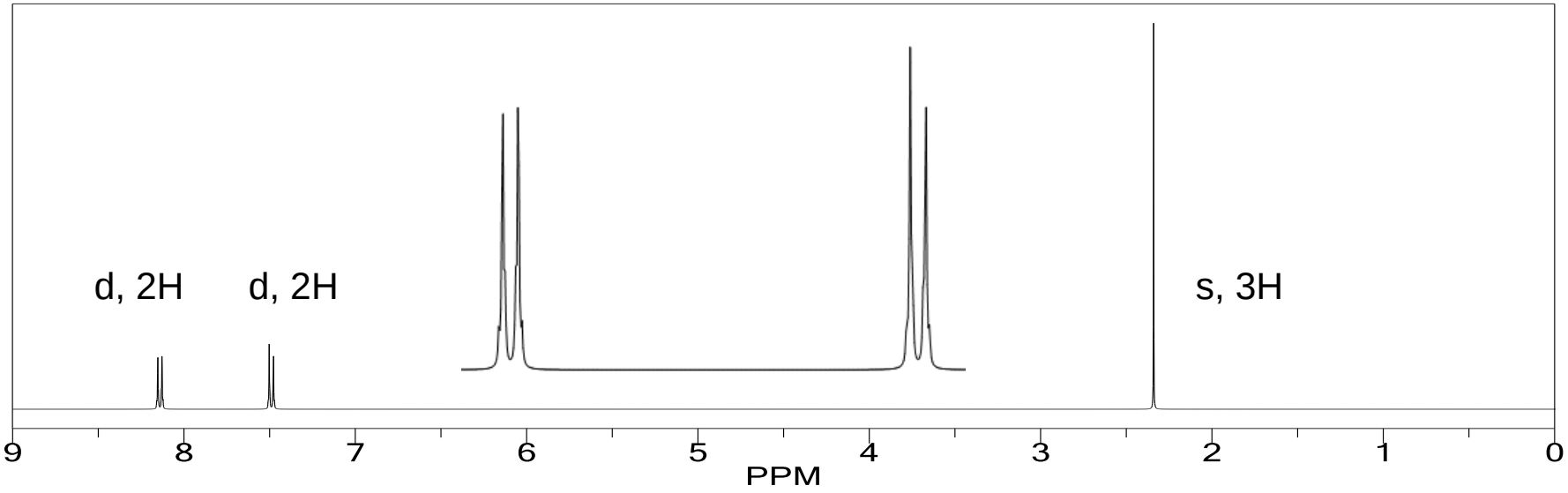


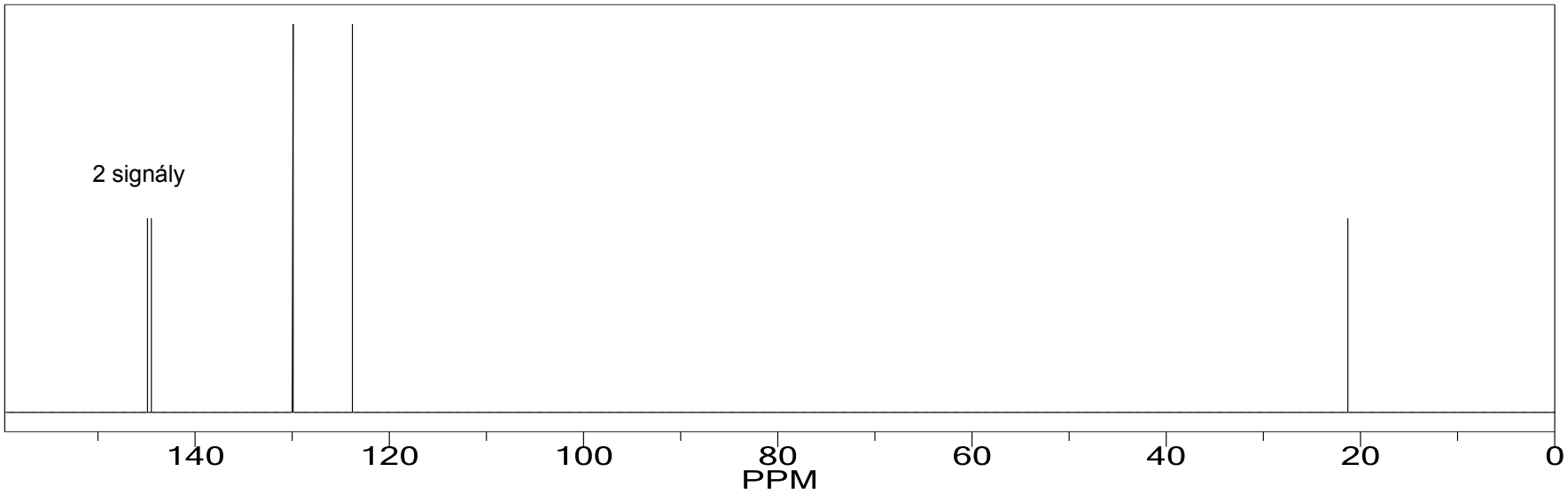
m/z: 74.04 (100.0 %), 75.04 (3.4 %)



Nukleární magnetická rezonance ^{1}H, ^{13}C, IČ, MS

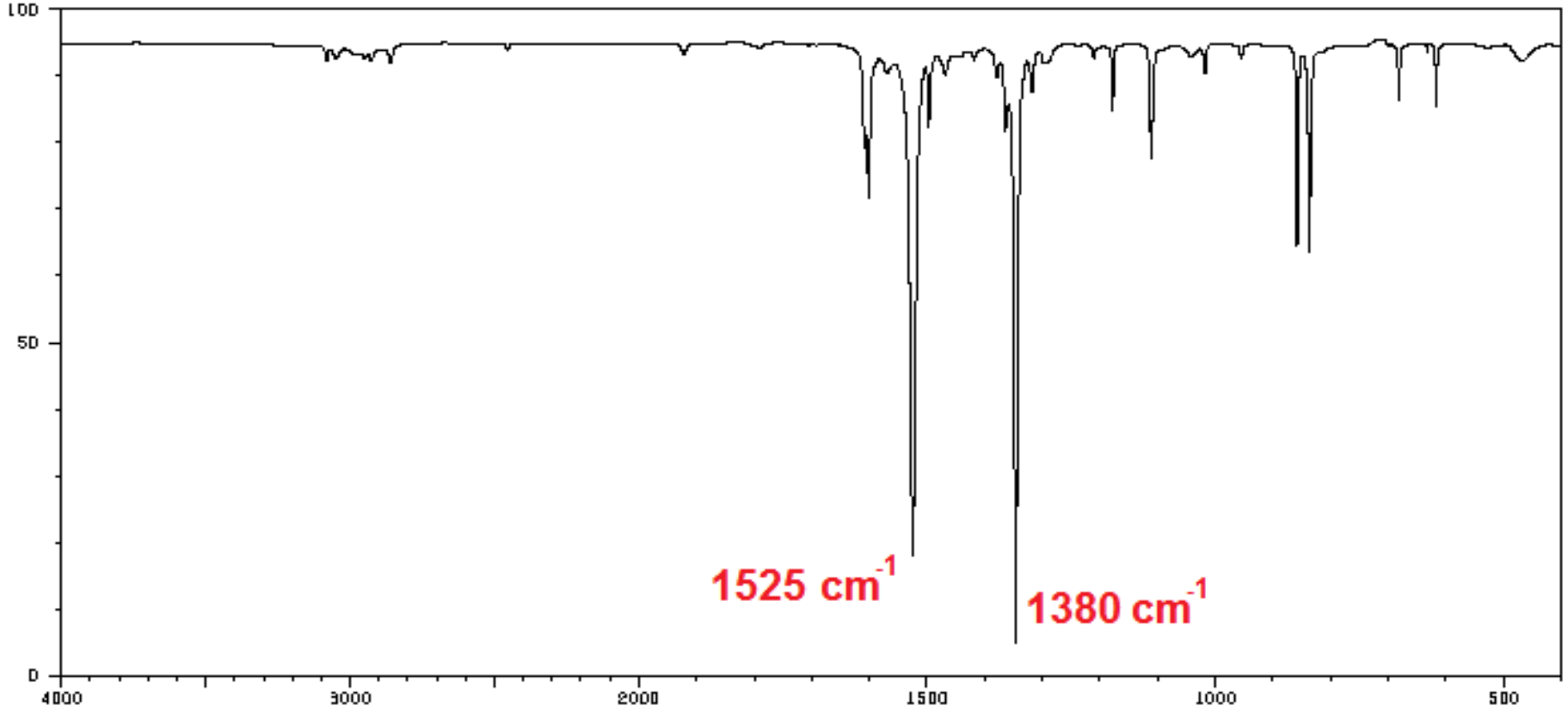
Navrhněte strukturu:





Nukleární magnetická rezonance ^{1}H, ^{13}C, IČ, MS

Navrhněte strukturu:



m/z: 137,05 (100,0 %), 138,05 (7,7 %)