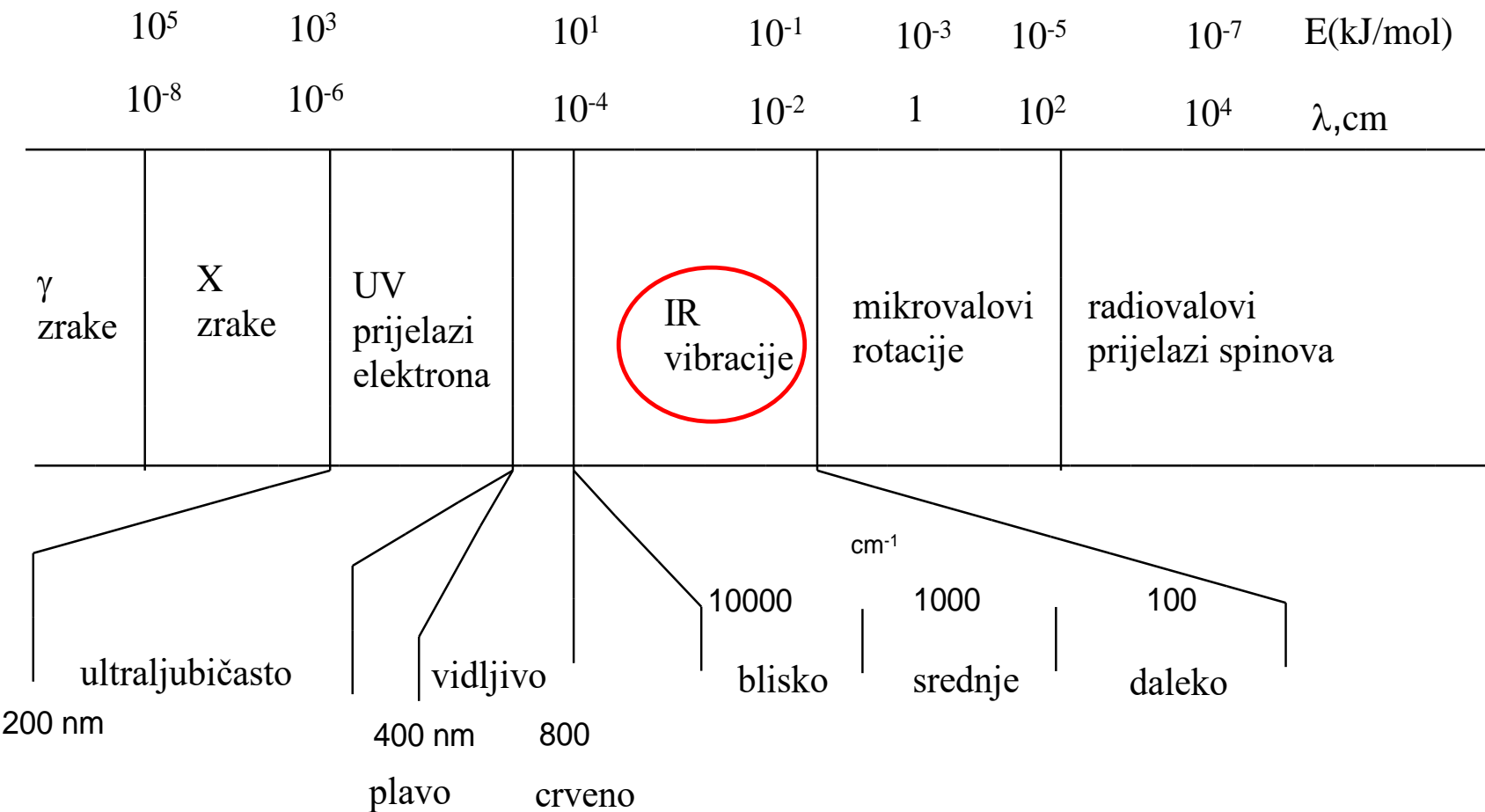


# Spektar elektromagnetnoga zračenja



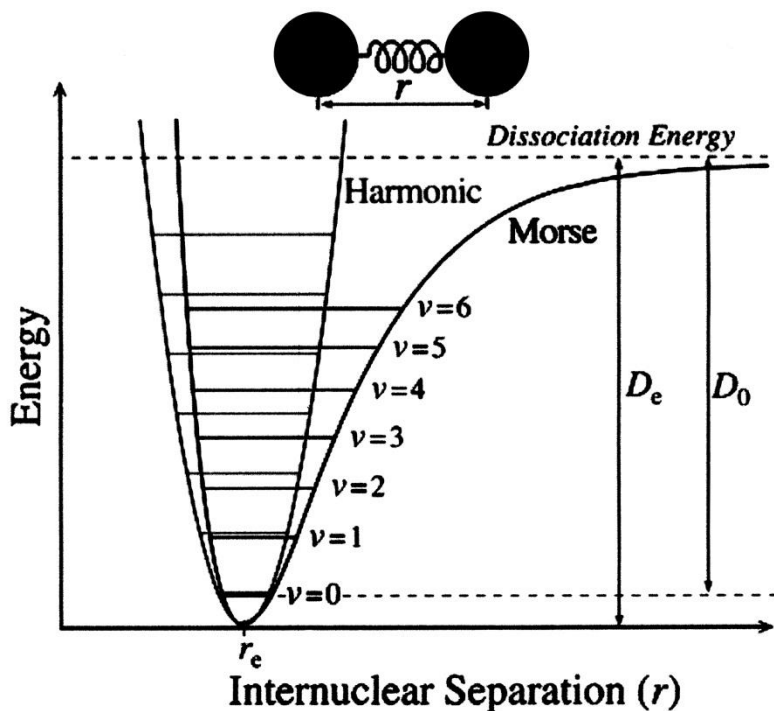
# Vibracijska spektroskopija

- Infracrvena spektroskopija (IR)
  - Apsorpcija, promjena dipolnog momenta
  - Srednji IR: temeljne ili osnovne vibracije
  - Bliski IR: gornji tonovi, složene (kombinirane) vibracije
- Ramanova spektroskopija
  - Neelastično raspršenje, promjena polarizabilnosti
  - Ramanov spektar: temeljne ili osnovne vibracije

# SPEKTROSKOPIJA IR

## PODRUČJA INFRACRVENOG ZRAČENJA

IR područje	$\lambda / \mu\text{m}$	$\tilde{\nu} / \text{cm}^{-1}$	$\nu / \text{Hz}$
Blisko	0,78 – 2,50	12 800 – 4 000	$3,8 \times 10^{14} - 1,2 \times 10^{14}$
Srednje	2,50 – 50	4 000 – 200	$1,2 \times 10^{14} - 6,0 \times 10^{12}$
Daleko	50 – 1 000	200 – 10	$6,0 \times 10^{12} - 3,0 \times 10^{11}$
Uobičajeno	2,50 – 25	4 000 – 400	$1,2 \times 10^{14} - 2,0 \times 10^{13}$



## IZBORNA PRAVILA ZA INFRACRVENE SPEKTRE

$$\delta\mu/\delta q \neq 0$$

$$\Delta V = \pm 1, \pm 2, \pm 3, \dots \text{ (neharmoničnost)}$$

Posljedica : mogućnosti kombinacija

a) gornji ili viši tonovi (harmonici)

$$2\nu_i, 3\nu_i \dots$$

b) kombinacije osnovnih vibracija

$$\nu_i + \nu_j \text{ ili } \nu_i - \nu_j$$

## IR

Apsorpcija

$$T = \frac{I}{I_0} (\%)$$

$$A = \log\left(\frac{I_0}{I}\right) = abc = \epsilon bc$$

## Raman

Raspršenje

linearni intenzitet

Stokes:  $h\nu' = h\nu_0 - h\nu_{\text{vib}}$

anti-Stokes:  $h\nu' = h\nu_0 + h\nu_{\text{vib}}$

### Izborna pravila (samo vibracije)

$$\frac{\partial\mu}{\partial q} \neq 0$$

$$\Delta\nu = \pm 1$$

$$\Delta\nu = \pm 1, \pm 2, \pm 3\dots$$

harmonično

neharmonično

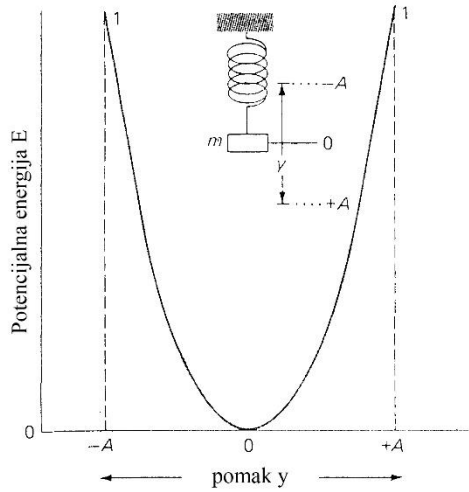
$$\frac{\partial\alpha}{\partial q} \neq 0$$

$$\Delta\nu = \pm 1$$

$$\Delta\nu = \pm 1, \pm 2, \pm 3\dots$$

### Pravilo uzajamnoga isključenja

## HARMONIČNI OSCILATOR



Klasično:

$$F = -ky = -k(r - r_e)$$

$$dE = -Fdy = kydy$$

$$\int_0^E dE = k \int_0^y ydy$$

$$E = \frac{1}{2}ky^2$$

$$F = ma$$

$$F = m \frac{\partial^2 y}{\partial t^2}$$

$$y = -\frac{m}{k} \frac{\partial^2 y}{\partial t^2}$$

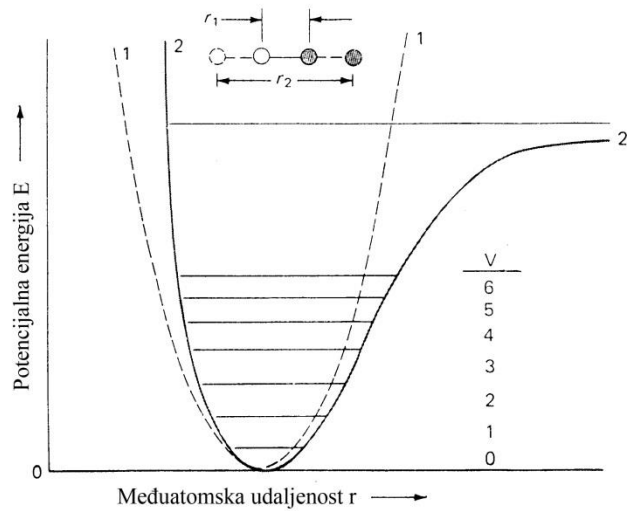
$$y = A \cos 2\pi vt$$

$$v = \frac{1}{2\pi} \sqrt{\frac{k}{m}}$$

$$v = \frac{1}{2\pi} \sqrt{\frac{k}{m}} = \frac{1}{2\pi} \sqrt{\frac{k(m_1 + m_2)}{m_1 m_2}}$$

Hookeov zakon

## NEHARMONIČNI OSCILATOR



Kvantno-mehanički:

$$E = (v + \frac{1}{2}) \frac{h}{2\pi} \sqrt{\frac{k}{\mu}}$$

$$E = (v + \frac{1}{2}) h\nu$$

$$\Delta E = h\nu = \frac{h}{2\pi} \sqrt{\frac{k}{\mu}}$$

$$v = \frac{h}{2\pi} \sqrt{\frac{k}{\mu}}$$

$$\tilde{\nu} = \frac{h}{2\pi c} \sqrt{\frac{k}{\mu}}$$

$$\Delta v = \pm 1$$

$$\Delta v = \pm 1, \pm 2, \dots$$

$$E_0 = \frac{1}{2} h\nu$$

$$E_1 = \frac{3}{2} h\nu$$

harmonični oscilator  
neharmonični oscilator

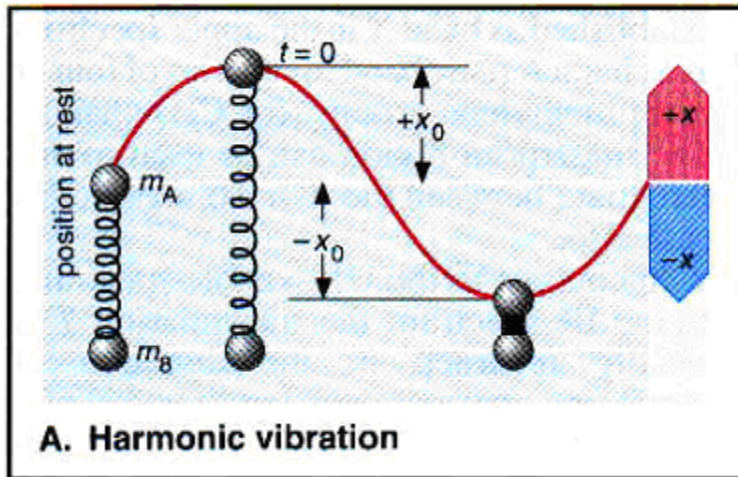
# SPEKTROSKOPIJA IR

područje:  $\bar{\nu} = 12800 - 10 \text{ cm}^{-1} \rightarrow \lambda = 0,78 - 1000 \text{ }\mu\text{m}$

podjela:

- blisko (NIR)
- srednje (2,5-50  $\mu\text{m}$ ; 4000-200  $\text{cm}^{-1}$ ) (MIR)
- daleko (FIR)

Hookeov zakon:  $F = -kx$



$$\nu = \frac{1}{2\pi} \sqrt{\frac{k}{\mu}} \quad \bar{\nu} = \frac{1}{2\pi c} \sqrt{\frac{k}{\mu}} \quad \mu = \frac{m_1 m_2}{m_1 + m_2}$$

konstanta sile veze:

- jednostruke:  $5 \times 10^2 \text{ N/m}$
- dvostruke:  $1 \times 10^3 \text{ N/m}$
- trostruke:  $1,5 \times 10^3 \text{ N/m}$

Ovisnost apsorpcijskog valnog broja o molarnoj energiji veze  $\Delta E_m$  i o masi atoma;

$k$  je pripadna konstanta sile veze\*

Veza	$\nu(\text{C}\cdots\text{X})$ $\text{cm}^{-1}$	$\Delta E_m$ $\text{kJ mol}^{-1}$	$k$ $\text{mdin } \text{Å}^{-1}$	Relativna atomska masa X	Veza	$\nu(\text{C}\cdots\text{C})$ $\text{cm}^{-1}$	$\Delta E_m$ $\text{kJ mol}^{-1}$	$k$ $\text{mdin } \text{Å}^{-1}$
-C-H	3000	420	4,8	1	-C $\equiv$ C-	2000	890	15,6
-C-C-	1000	370	4,5	12	C=C	1600	680	9,6
-C-Cl	700	335	3,6	35	-C-C-	1000	370	4,5

\*Pretvorbene faktori za uobičajene jedinice u jedinice SI jesu:  $1 \text{ mdin}/\text{Å} = 1 \text{ aJ}/\text{Å}^2 = 10^2 \text{ N/m}$ ;

$1 \text{ mdin} \cdot \text{Å} = 10^{-18} \text{ J} = 1 \text{ aJ}$ .

$N_{\text{viši}}/N_{\text{niži}} = \exp(-\Delta E/kT)$  Boltzmanova raspodijela

$$N_{v=1}/N_{v=0} = \exp\{-6.63 \times 10^{-34} \times 3 \times 10^{10} \times 10^3 / 1.38 \times 10^{-24} \times 300\}$$
$$\approx \exp(-4.8) \approx 0.008$$

napučenost  $v=1$  je približno 0.01 ili 1% od ukupne napučenosti osnovnog nivoa

prijelazi  $v = 1 \rightarrow v = 2, 3..$  se mogu zanemariti

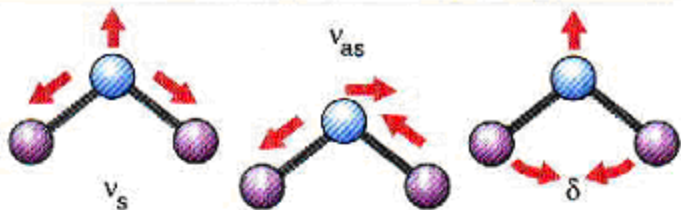
$v = 0 \rightarrow v = 1$ ,  $\Delta v = \pm 1$  fundamentalna (osnovna) vrpca

$v = 0 \rightarrow v = 2$ ,  $\Delta v = \pm 2$  prvi viši harmonik (prvi "overtone")

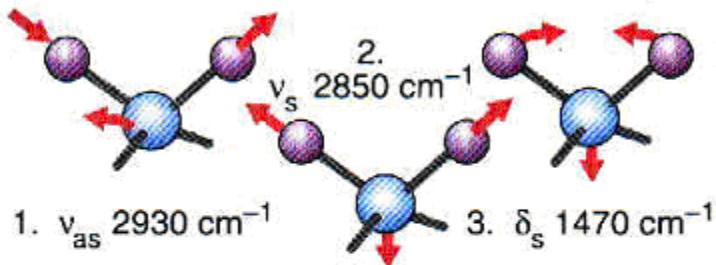
$v = 0 \rightarrow v = 3$ ,  $\Delta v = \pm 3$  drugi viši harmonik (drugi "overtone")

primjer HCl, vrpca kod  $2886 \text{ cm}^{-1}$  (jak intenzitet), vrpca kod  $5668 \text{ cm}^{-1}$  (slabiji intenzitet), vrpca kod  $8347 \text{ cm}^{-1}$  (vrlo slabi intenzitet)

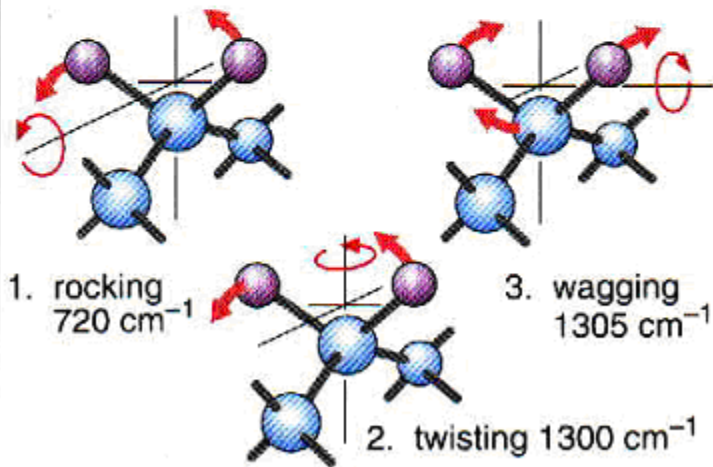




C. Natural vibration of a three-atom bent molecule



D. Normal vibrations of the CH<sub>2</sub> fragment



E. Bending vibrations of the CH<sub>2</sub> fragment in alkanes

## vibracije:

- rastezanje
- svijanje

## broj vibracija:

- linearne molekule:  $3N-5$
- nelinearne molekule:  $3N-6$

**uvjet IR-aktivnosti:**  
promjena dipolnog momenta

# VIBRACIJE VIŠEATOMNIH MOLEKULA

Broj temeljnih ili osnovnih vibracija

$3N - 5$  linearne molekule

$3N - 6$  nelinearne molekule

Sprege vibracija

- 1) vibracije koje se sprežu moraju biti iste simetrije
- 2) najača interakcija među vibracijama bliskih frekvencija (sličnih energija)
- 3) jaka sprega između vibracija rastezanja, ako dvije vibracije uključuju zajednički atom
- 4) sprega između vibracija savijanja, ako dvije vibracije uključuju zajedničku vezu
- 5) sprega između vibracija savijanja i rastezanja, ako je veza koja se rasteže sastavni dio kuta koji se savija
- 6) slaba sprega ako su vibracije odvojene s više od dvije veze

## DEFINICIJA SKUPINSKE VIBRACIJE

1. Vibracija čija se vrpca uvijek nalazi u spektru molekule koja sadrži dotičnu funkcionalnu skupinu, te se nalazi u uskom području spektra
  - a) ponekad izostaje ovaj dvostruki uvijet
  - b) postoje IR i Ramanove skupinske vibracije, najčešće komplementarne (ako je jedna jaka druga je slaba)
2. Frekvencija vibracije je približno ista za svaku molekulu koja sadrži tu skupinu zbog oblika vibracije tj. načina gibanja atoma
3. Skupinska vibracija i nena frekvencija određuju se empirijski proučavanjem spektara srodnih molekula

Poželjne značajke skupinske vibracije:

- usko područje  $\pm 30 \text{ cm}^{-1}$
- intenzivna vrpca
- točan položaj
- jedinstvena vrpca
- pouzdana vrpca

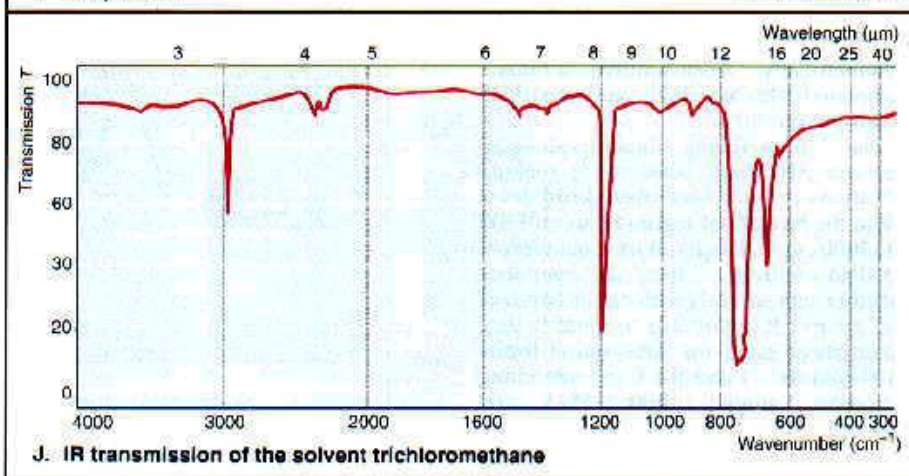
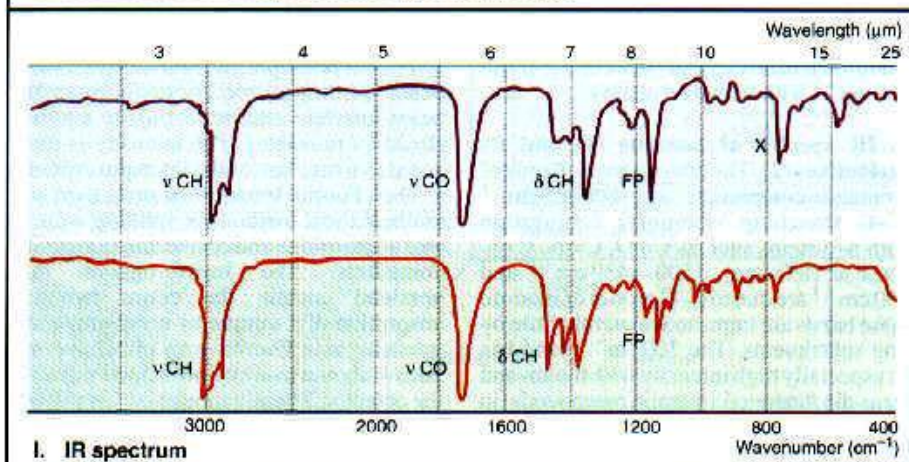
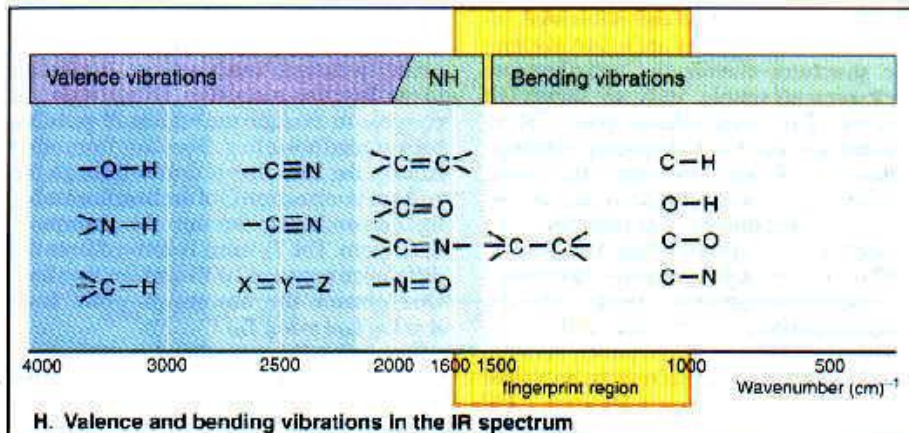
# INTERPRETACIJA INFRACRVENIH I RAMANOVIH SPEKTARA

## SKUPINSKE VIBRACIJE

1. Karakteristične za skupine atoma:  $-\text{CH}_2$ ,  $-\text{CH}_3$ ,  $-\text{C}\equiv\text{N}$ ,  $-\text{NO}_2$ ,  $-\text{C}_6\text{H}_5$ ,  $-\text{OH}$ .....
2. Ove su vibracije uglavnom lokalizirane unutar skupine

## OTISAK PRSTIJU

1. Karakteristične za specifičnu molekulu
2. Vibracije molekule kao cjeline
3. Brojčane vrijednosti frekvencija ne mogu se predvidjeti empirijski
4. Važne za karakterizaciju molekule



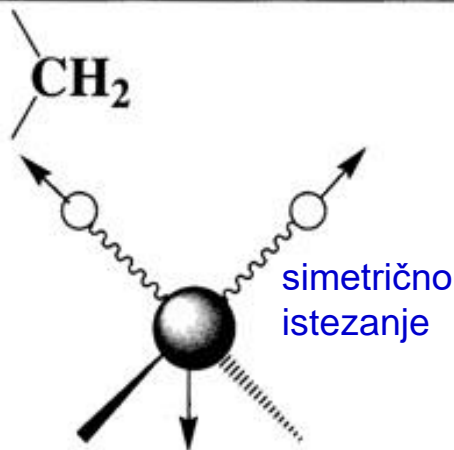
⇒ funkcijske skupine

⇒ **heksan-2-on:**  
 $(\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{COCH}_3)$

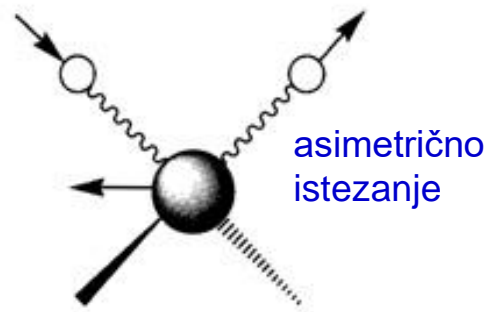
⇒ **heksan-3-on:**  
 $(\text{CH}_3\text{CH}_2\text{CH}_2\text{COCH}_2\text{CH}_3)$

⇒ otapalo

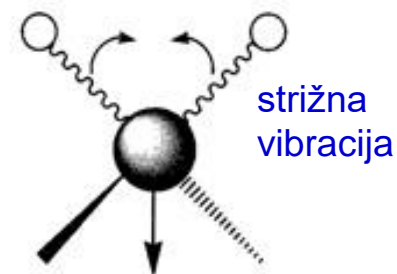
# Koncept skupinskih vibracija -karakteristične vibracije u spektru IR



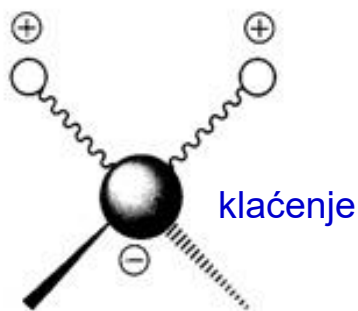
Symmetrical  
stretching ( $\nu_s$  CH<sub>2</sub>)  
~2853 cm<sup>-1</sup>



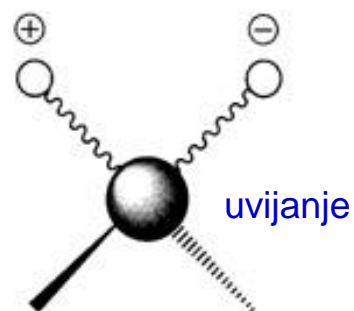
Asymmetrical  
stretching ( $\nu_{as}$  CH<sub>2</sub>)  
~2926 cm<sup>-1</sup>



In-plane bending  
or scissoring ( $\delta_s$  CH<sub>2</sub>)  
~1465 cm<sup>-1</sup>



Out-of-plane bending  
or wagging ( $\omega$  CH<sub>2</sub>)  
1350-1150 cm<sup>-1</sup>

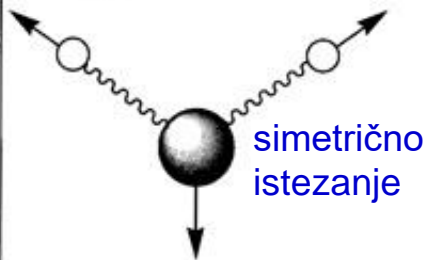


Out-of-plane bending  
or twisting ( $\tau$  CH<sub>2</sub>)  
1350-1150 cm<sup>-1</sup>

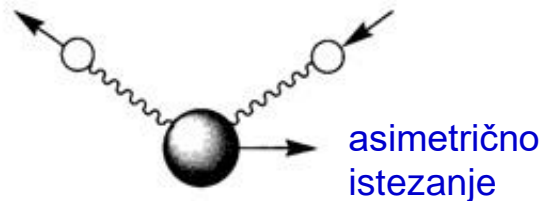


In-plane bending  
or rocking ( $\rho$  CH<sub>2</sub>)  
~720 cm<sup>-1</sup>

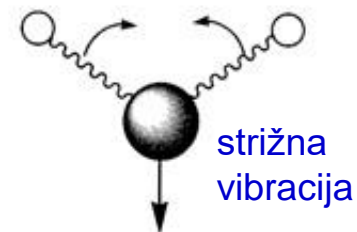
**H<sub>2</sub>O**



Symmetrical stretching ( $\nu_s$  OH)  
3652 cm<sup>-1</sup>



Asymmetrical stretching ( $\nu_{as}$  OH)  
3756 cm<sup>-1</sup>



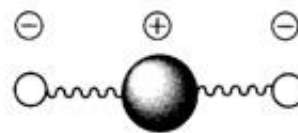
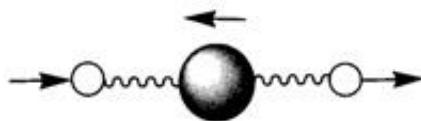
Scissoring ( $\delta_s$  OH)  
1596 cm<sup>-1</sup>

**CO<sub>2</sub>**



(1) Symmetrical stretching ( $\nu_s$  CO<sub>2</sub>)  
1340 cm<sup>-1</sup>

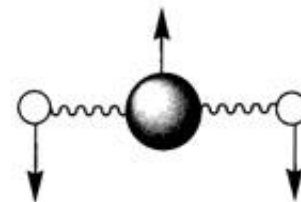
asimetrično istežanje  
(2) Asymmetrical stretching ( $\nu_{as}$  CO<sub>2</sub>)  
2350 cm<sup>-1</sup>



(3) Scissoring (bending) ( $\delta_s$  CO<sub>2</sub>)  
665 cm<sup>-1</sup>

strižna vibracija

(4) Scissoring (bending) ( $\delta_s$  CO<sub>2</sub>)  
665 cm<sup>-1</sup>

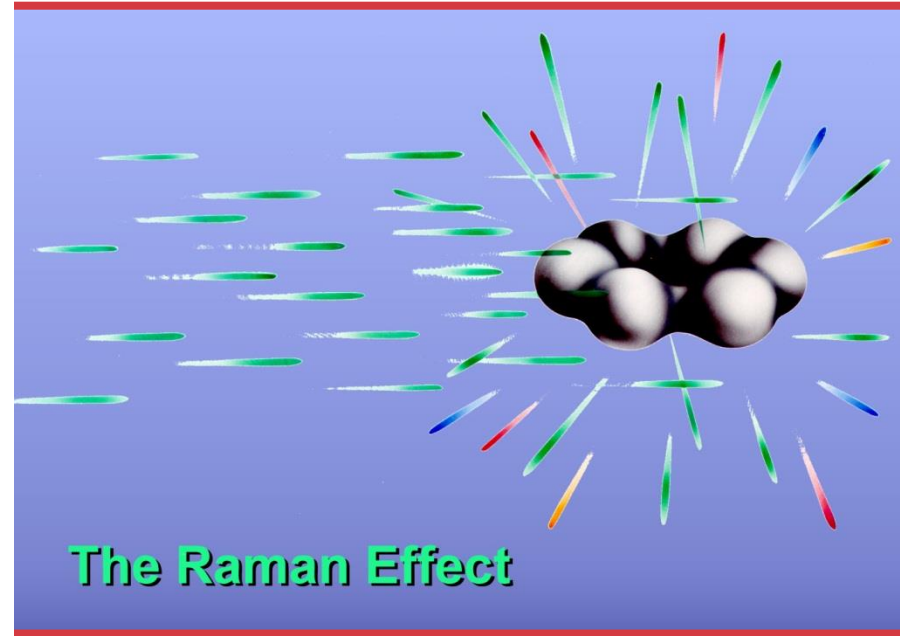


# RAMANOV EFEKT

Osvijetliti (ozračiti) uzorak **monokromatskim zračenjem** (npr. laserska svjetlost valne duljine od 300 do 1064 nm)

Promatrati sljedeće fizikalne efekte:

1. Glavni dio zračenja obasjava uzorak bez interakcije
2. Oko  $10^{-4}$  zračenja raspršuje se elastično, tj. bez interakcije  
– **Raleighovo zračenje**
3. Dio zračenja se putem elektronskih prijelaza apsorbira i emitira kao **fluorescencija**
4. Samo oko  $10^{-8}$  upadnoga zračenja se raspršuje neelastično, pri čemu se odvija energijski prijelaz – **Ramanov spektar**

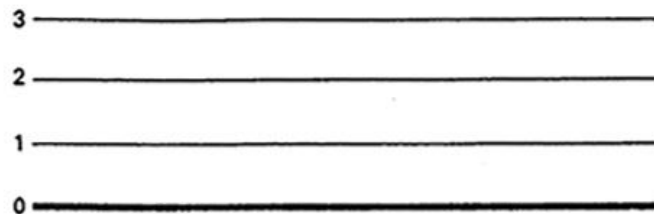




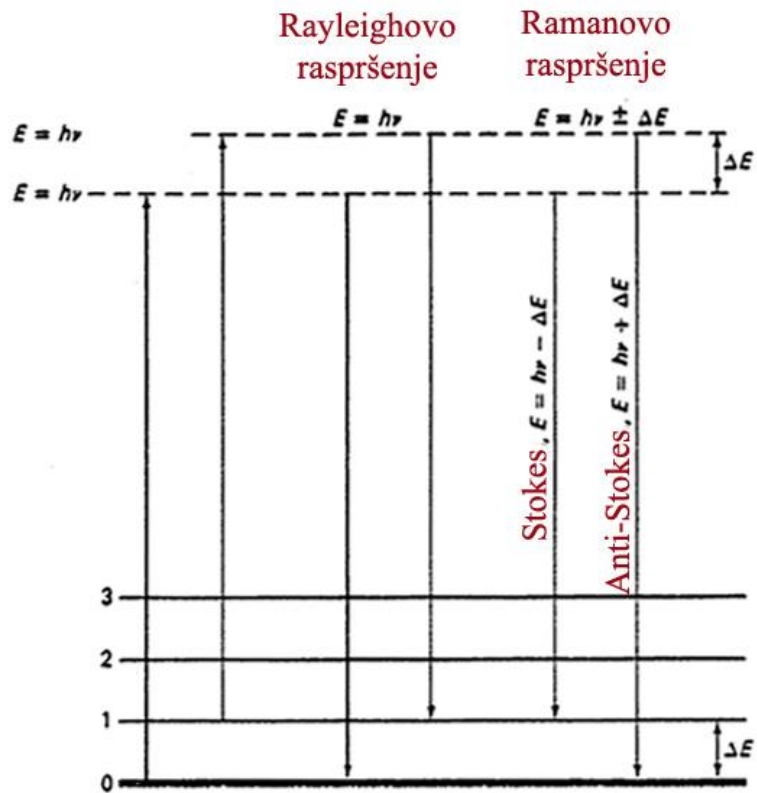
# Ramanova spektroskopija

$$\delta\alpha/\delta r \neq 0$$

najniže  
pobuđeno elektronsko  
stanje



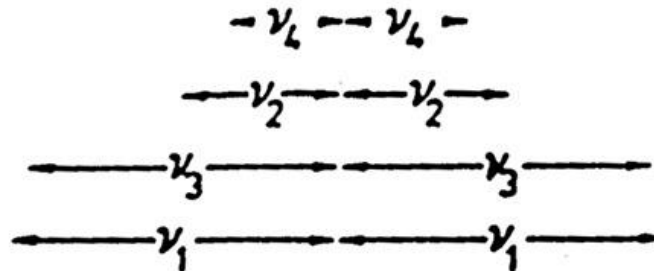
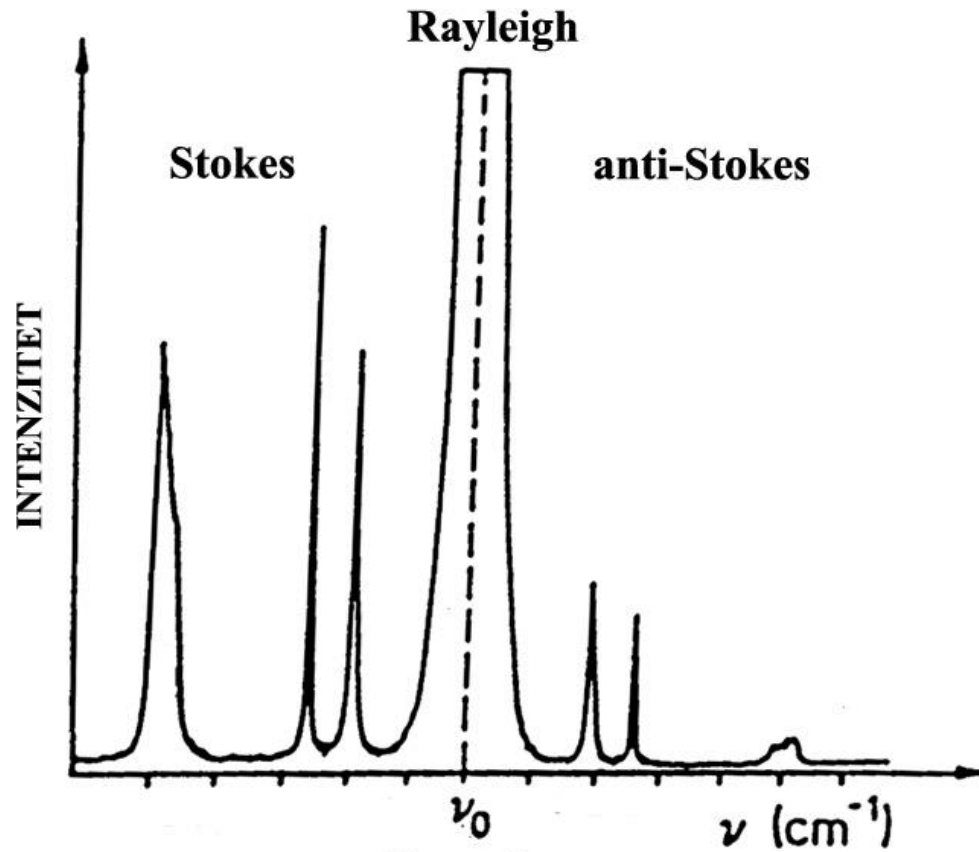
virtuelna stanja



osnovno  
elektronsko  
stanje



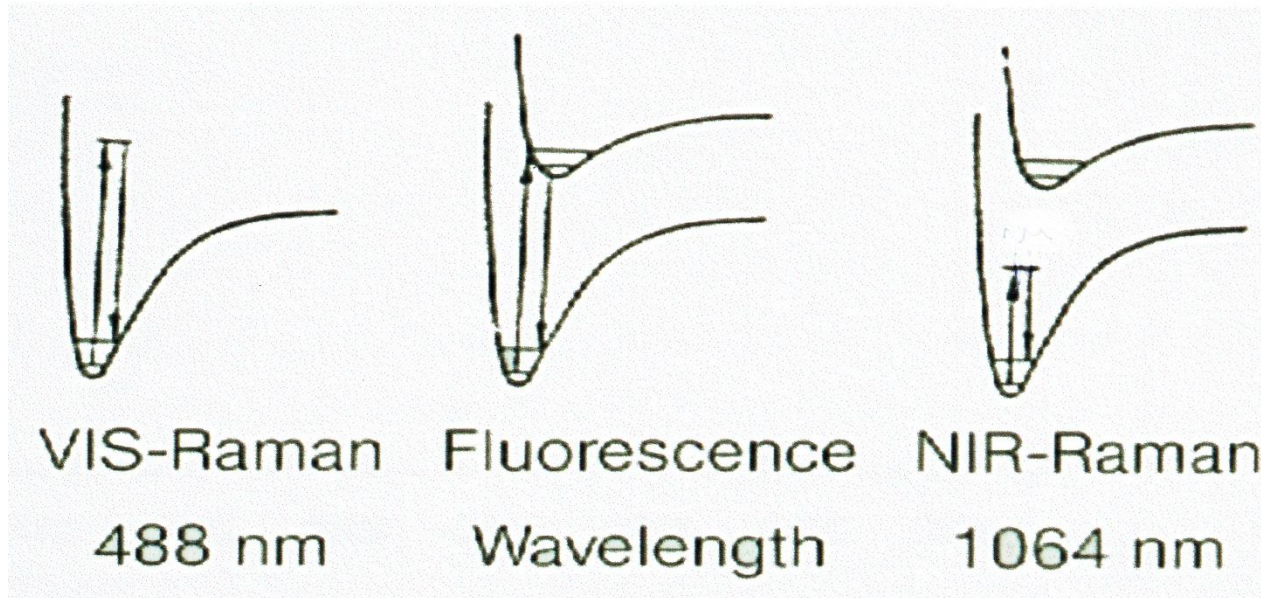
pobuda:  $\lambda = 488 \text{ nm}$



Ramanov pomak

$\Delta \nu_i \text{ (cm}^{-1}\text{)}$

## Zašto NIR-Raman?



Nd-YAG laser  
1064 nm

Ar 488 nm

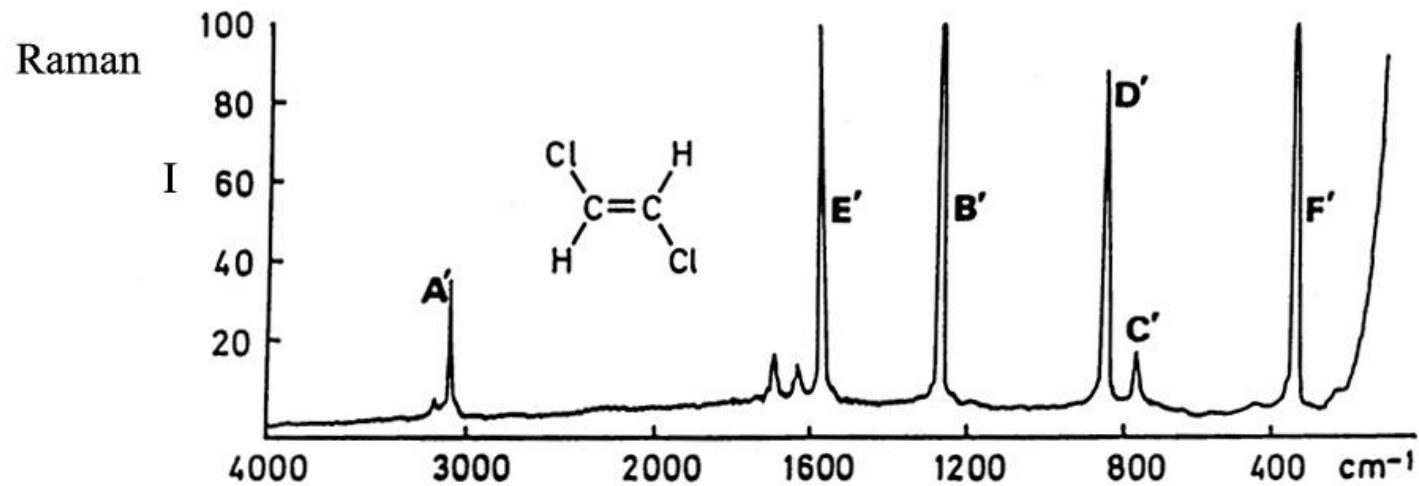
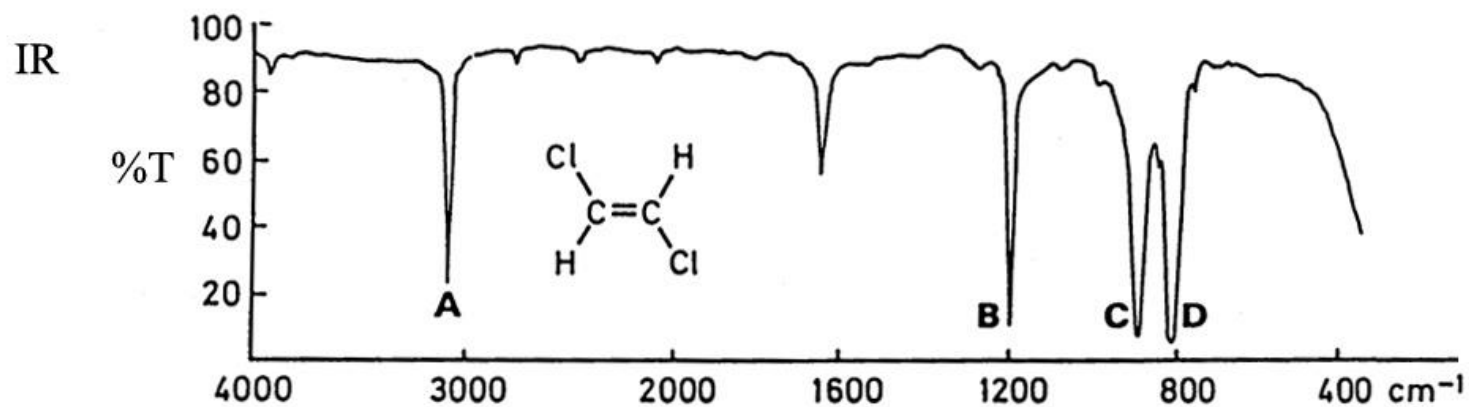
He-Ne 632 nm

Diodni laseri 782 i 830 nm

# Najčešće vrste Ramanove spektroskopije

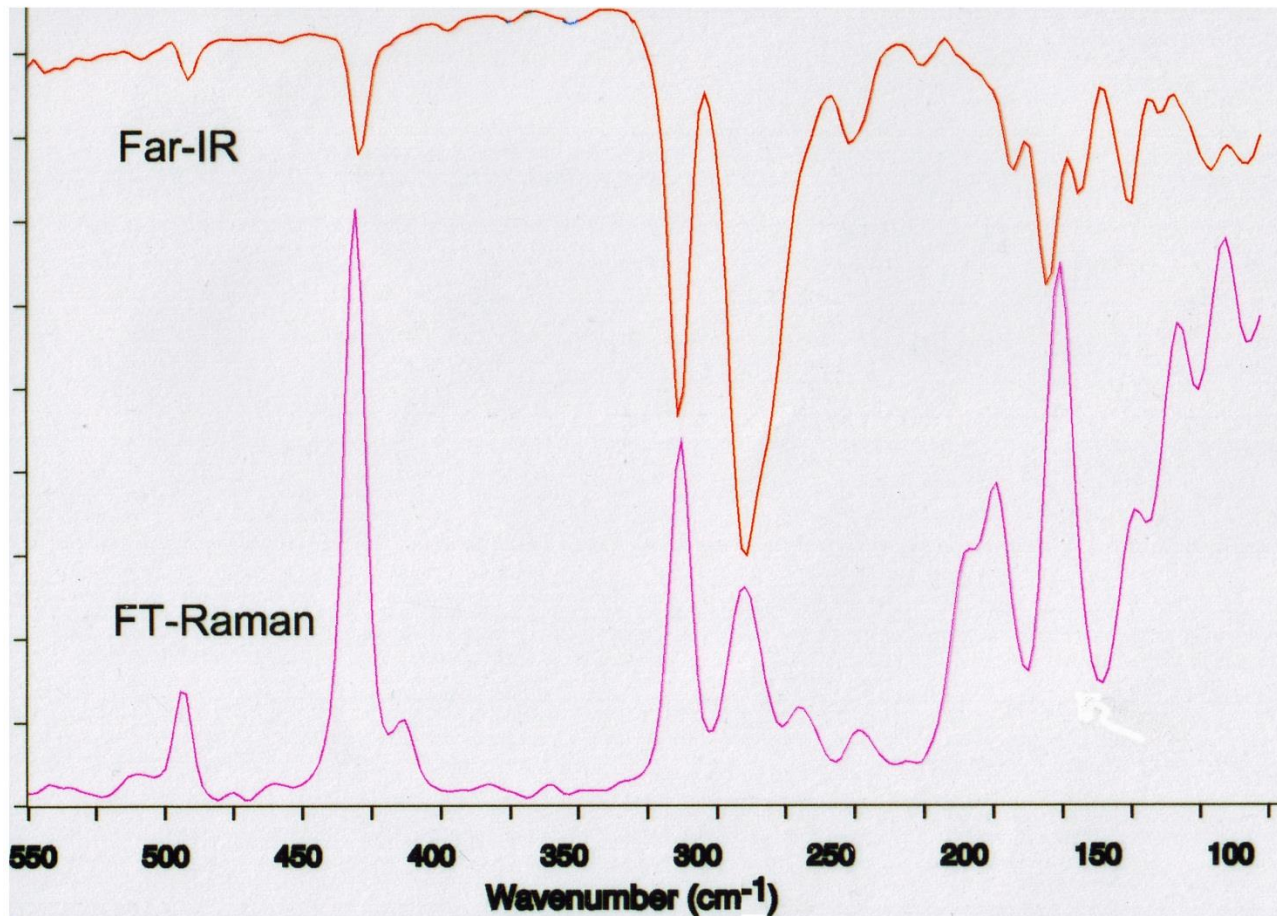
- FT Ramanova spektroskopija
- Disperzna Ramanova spektroskopija
- Rezonantna Ramanova spektroskopija
- Površinski pojačana Ramanova spektroskopija (SERS-Surface enhanced Raman spectroscopy)
- Površinski pojačana rezonantna Ramanova spektroskopija (SERRS)
- Nelinearna Ramanova spektroskopija- CARS (koherentna anti-Stokesova ramanova spektroskopija)
- Ramanova optička aktivnost (ROA)

# Pravilo isključenja



Način vibracije	asimetričan način vibracije (IR-aktivan)	IR-vrpca (cm <sup>-1</sup> )	simetričan način vibracije (Raman-aktivan)	Ramanova vrpca (cm <sup>-1</sup> )
$\nu$ (C—H)		3090 (A)		3070 (A')
$\nu$ (C—Cl)		817 (D)		844 (D')
$\delta$ (C—H)		1200 (B)		1270 (B')
$\gamma$ (C—H)		895 (C)		760 (C')
$\nu$ (C=C)	-	-		1576 (E')
$\delta$ (C—Cl)	< 300 cm <sup>-1</sup>	-		350 (F')

Uzorak: kompleks bakra



Komplementarne informacije

# VIBRACIJSKE FREKVENCije VEZA X-H/cm<sup>-1</sup>

## ELEKTRONEGATIVNOST X

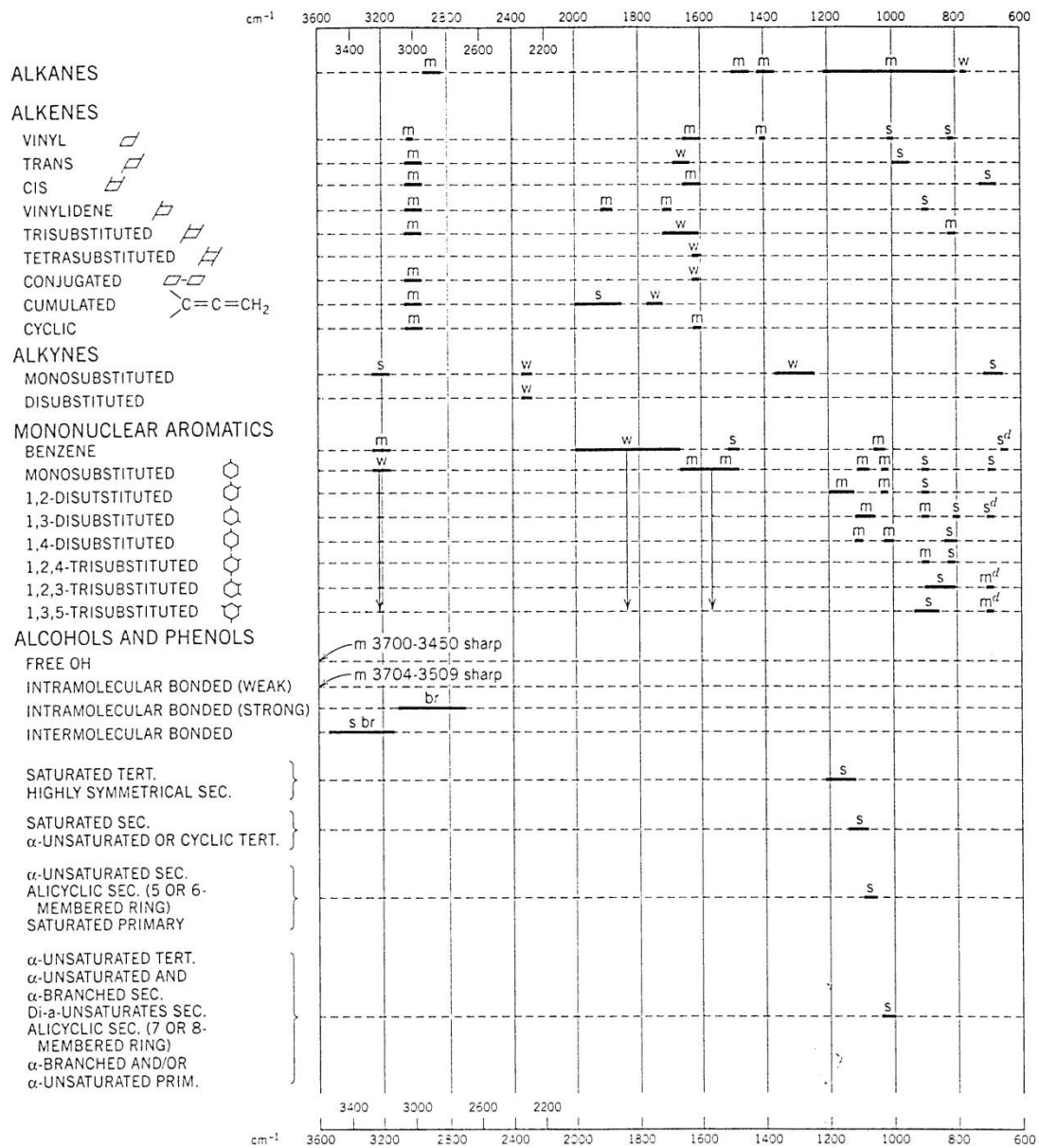
M A S A X	BH 2500	CH 3000	NH 3400	OH 3600	FH 3960	E L E K T R O N E G I V N O S T X
	AlH 1820	SiH 2150	PH 2350	SH 2570	ClH 2890	
		GeH 2070	AsH 2150	SeH 2300	BrH 2560	
		SnH 1850	SbH 1890		IH 2230	

MASA X

## USPOREDBA INTENZITETA NEKIH VIBRACIJA

IR	jak	slab	jak
Raman	slab	jak	jak
	C-F rast.	C≡C rast.	C≡N rast.
	O-H rast.	C=C rast.	C=O rast.
	N-H rast.	C-C rast.	C-Cl rast.
	C-H rast.	S-H rast.	NO <sub>2</sub> rast.
		C=S rast.	
		C-S rast.	
		S-S rast.	
		CH <sub>2</sub> uv. ili njih.	



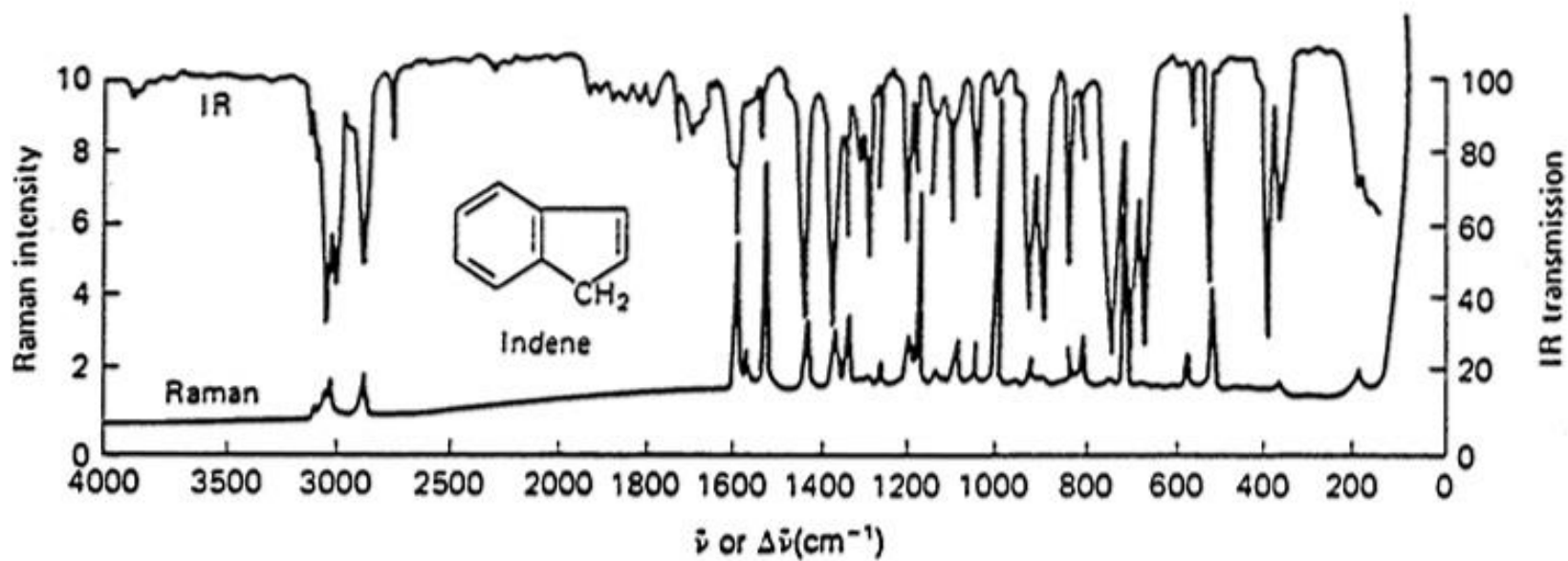
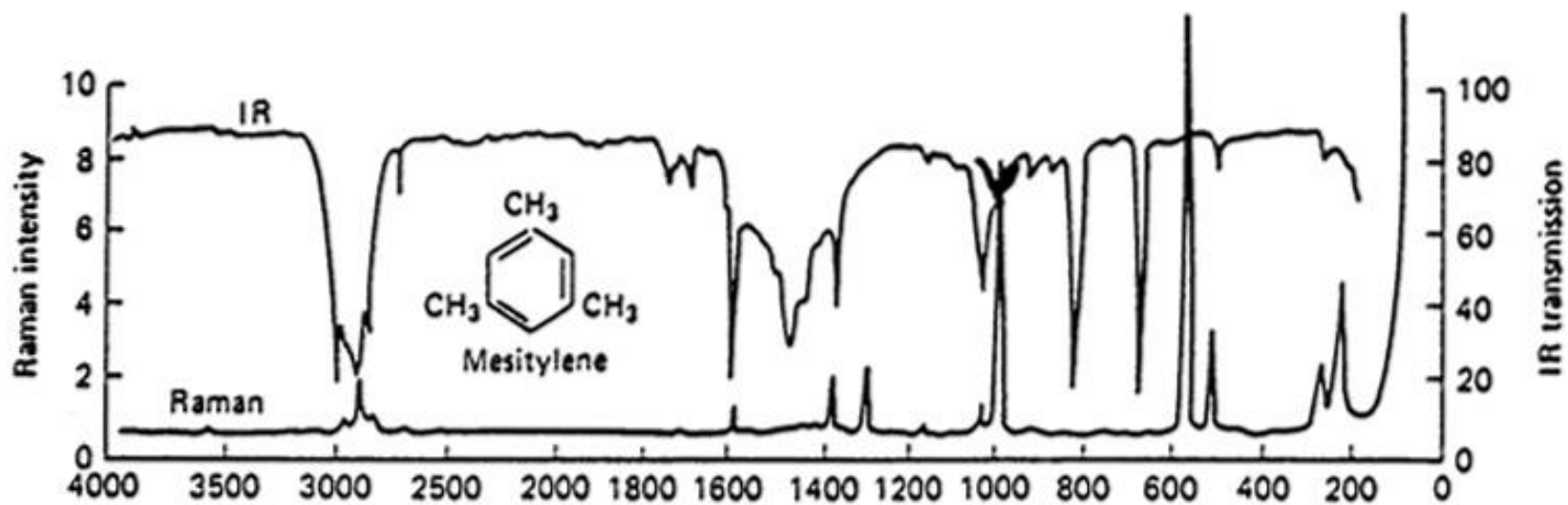


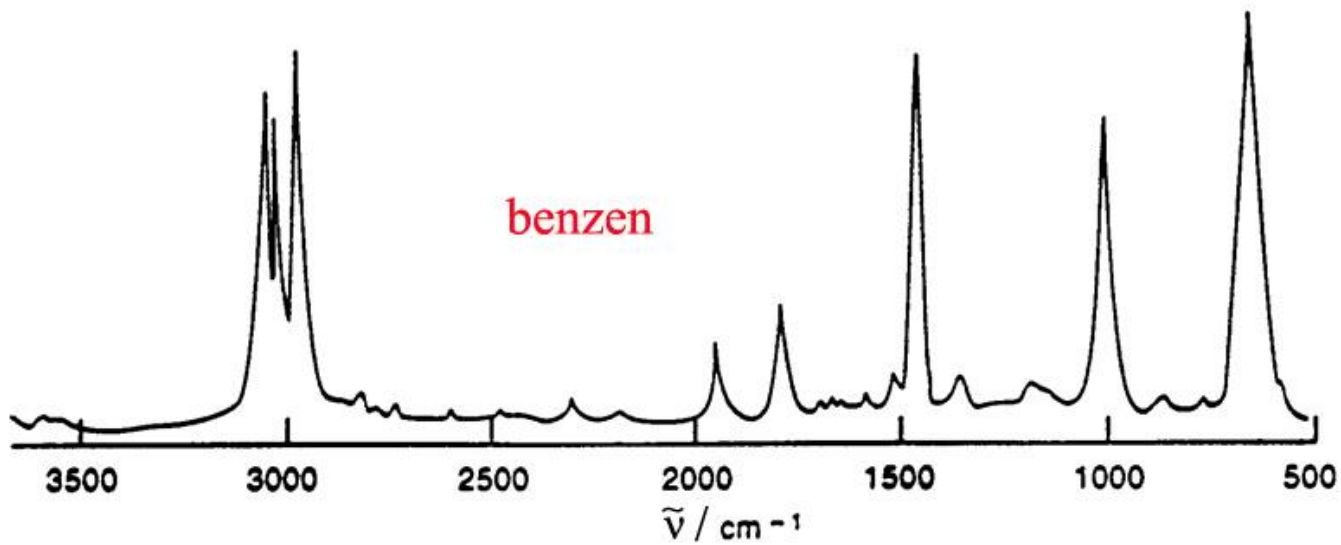
\* Absorptions are shown by heavy bars. s = strong, m = medium, w = weak, sh = sharp, br = broad. Two intensity designations over a single bar indicate that two peaks may be present.

<sup>b</sup> May be absent.

<sup>c</sup> Frequently a doublet.

<sup>d</sup> Ring bending bands.





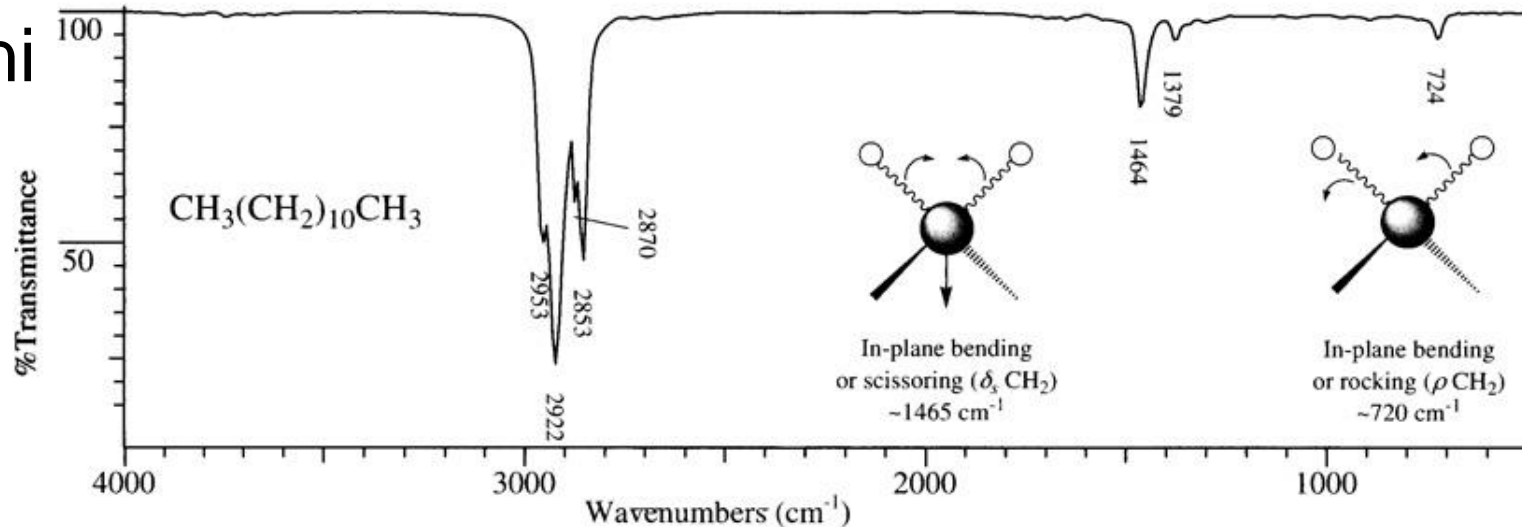
# Primjena IR spektroskopije

- **NIR :**
  - Kvantitativna analiza uzoraka u industriji (udio vode, fenola, alkohola...) i analiza plinovitih smjesa
- **MID-IR :**
  - Kvalitativna analiza čvrstih, tekućih i plinovitih uzoraka
  - Kvantitativna analiza
  - U sprezi s kromatografijom, LC-IR, analiza smjese spojeva
- **FAR-IR :**
  - Kvalitativna analiza anorganskih spojeva i organometalnih spojeva

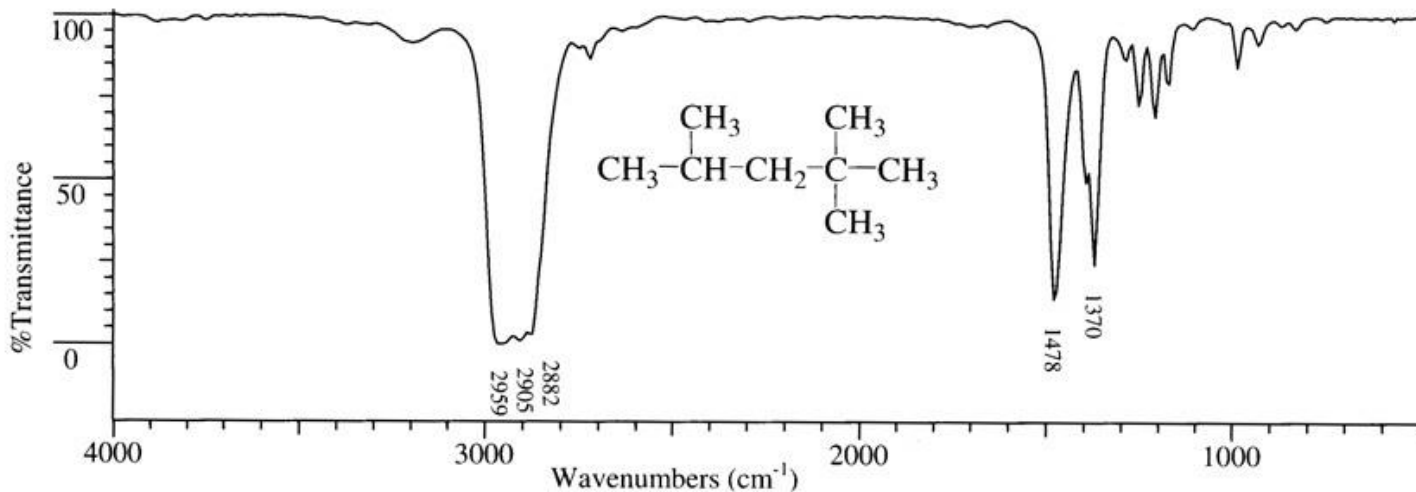
# Primjena Ramanove spektroskopije

- Kvalitativna i kvantitativna analiza uzoraka u vodenoj otopini
- Analiza anorganskih spojeva: veze metal-ligand (100-700  $\text{cm}^{-1}$ ), koordinacijski spojevi ((halogenidni i oksikompleksi s metalima, npr.  $\text{VO}_4^{3-}$ ,  $\text{Al}(\text{OH})_4^-$ ))
- Analiza organskih spojeva: olefini, cikloalkani (veličina prstena)
- Analiza bioloških uzoraka

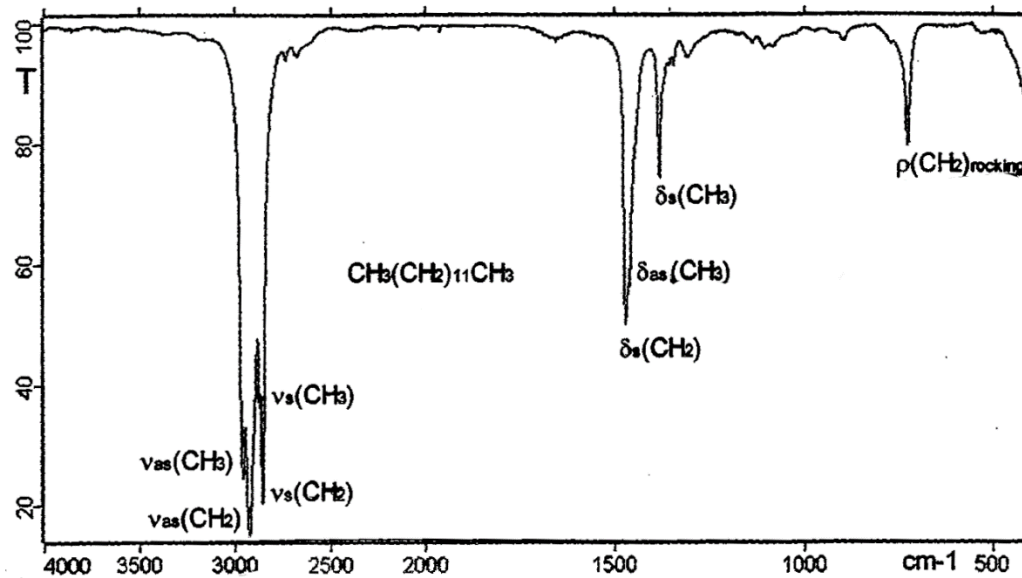
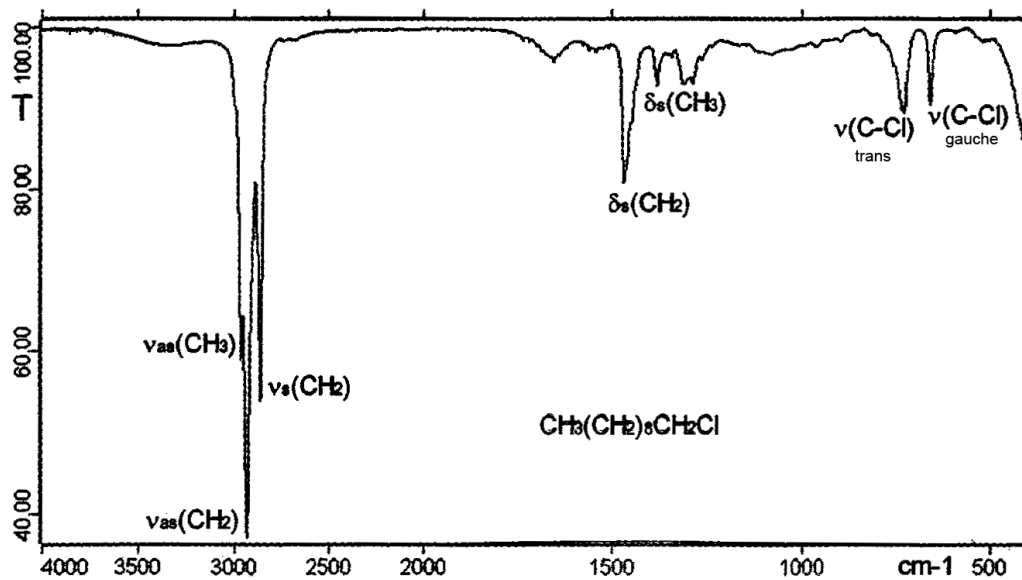
alkani



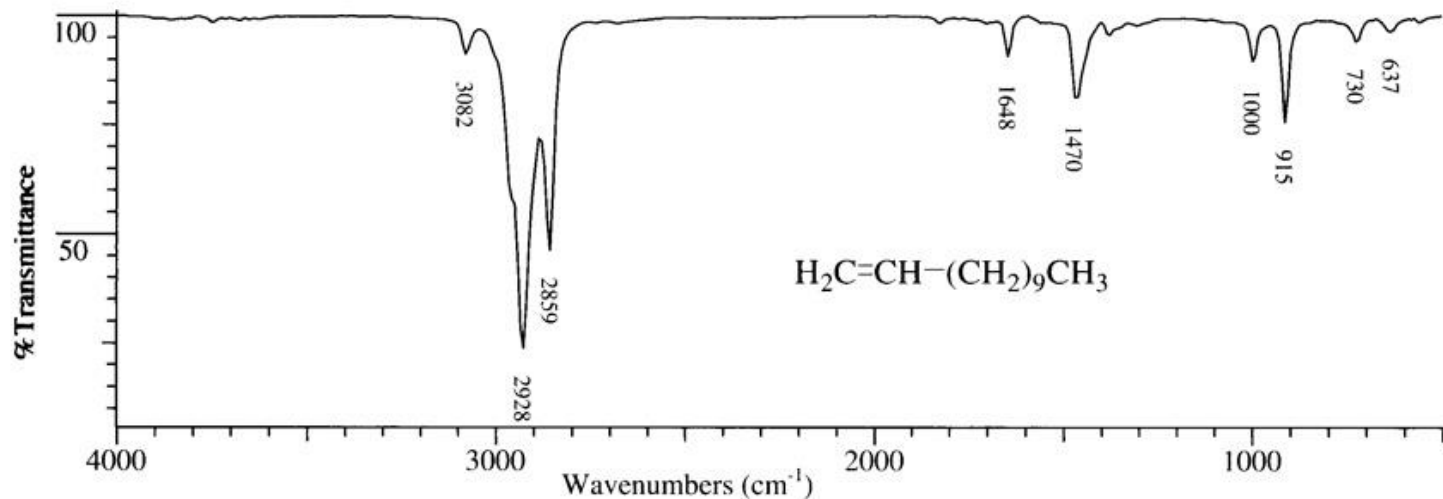
Dodecane. C—H stretch: 2953 cm<sup>-1</sup>  $\nu_{as}$ CH<sub>3</sub>, 2870 cm<sup>-1</sup>  $\nu_s$ CH<sub>3</sub>, 2922 cm<sup>-1</sup>  $\nu_{as}$ CH<sub>2</sub>, 2853 cm<sup>-1</sup>  $\nu_s$ CH<sub>2</sub>.  
C—H bend: 1464 cm<sup>-1</sup>  $\delta_s$ CH<sub>2</sub>, 1450 cm<sup>-1</sup>  $\delta_{as}$ CH<sub>3</sub>, 1379 cm<sup>-1</sup>  $\delta_s$  CH<sub>3</sub>. CH<sub>2</sub> rock: 724 cm<sup>-1</sup>  $\rho$  CH<sub>2</sub>.



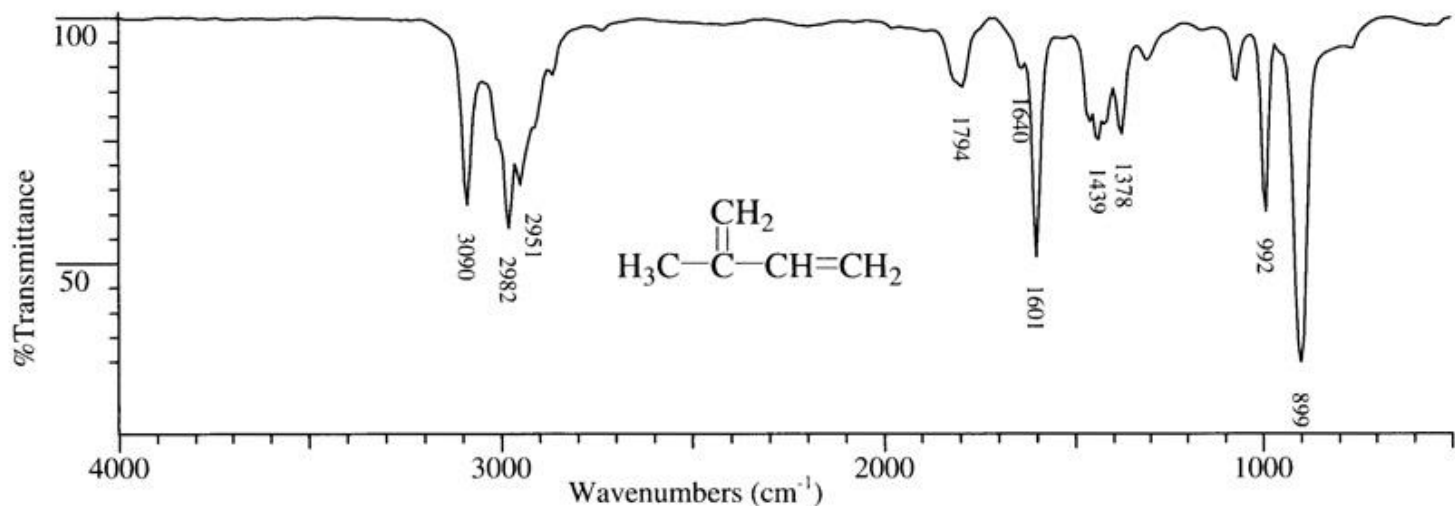
2,2,4-Trimethylpentane. C—H stretch. C—H bend. There are overlapping doublets for the *t*-butyl and the isopropyl groups at 1400–1340 cm<sup>-1</sup>.



alkeni



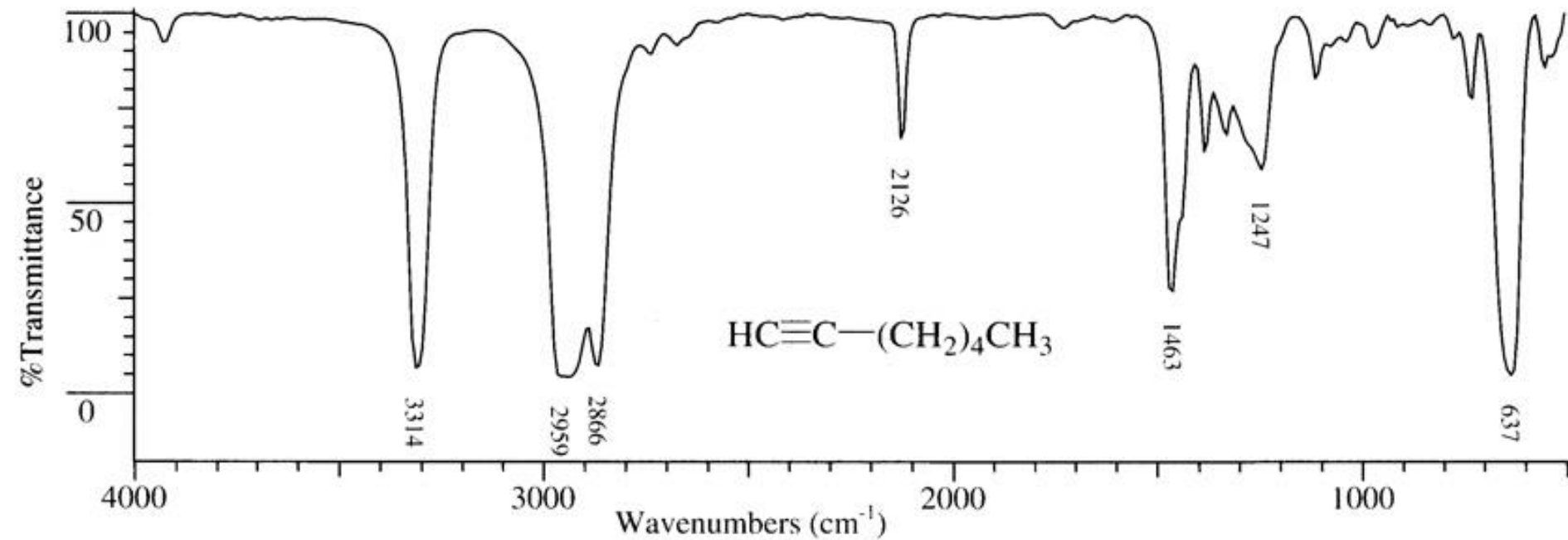
1-Dodecene. C—H stretch. Note alkene C—H stretch at 3082 cm<sup>-1</sup>. C=C stretch, 1648 cm<sup>-1</sup>. Out-of-plane C—H bend: 1000 cm<sup>-1</sup>, (alkene) 915 cm<sup>-1</sup>. Methylene rock: 730 cm<sup>-1</sup>.



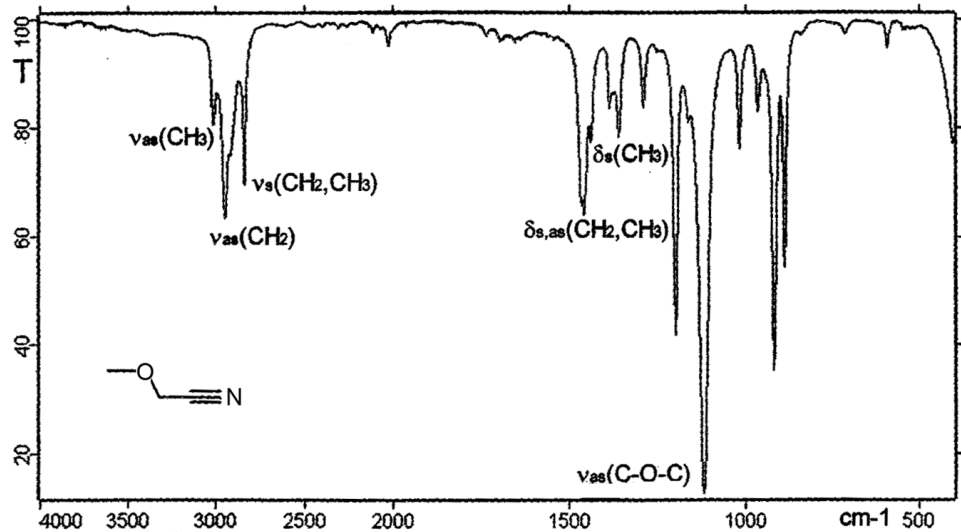
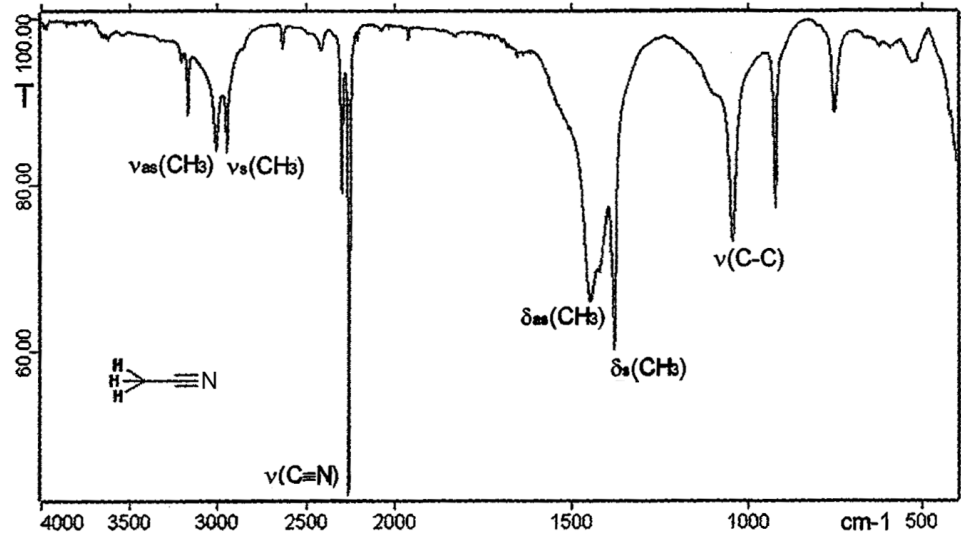
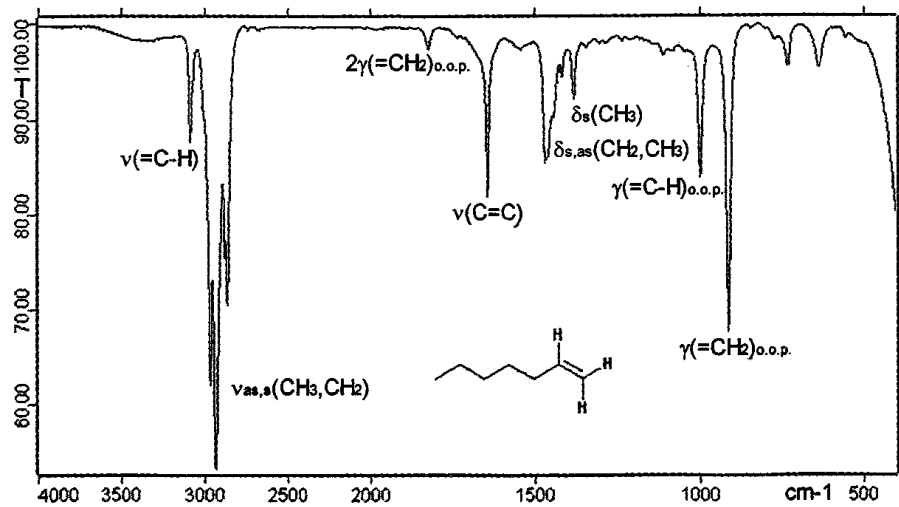
Isoprene. C—H stretch: =C—H 3090 cm<sup>-1</sup>. Coupled C=C—C=C stretch: symmetric 1640 cm<sup>-1</sup> (weak), asymmetric 1601 cm<sup>-1</sup> (strong). C—H bend (saturated, alkene in-plane). C—H out-of-plane bend: 992 cm<sup>-1</sup>, 899 cm<sup>-1</sup>.

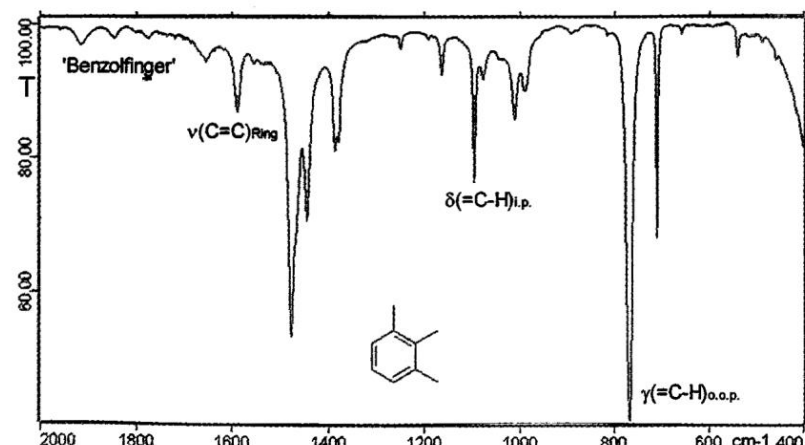
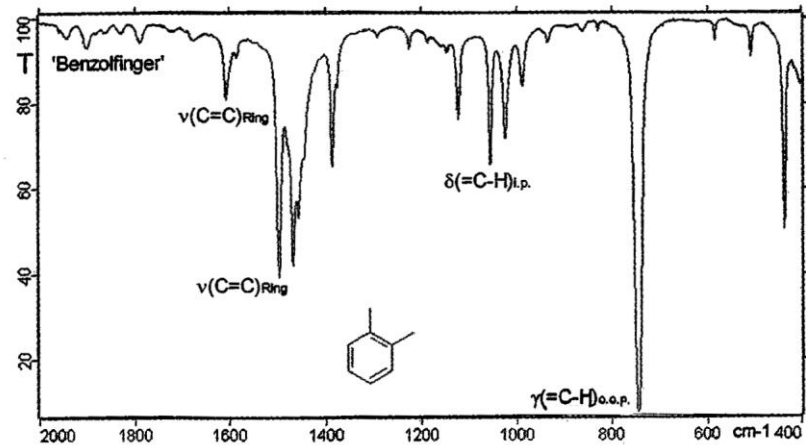
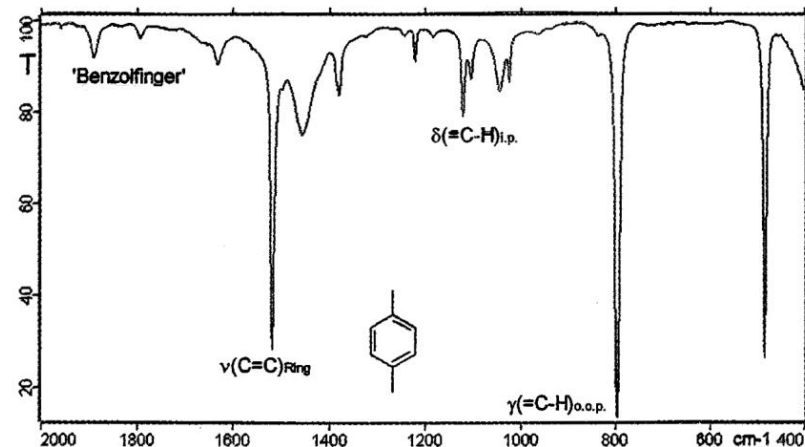
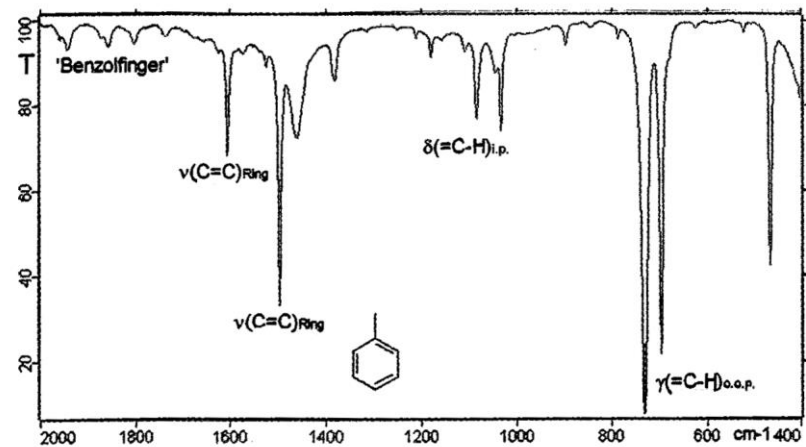
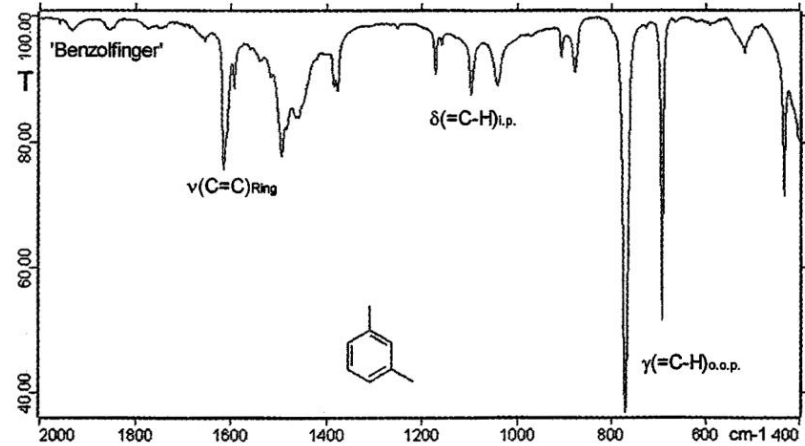
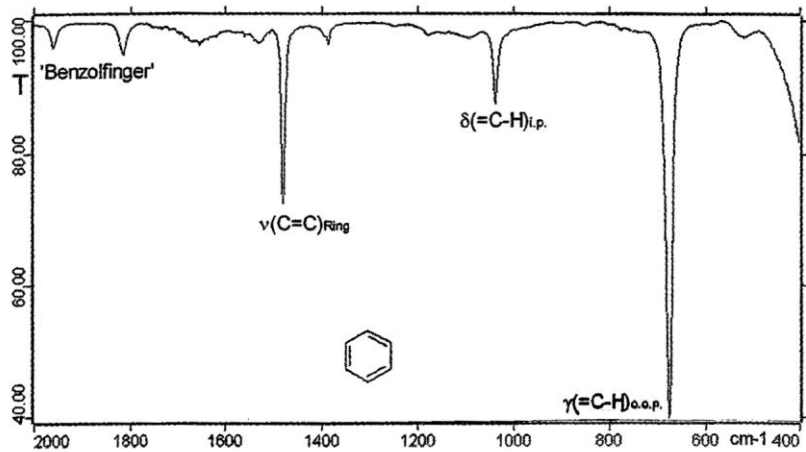


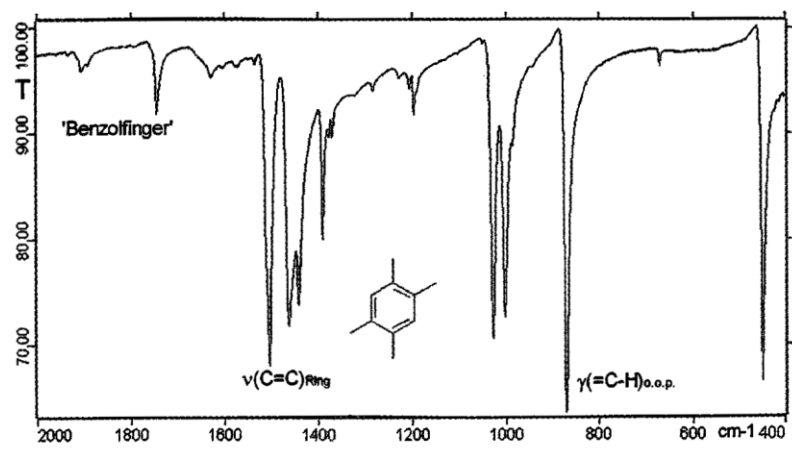
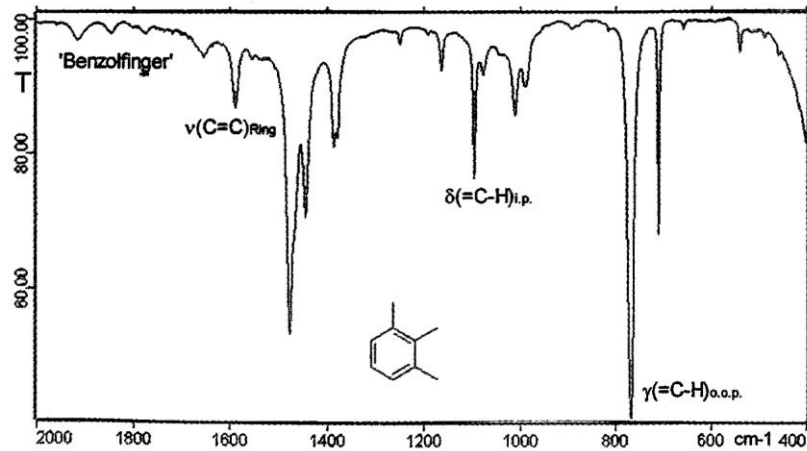
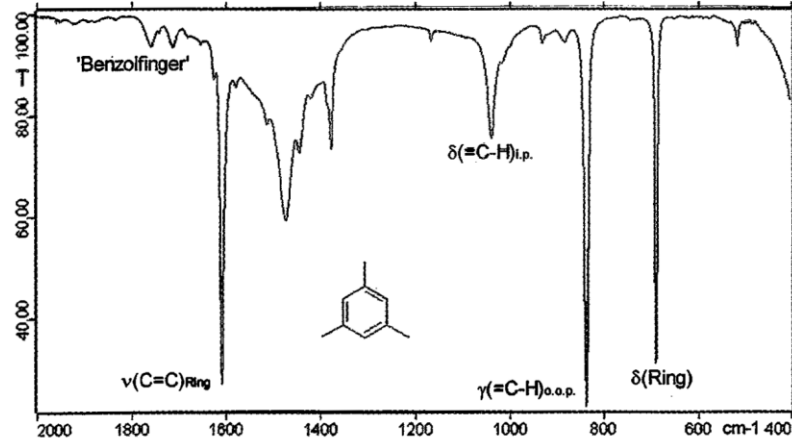
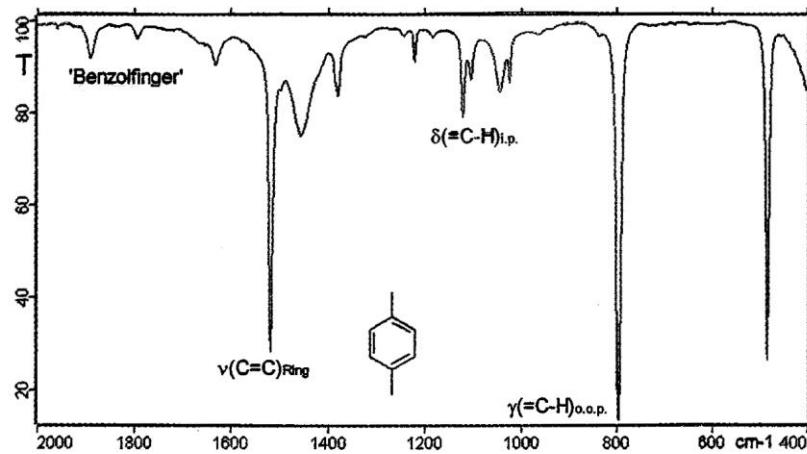
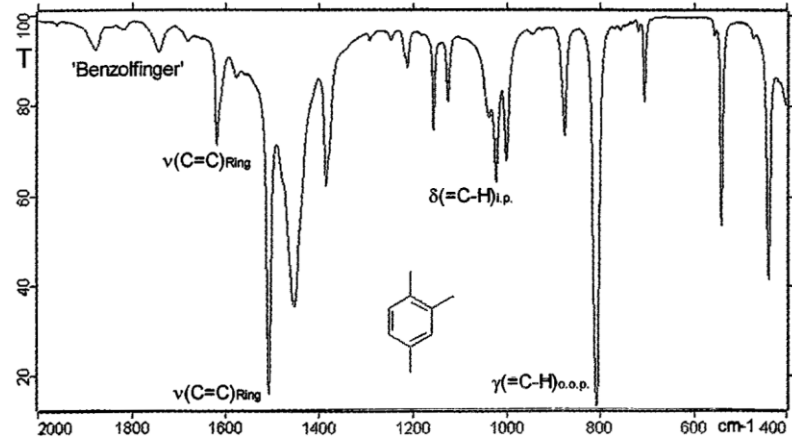
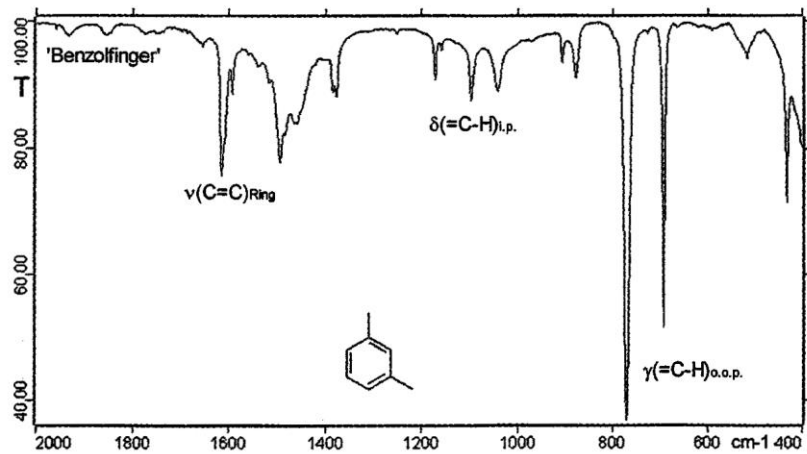
# alkini

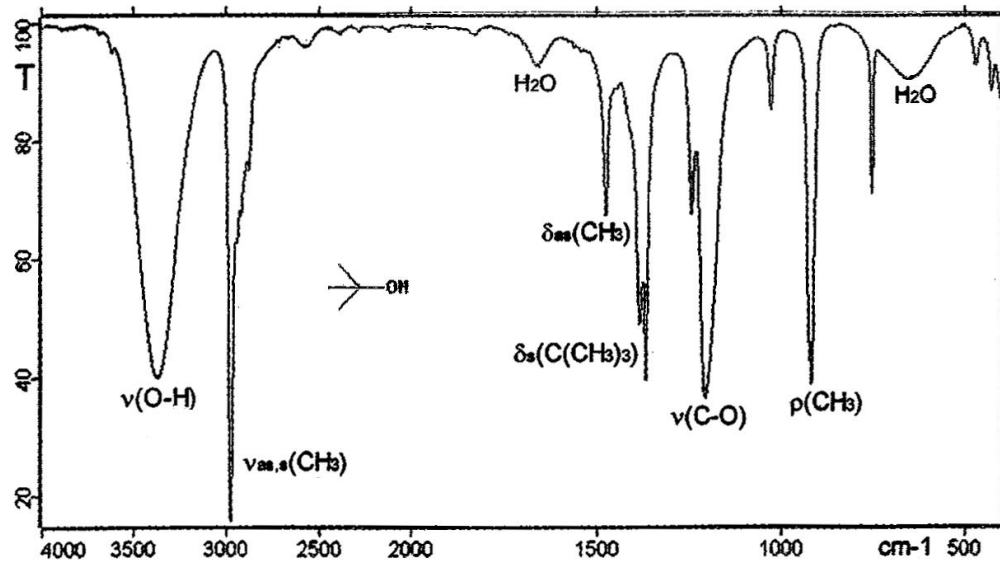
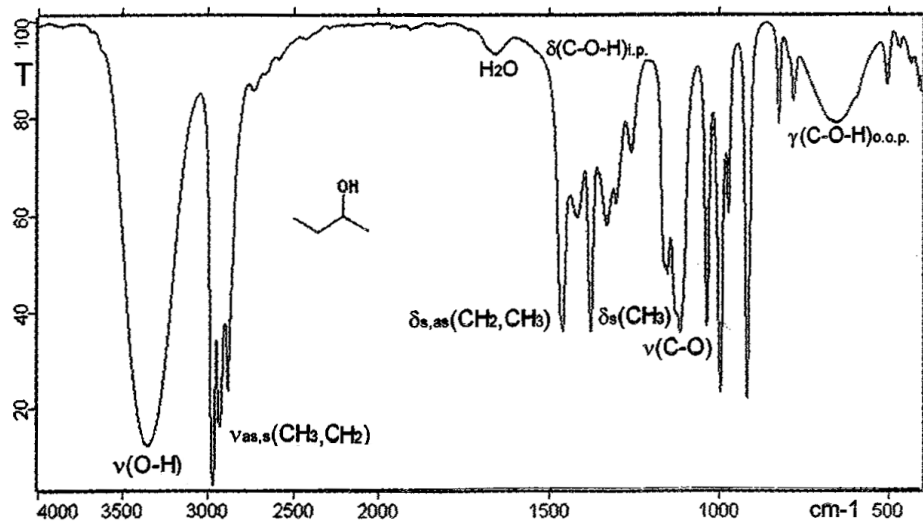
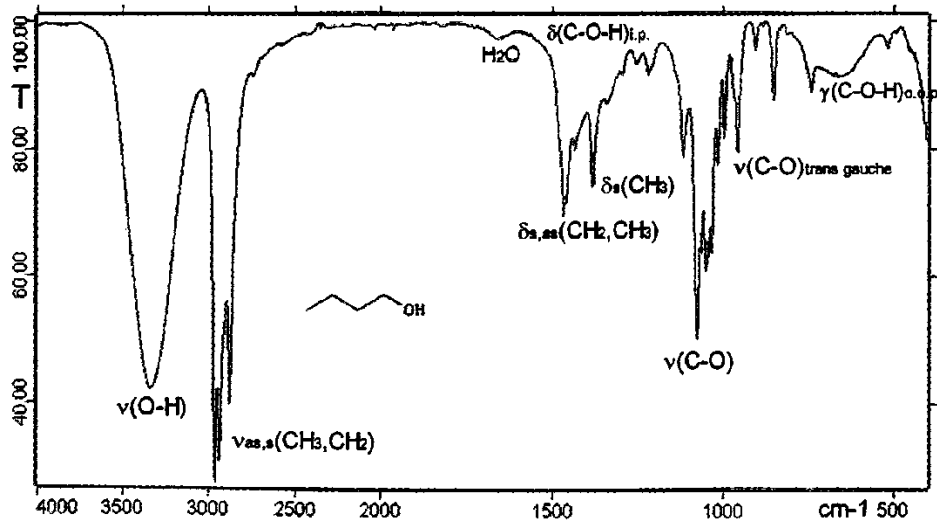


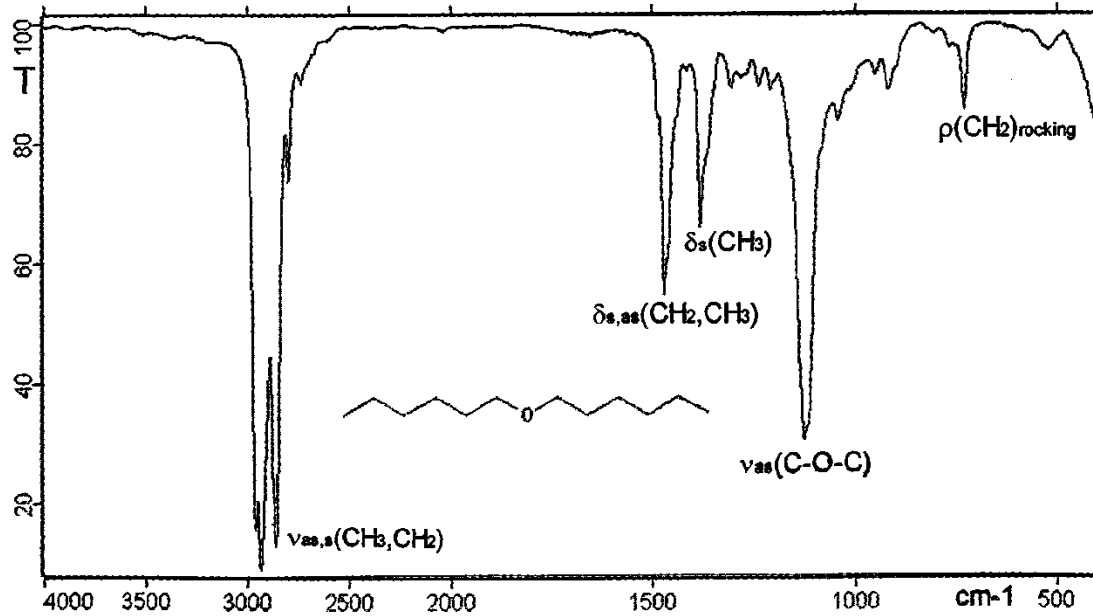
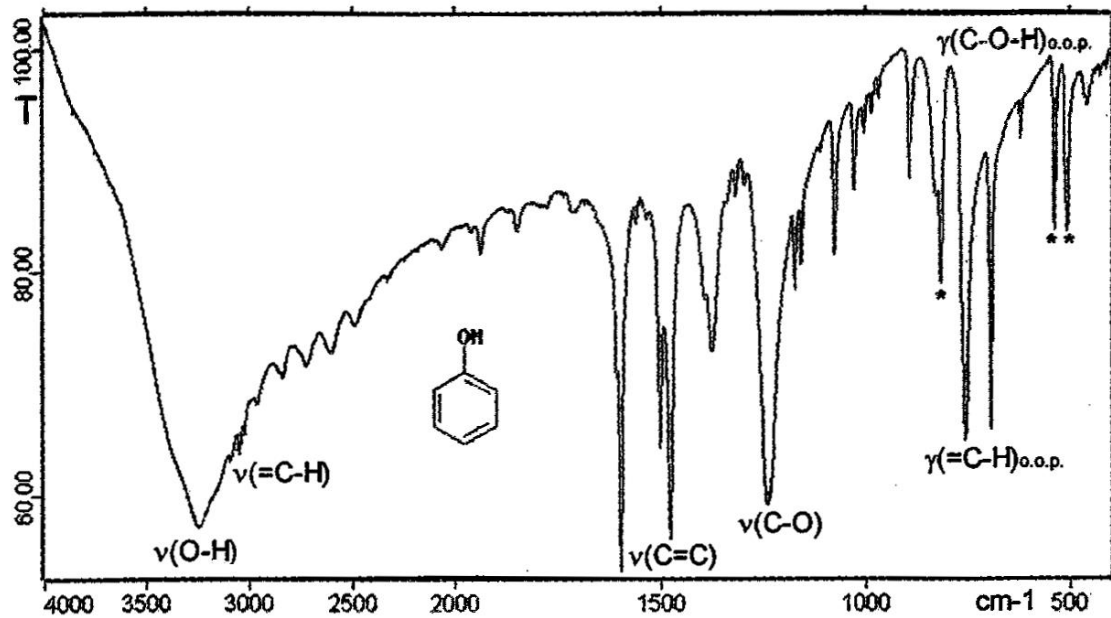
1-Heptyne.  $\equiv\text{C}-\text{H}$  stretch,  $3314\text{ cm}^{-1}$ . Alkyl  $\text{C}-\text{H}$  stretch  $1450-1360\text{ cm}^{-1}$ ,  $2960-2860\text{ cm}^{-1}$ .  $\text{C}\equiv\text{C}$  stretch,  $2126\text{ cm}^{-1}$ .  $\text{C}-\text{H}$  bend:  $1463\text{ cm}^{-1}$   $\delta_s\text{CH}_2$ ,  $1450\text{ cm}^{-1}$   $\delta_{as}\text{CH}_3$ .  $\equiv\text{C}-\text{H}$  bend overtone,  $1247\text{ cm}^{-1}$ .  $\equiv\text{C}-\text{H}$  bend fundamental,  $637\text{ cm}^{-1}$ .

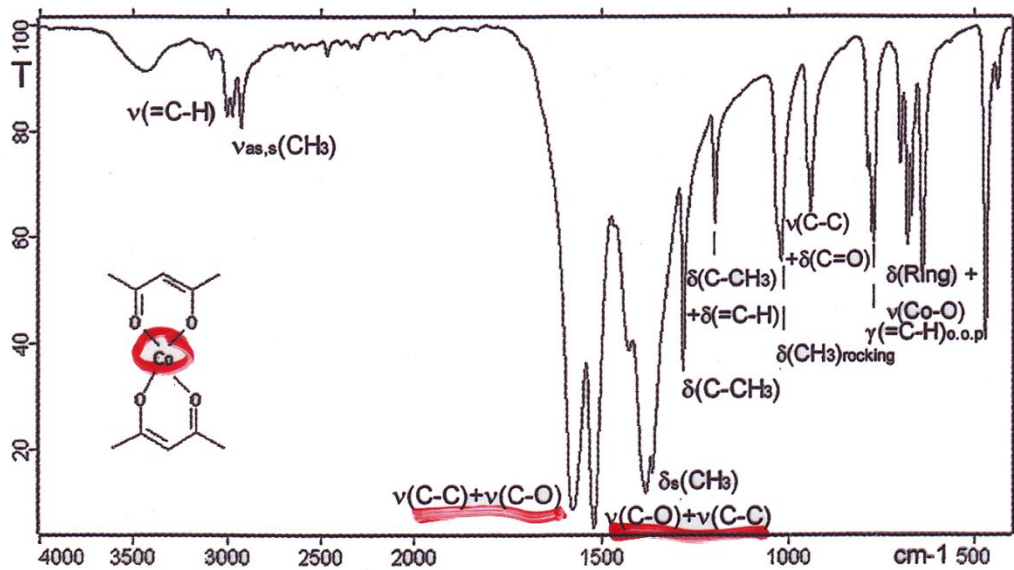
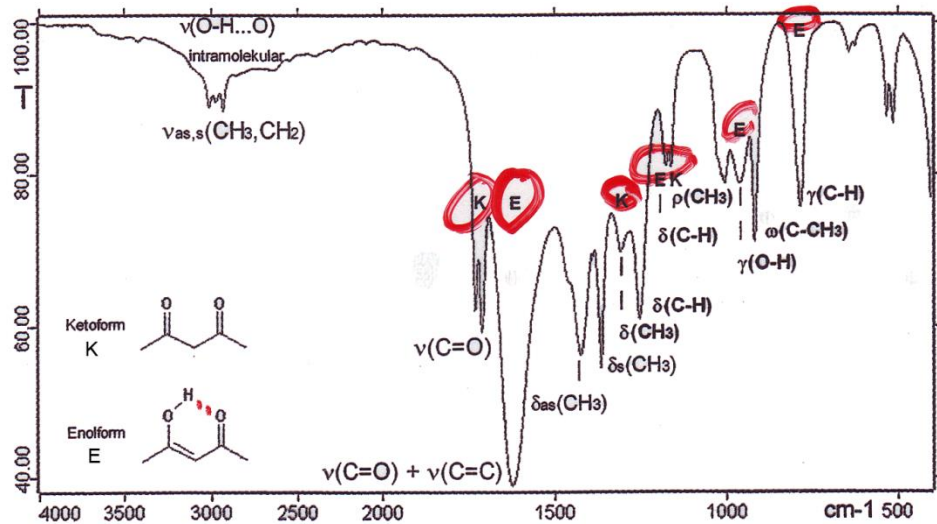
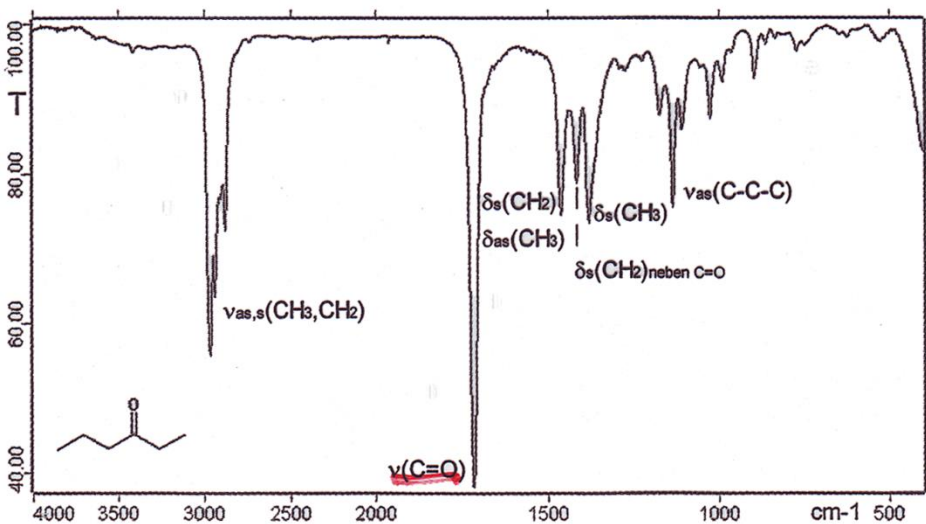


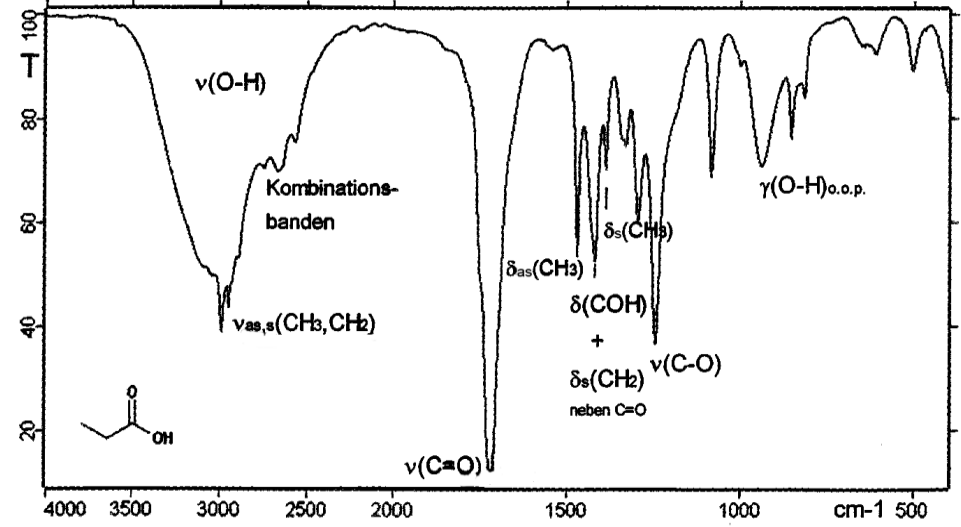
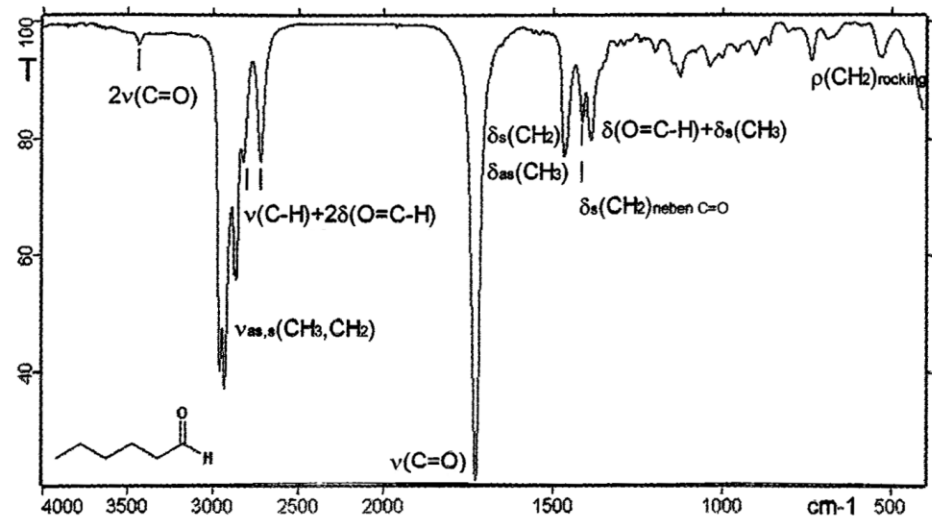




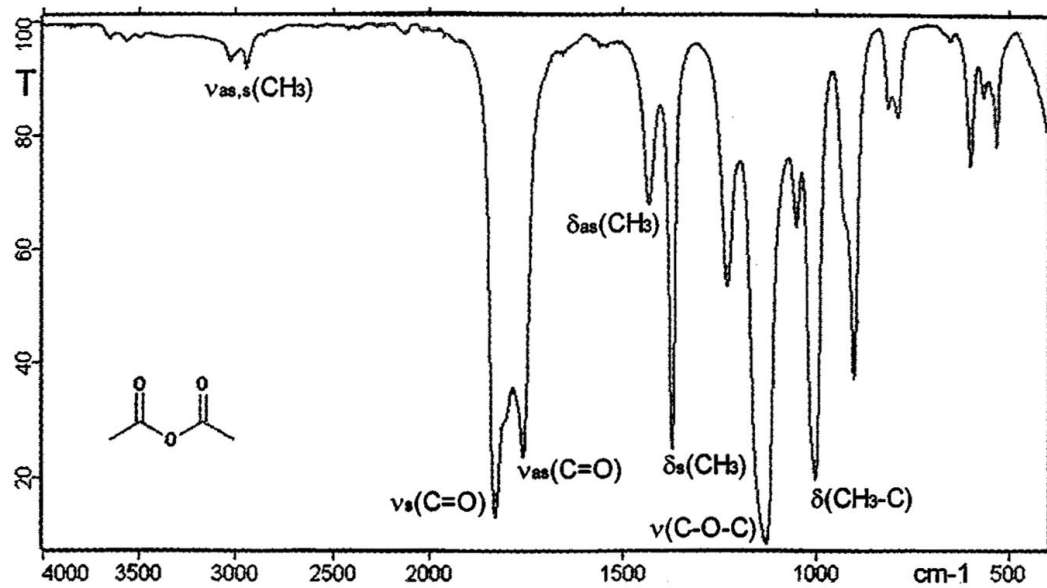
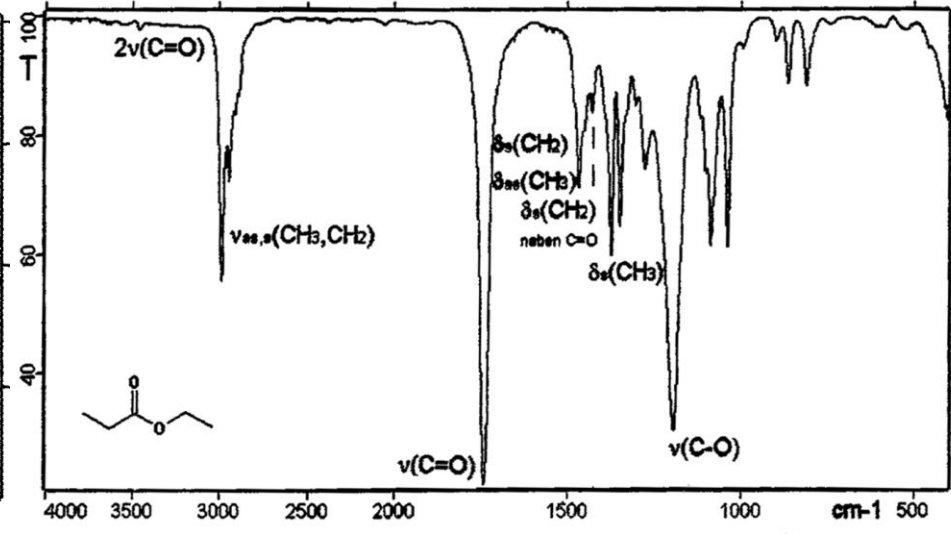
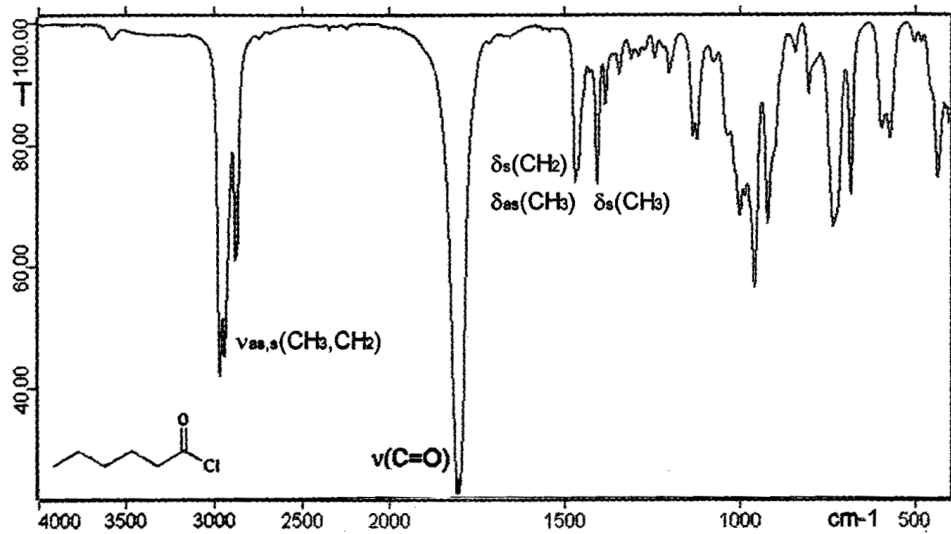


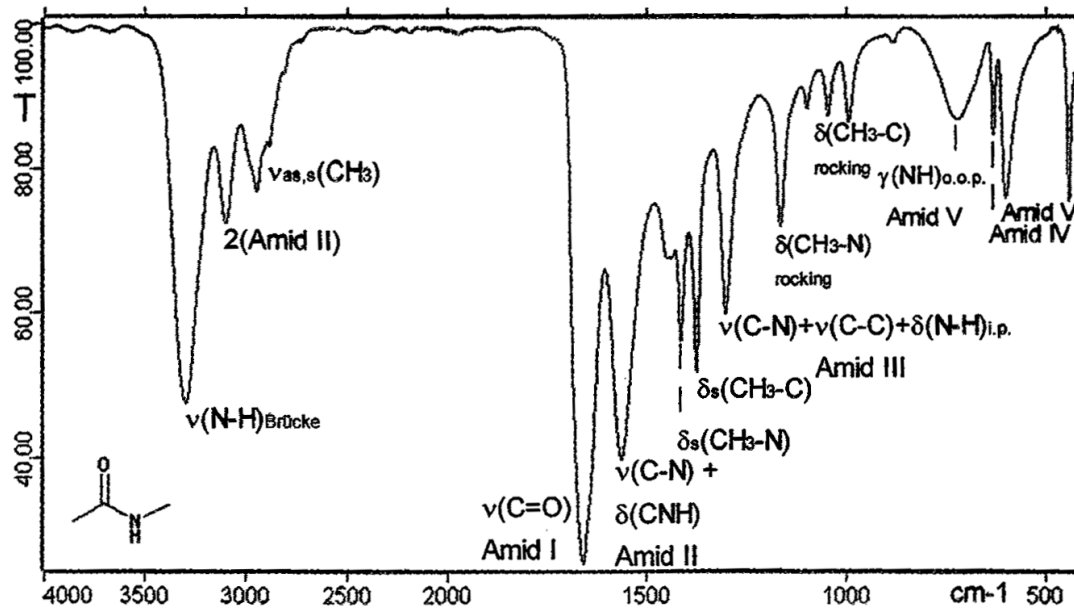
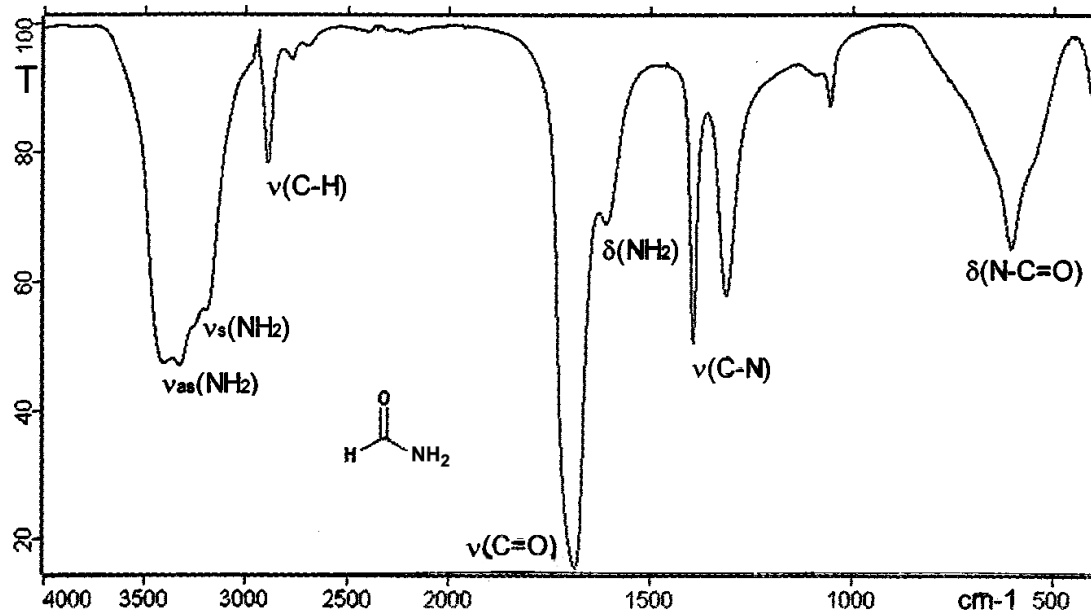


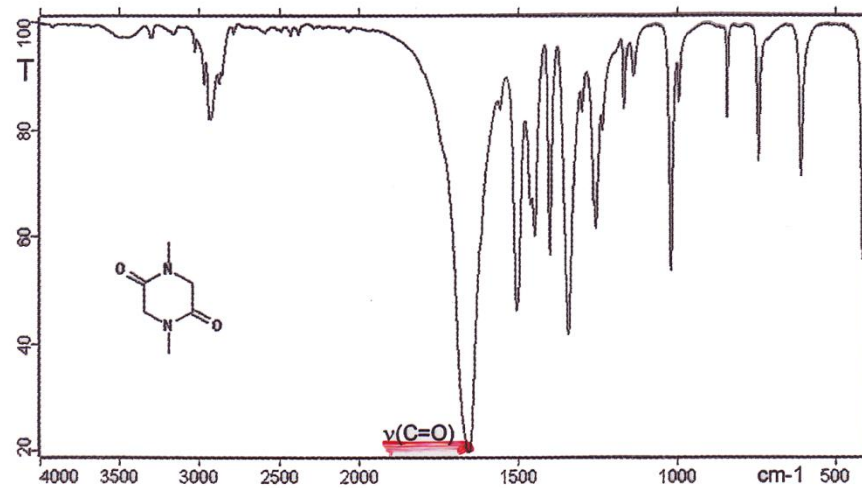
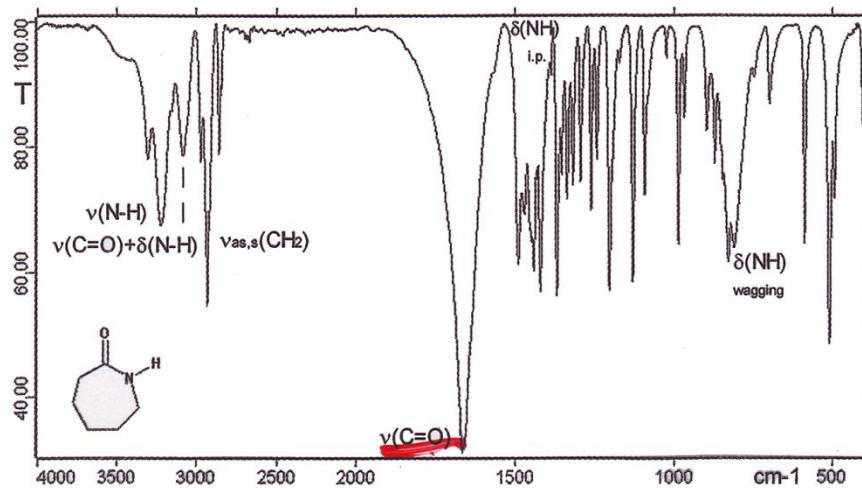




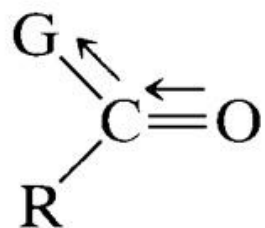






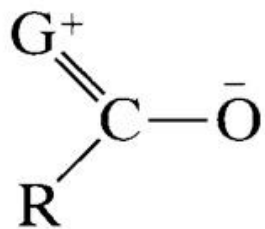


## G Effect Predominantly Inductive



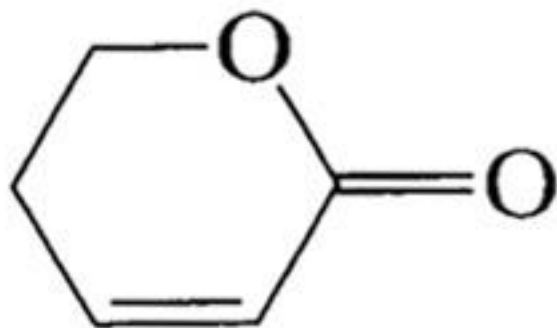
G	$\nu$ C=O (cm <sup>-1</sup> )
Cl	1815–1785
F	~1869
Br	1812
OH (monomer)	1760
OR	1750–1735

## G Effect Predominantly Resonance

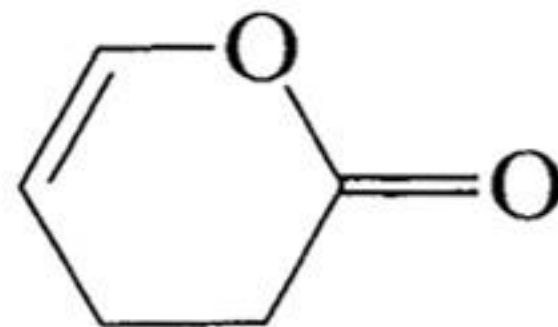


G	$\nu$ C=O (cm <sup>-1</sup> )
NH <sub>2</sub>	1695–1650
SR	1720–1690

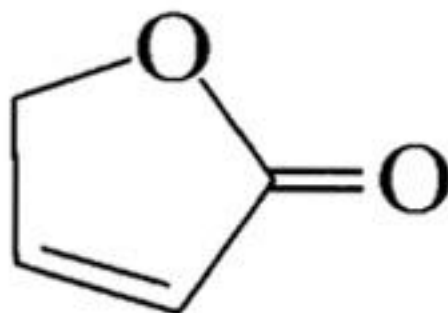
# laktoni



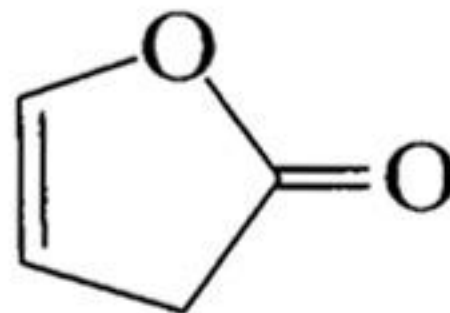
1720  $\text{cm}^{-1}$



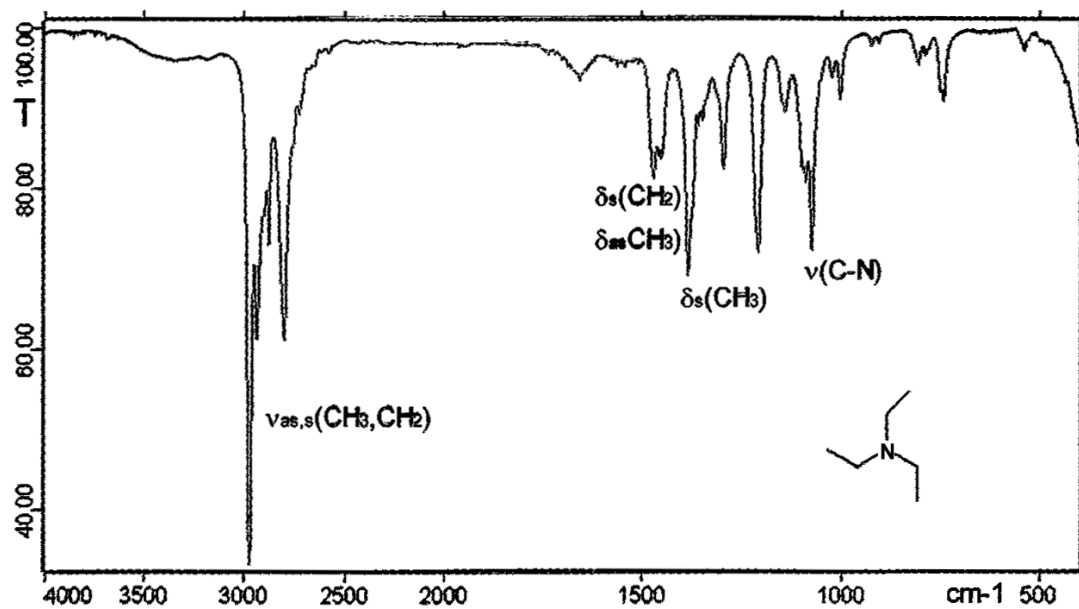
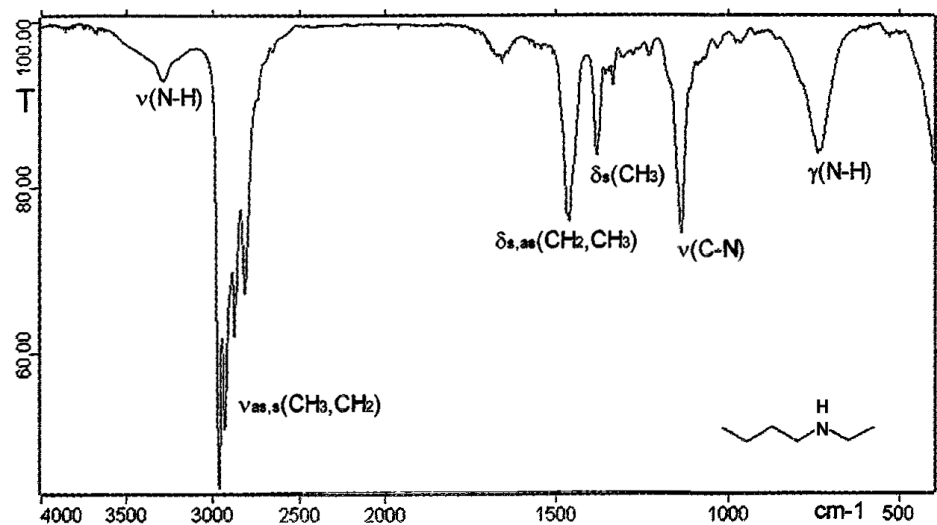
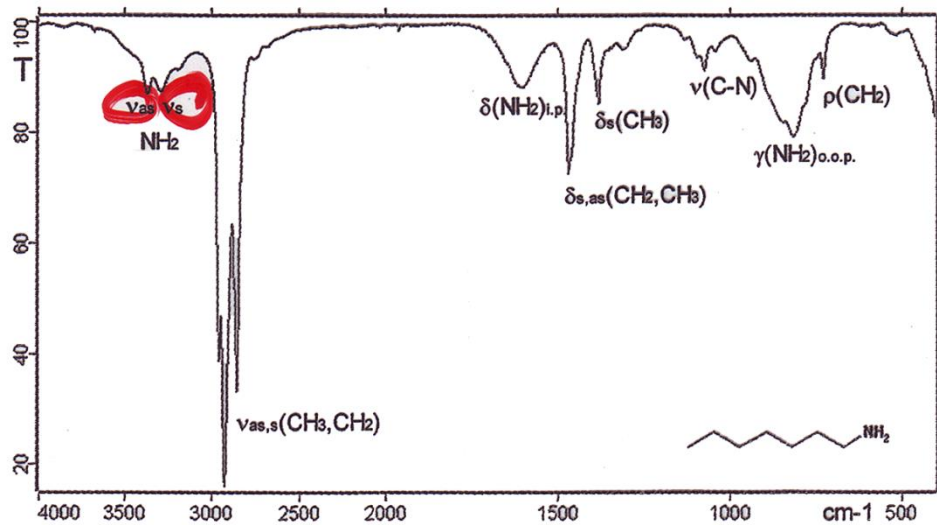
1760  $\text{cm}^{-1}$

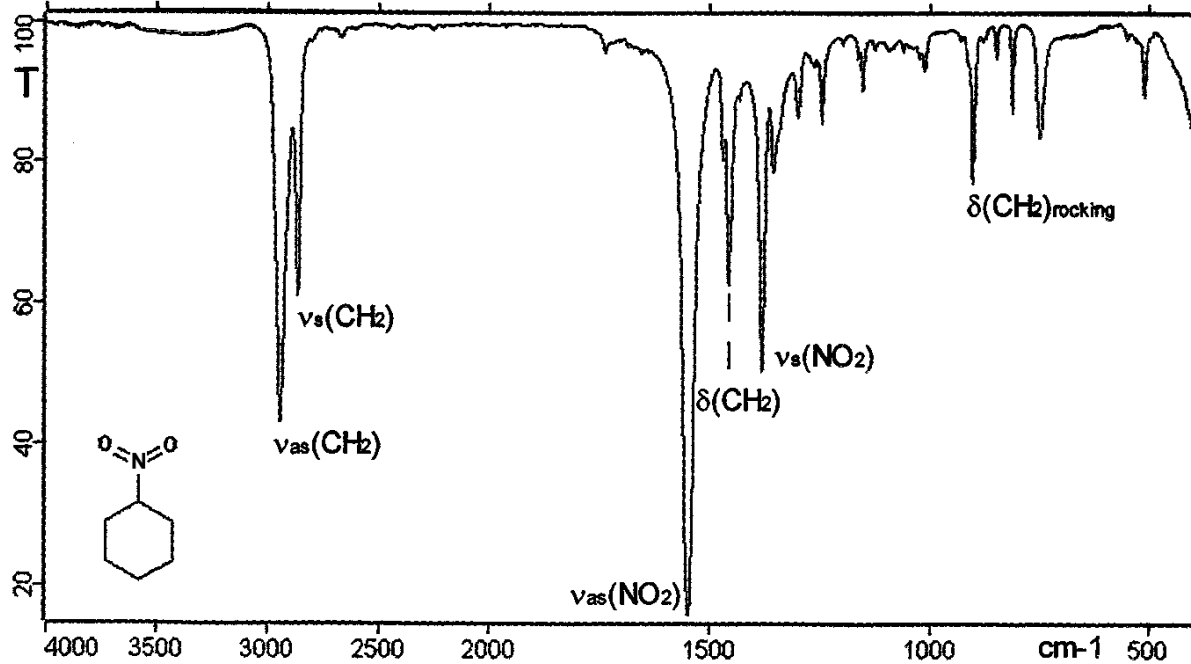
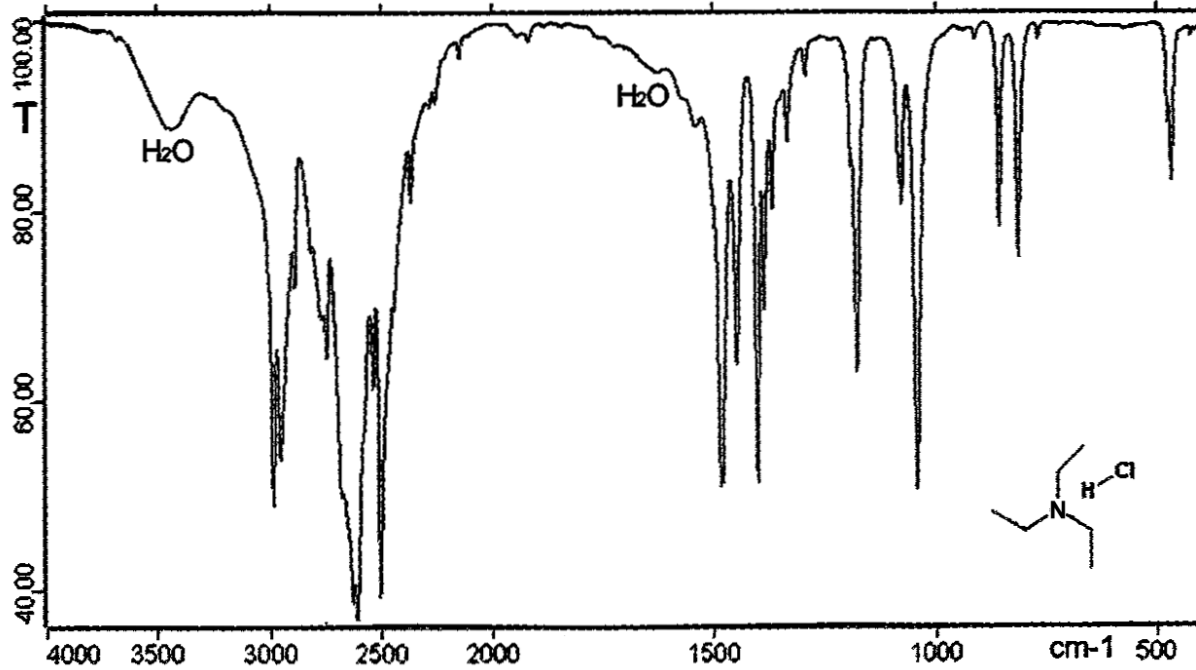


1750  $\text{cm}^{-1}$



1800  $\text{cm}^{-1}$



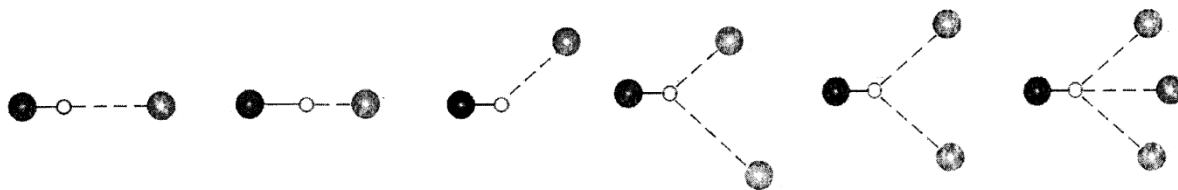


# Vodikova veza

opći izraz  $D-H \cdots A$ , privlačna je interakcija između proton-donorske skupine  $D-H$  i proton-akceptorske skupine  $A$ ,

$D$  atom elektronegativniji od vodika, a  $A$  skupina sadrži nevezni elektronski par elektronegativnog atoma ( $\sigma$ -elektron-donor) ili  $\pi$ -orbitalu nezasićenog sustava.

<b>Donori</b>	<b>C-H, P-H, S-H, Se-H</b>	<b>-O-H, =N-H, P-O-H</b>	<b>[=O<math>\cdots</math>H]<sup>+</sup>, [<math>\equiv</math>N<math>\cdots</math>H]<sup>+</sup></b>
<b>Akceptori</b>	C-Hal:, =S:, =Se:, $\pi$ -veza	=O:, $\equiv$ N:, P=O:	[Hal] <sup>-</sup> , [-O] <sup>-</sup> , [P-O] <sup>-</sup>
<b>Vodikove veze</b>	C-H $\cdots$ O C-H $\cdots$ N C/O/N-H $\cdots$ Hal-C C/O/N-H $\cdots$ $\pi$ -veza	-O-H $\cdots$ O= -N-H $\cdots$ O= -O-H $\cdots$ N $\equiv$ -N-H $\cdots$ N $\equiv$ $\cdots$ O-H $\cdots$ O-H $\cdots$ $\cdots$ O=C-C=C-OH $\cdots$ $\cdots$ O=C-C=C-N(R)H $\cdots$	[H <sub>2</sub> O $\cdots$ H $\cdots$ OH <sub>2</sub> ] <sup>+</sup> [ $\equiv$ N $\cdots$ H $\cdots$ N $\equiv$ ] <sup>+</sup> [F $\cdots$ H $\cdots$ F] <sup>-</sup> [RCOO $\cdots$ H $\cdots$ OOCR] <sup>-</sup> [O <sub>3</sub> SO $\cdots$ H $\cdots$ OSO <sub>3</sub> ] <sup>-</sup> R <sub>3</sub> N <sup>+</sup> -H $\cdots$ <sup>-</sup> OOCR $\cdots$ O=C-C=C-OH $\cdots$ $\cdots$ O=C-C=C-N(R)H $\cdots$



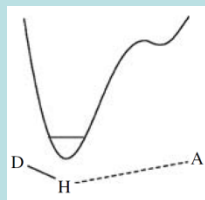
Strukture vodikovih veza: **a)** asimetrična linearna, **b)** simetrična linearna, **c)** svijena, **d)** asimetrična bifurkatna, **e)** simetrična bifurkatna, **f)** trifurkatna



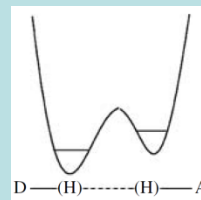
	Vodikova veza D–H...A		
<b>Obilježja veze</b>	Slaba	Umjereno jaka	Jaka
<b>Tip interakcije</b>	elektrostatska	elektrostatsko-kovalentna	pretežno kovalentna
<b>Duljine veza</b>	$d(D-H) \ll d(H...A)$	$d(D-H) < d(H...A)$	$d(D-H) \approx d(H...A)$
<b><math>d(H...A)</math> / Å</b>	3,2 – 2,2	2,2 – 1,5	1,5 – 1,2
<b><math>d(D...A)</math> / Å</b>	4,0 – 3,2	3,2 – 2,5	2,5 – 2,2
<b>Kut D–H–A / °</b>	90 – 150	130 – 180	165 – 180
<b>Smanjenje <math>d(H...A)</math> u odnosu na sumu van der Waalsovih radijusa atoma H i A / %</b>	< 20	20 – 40	40 – 55
<b>Energija / kcal mol<sup>-1</sup></b>	< 4	4 – 15	15 – 45
<b>Relativno smanjenje IR <math>\nu(D-H)</math> / %</b>	< 10	10 – 20	20 – 80
<b><sup>1</sup>H <math>\delta(DH)</math> / ppm</b>	–	< 14	14 – 22

**Kvalitativna krivulja  
potencijalne energije**

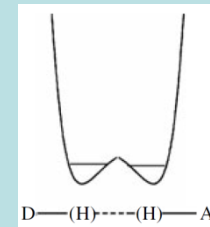
**asimetrična krivulja s  
jednostrukim minimumom i  
visokom energijskom  
barijerom**



**asimetrična krivulja s  
dvostrukim minimumom  
i srednje visokom energijskom  
barijerom**



**simetrična krivulja s  
dvostrukim  
minimumom i  
niskom energijskom barijerom**



ili

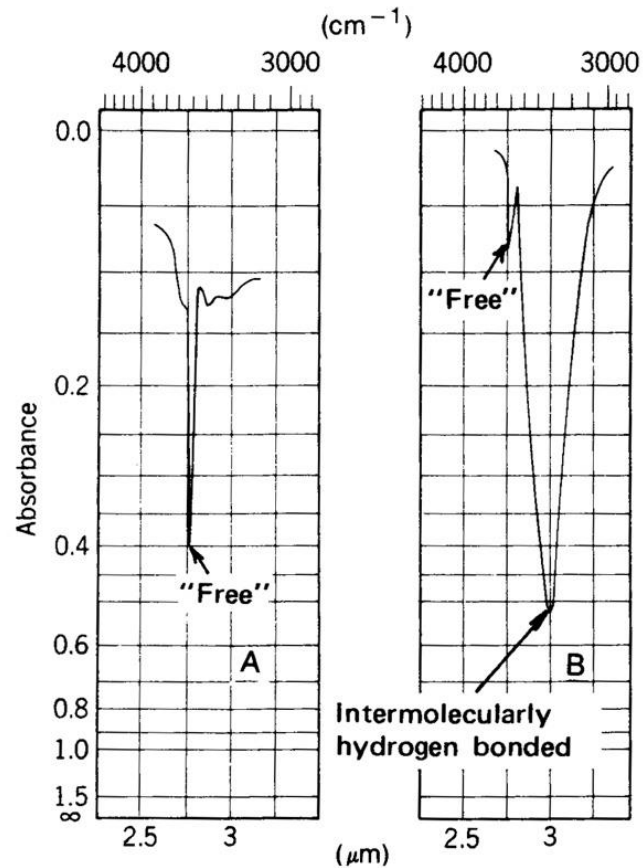


simetrična krivulja s jednostrukim  
minimumom

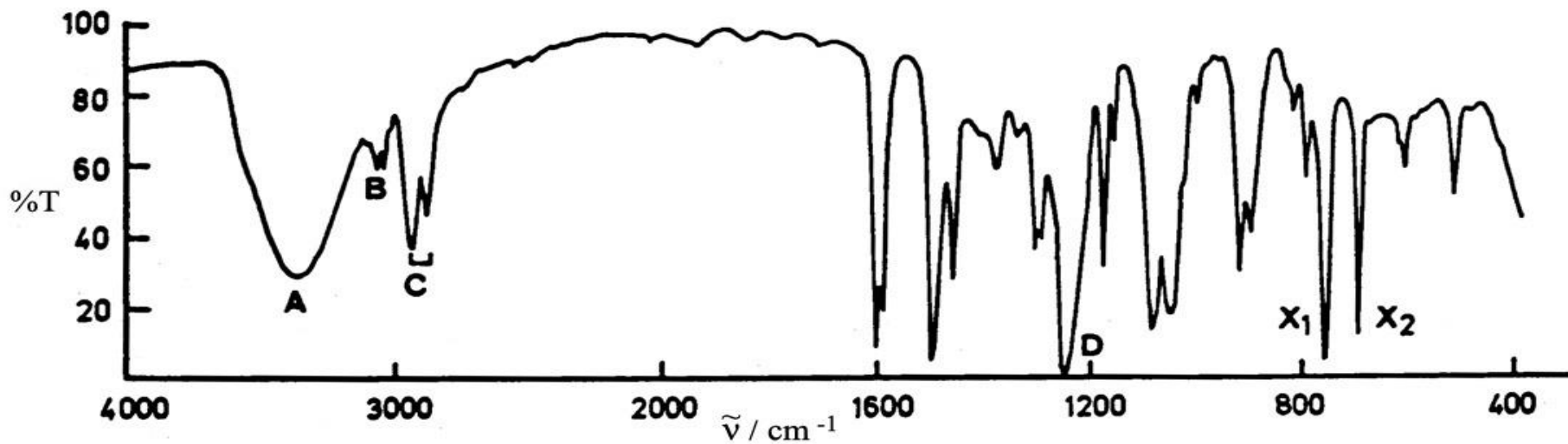
## Načini vibriranja sustava D-H···A.

IR područje / cm <sup>-1</sup>	Način vibracije		Opis vibracije
3500 – 2500	$\begin{array}{c} \leftarrow \quad \rightarrow \quad \rightarrow \\ \text{D}-\text{H}\cdots\text{A} \end{array}$	$v_s$	D-H istežanje
1700 – 1000	$\begin{array}{c} \uparrow \\ \text{D}-\text{H}\cdots\text{A} \\ \downarrow \end{array}$	$v_b$	D-H svijanje u ravnini
900 – 300	$\begin{array}{c} \pm \\ \text{D}-\text{H}\cdots\text{A} \end{array}$	$v_t$	svijanje izvan ravnine
250 – 100	$\text{D}-\text{H}\cdots\leftarrow\text{A}\rightarrow$	$v_\sigma$	H···D istežanje
< 200	$\begin{array}{c} \uparrow \\ \text{D}-\text{H}\cdots\text{A} \\ \downarrow \end{array}$	$v_\beta, v_\gamma$	H···D svijanje

Vodikove veze

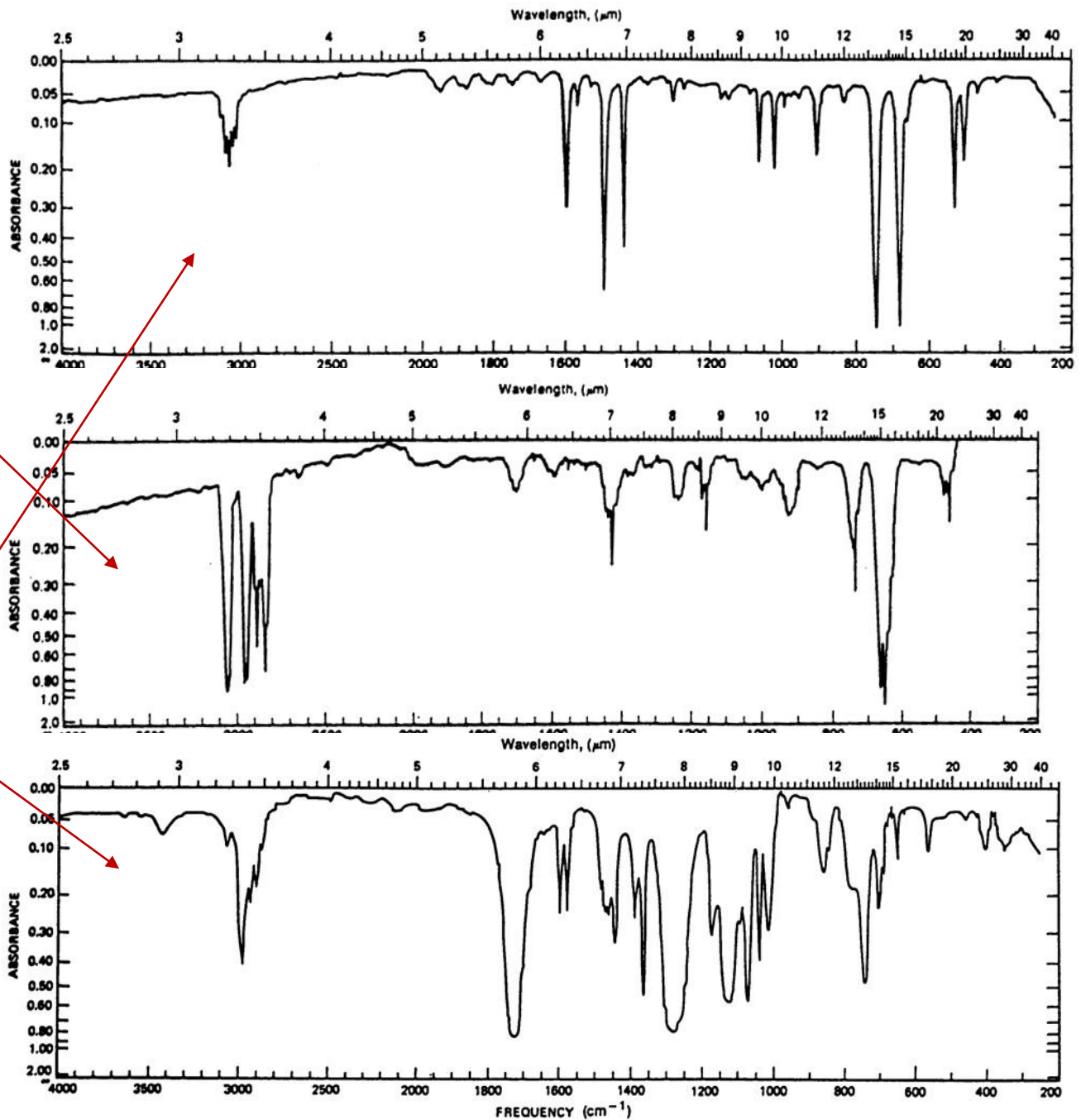
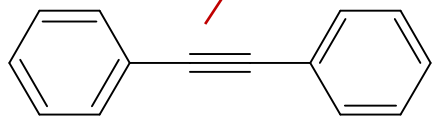
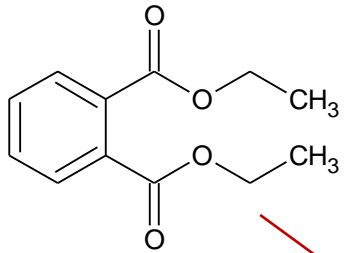


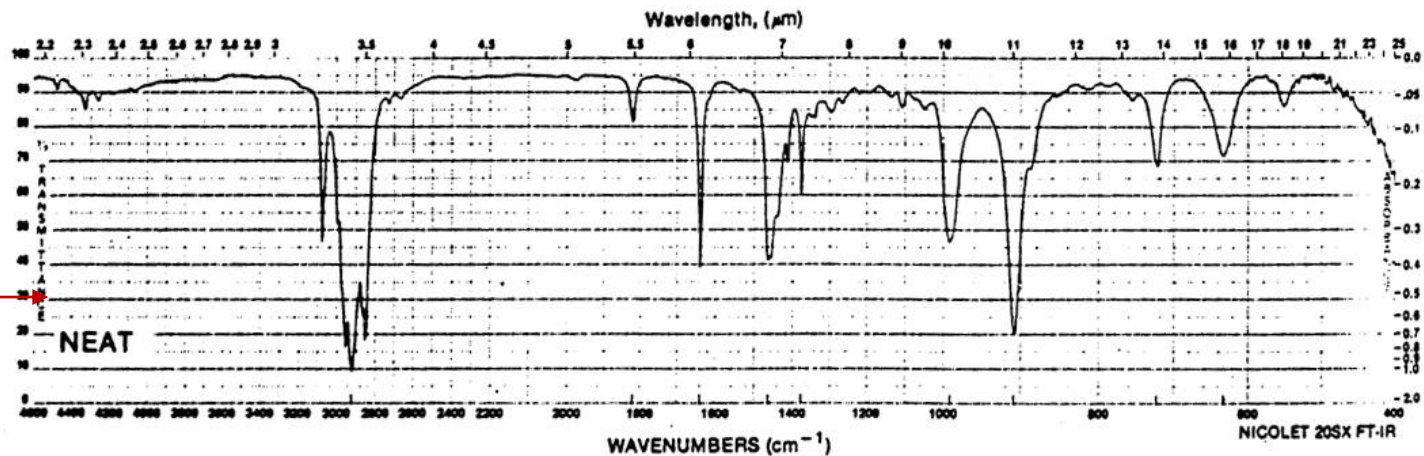
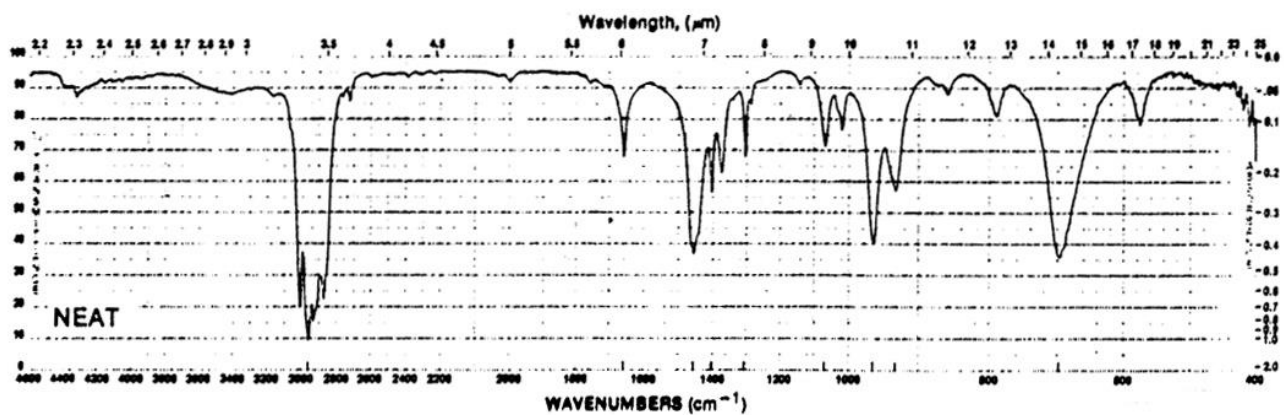
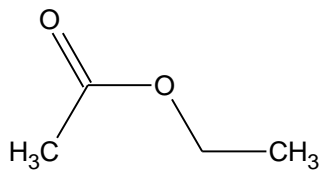
fenoksietanol



Koji spektar IR odgovara ovim spojevima?

1-okten





1,3-cikloheksa  
dien

2-penten

