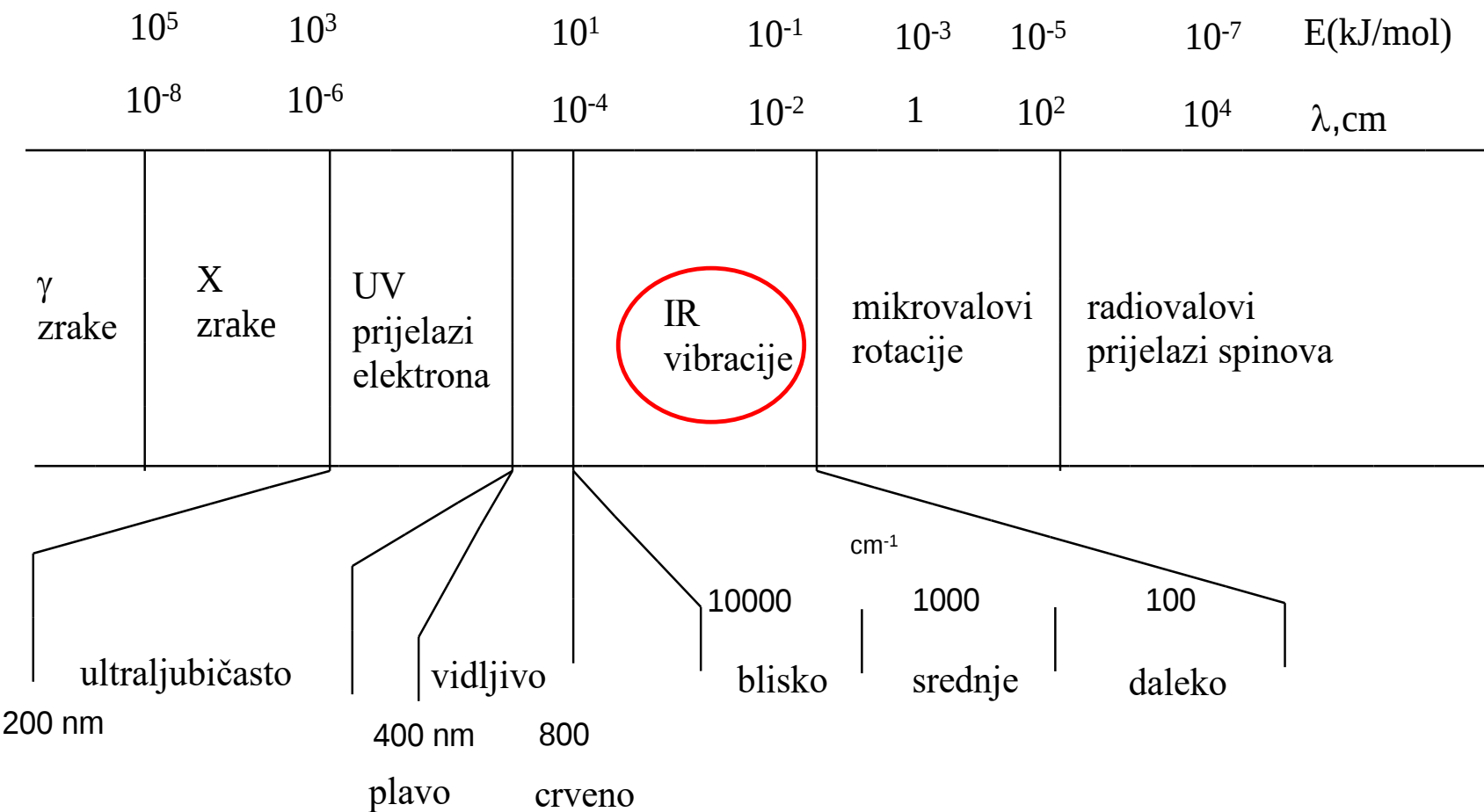


Spektar elektromagnetnoga zračenja



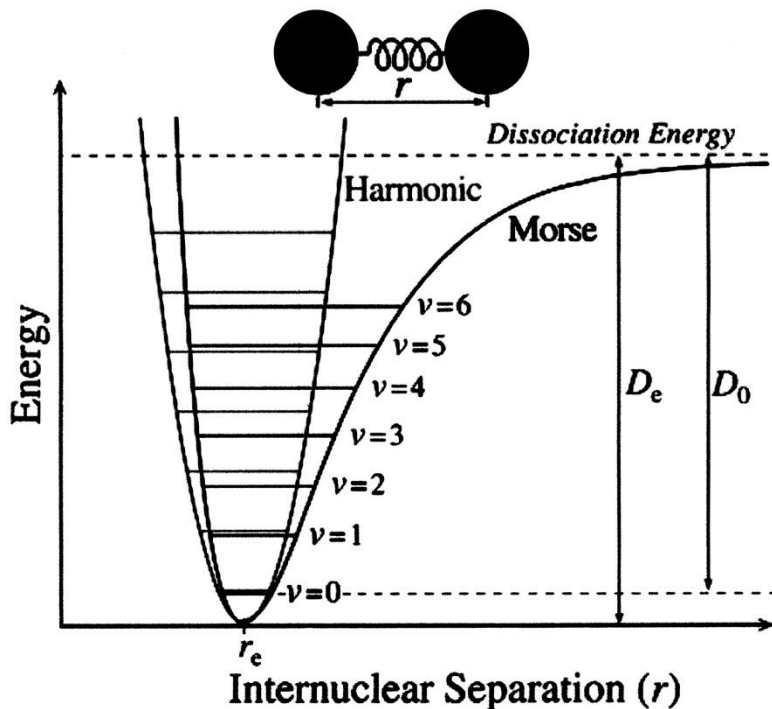
Vibracijska spektroskopija

- 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	λ / μm	$\tilde{\nu}$ / cm^{-1}	ν/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 INFRACRVE NE SPECTRE

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

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

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

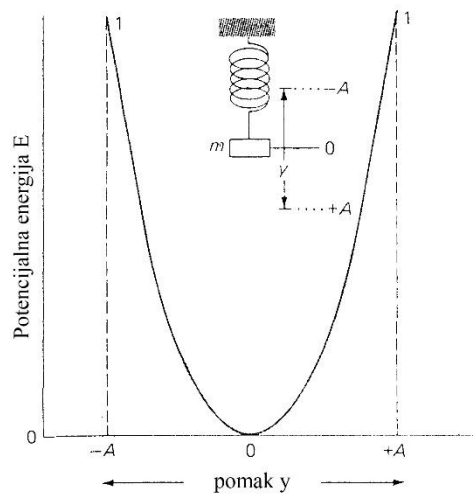
$$\frac{\partial \alpha}{\partial q} \neq 0$$

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

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

Pravilo uzajamnoga isključenja

HARMONIČNI OSCILATOR



Klasično:

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

$$dE = -Fdy = kydy$$

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

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

$$F = ma$$

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

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

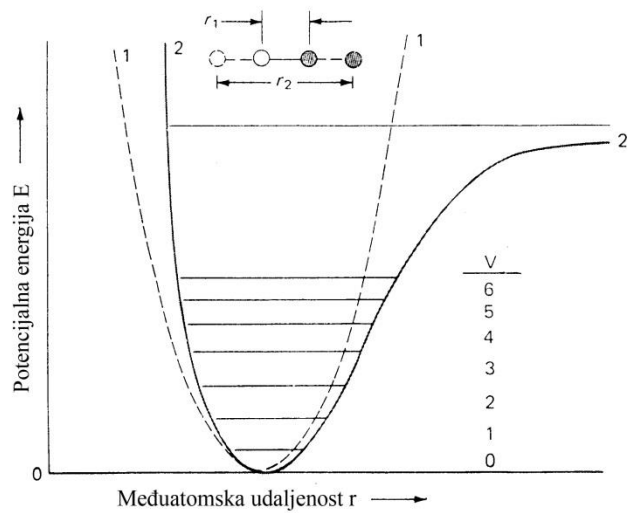
$$y = A \cos 2\pi \nu t$$

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

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

Hookeov zakon

NEHARMONIČNI OSCILATOR



Kvantno-mehanički:

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

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

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

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

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

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

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

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

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

harmonični oscilator
neharmonični oscilator

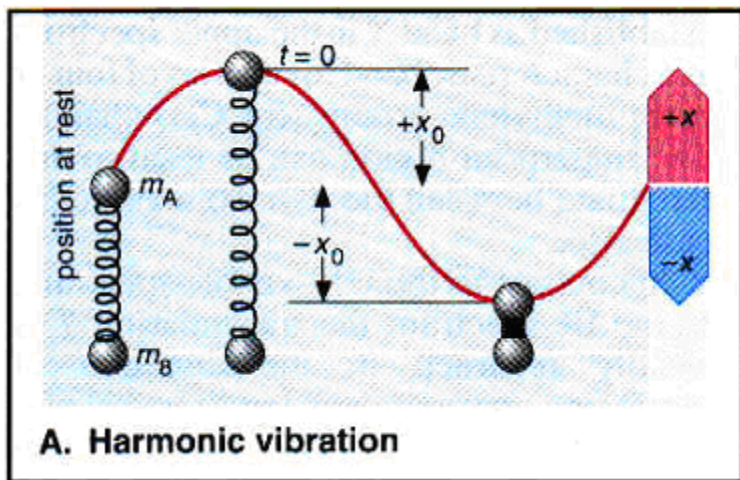
SPEKTROSKOPIJA IR

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

podjela:

- blisko (NIR)
- srednje (2,5-50 μm ; 4000-200 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 ΔE_m i o masi atoma;

k je pripadna konstanta sile veze*

Veza	$\nu(\text{C}\cdots\text{X})$	ΔE_m	k	Relativna	Veza	$\nu(\text{C}\cdots\text{C})$	ΔE_m	k
	cm^{-1}	kJ mol^{-1}	$\text{mdin } \text{\AA}^{-1}$	atomska		cm^{-1}	kJ mol^{-1}	$\text{mdin } \text{\AA}^{-1}$
				masa X				
-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

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

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

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

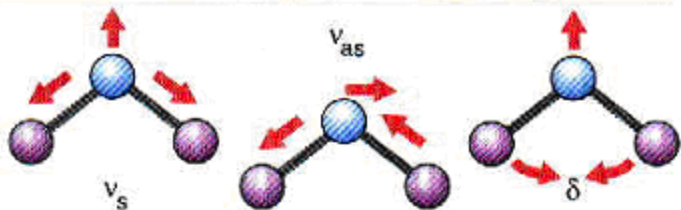
prijelazi $v = 1 \rightarrow v = 2, 3..$ se mogu zanemariti

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

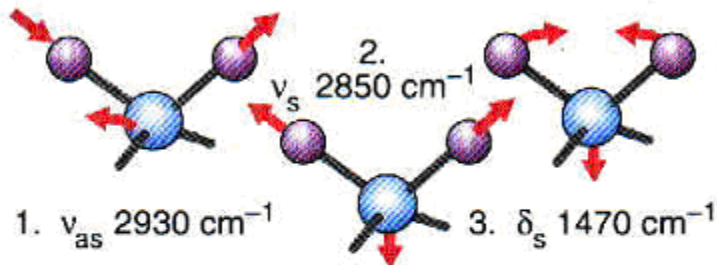
$v = 0 \rightarrow v = 2$, $\Delta v = \pm 2$ prvi viši harmonik (prvi "overtone")

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

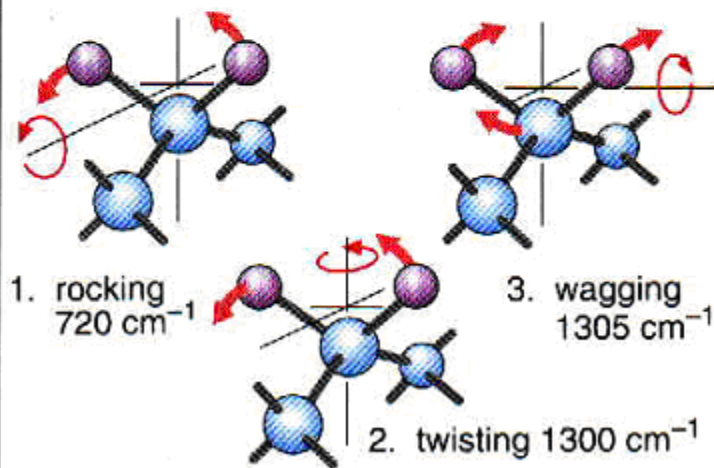
primjer HCl, vrpca kod 2886 cm^{-1} (jak intenzitet), vrpca kod 5668 cm^{-1} (slabiji intenzitet), vrpca kod 8347 cm^{-1} (vrlo slabi intenzitet)



C. Natural vibration of a three-atom bent molecule



D. Normal vibrations of the CH_2 fragment



E. Bending vibrations of the CH_2 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

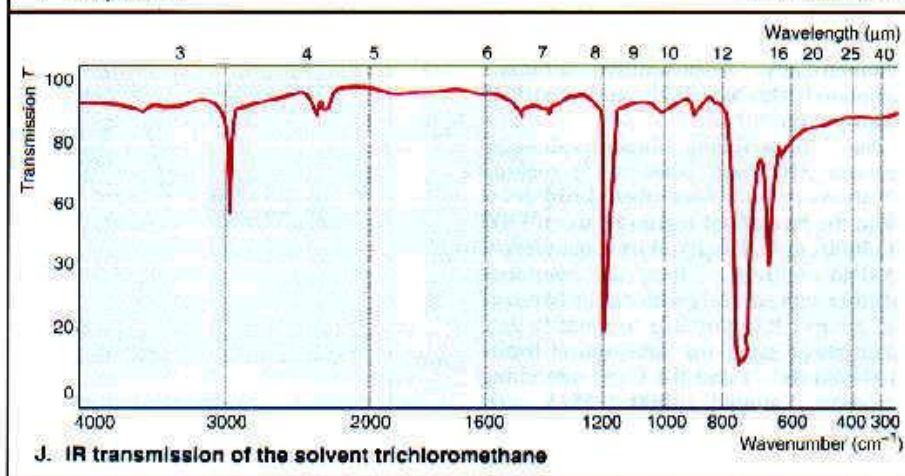
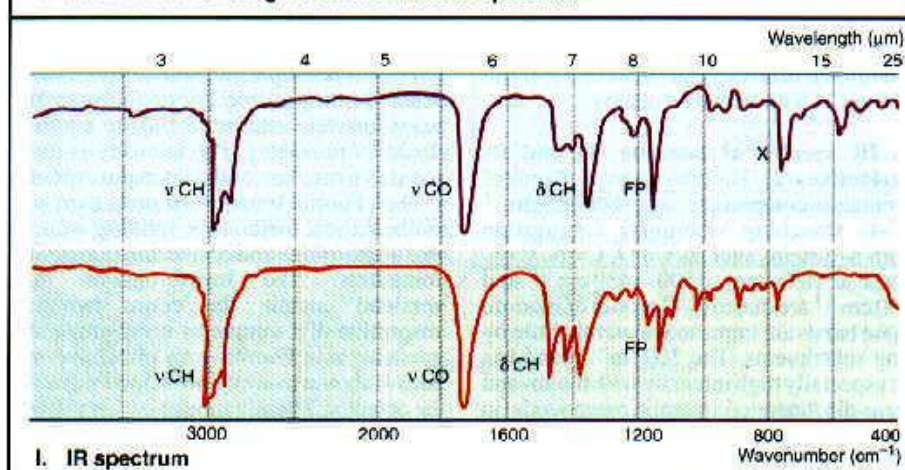
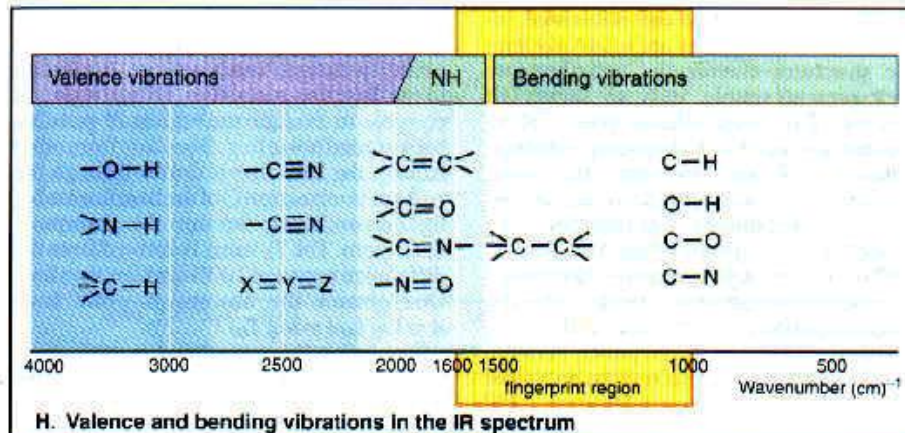
INTERPRETACIJA INFRACRVENIH I RAMANOVIH SPEKTARA

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

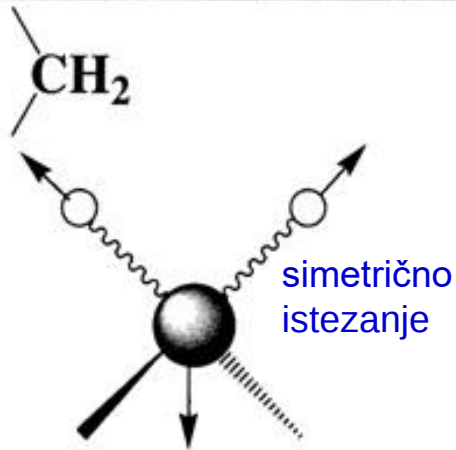
⇒ **heksan-2-on:**
(CH3CH2CH2CH2COCH3)

⇒ **heksan-3-on:**
(CH3CH2CH2COCH2CH3)

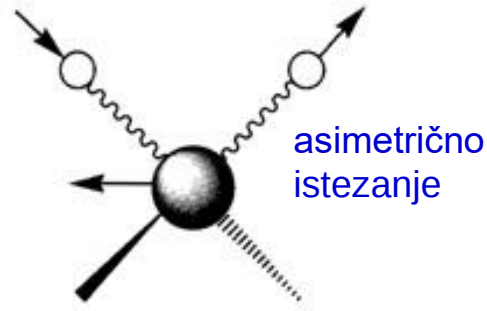
⇒ otapalo

Koncept skupinskih vibracija

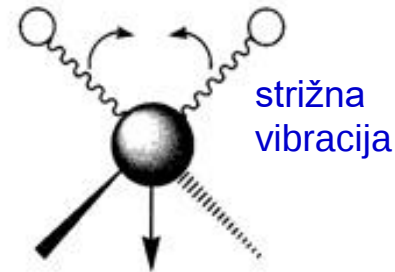
-karakteristične vibracije u spektru IR



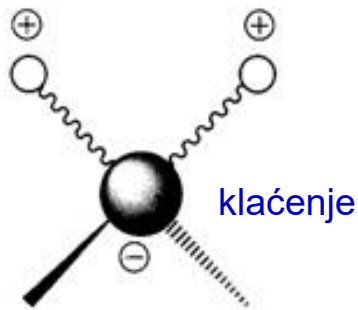
Symmetrical stretching (ν_s CH₂)
~2853 cm⁻¹



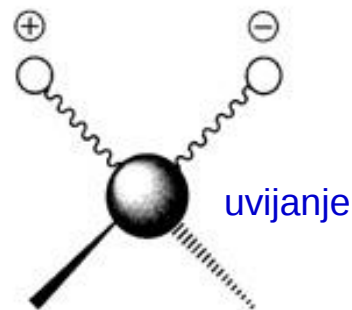
Asymmetrical stretching (ν_{as} CH₂)
~2926 cm⁻¹



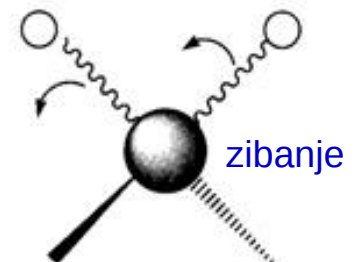
In-plane bending or scissoring (δ_s CH₂)
~1465 cm⁻¹



Out-of-plane bending or wagging (ω CH₂)
1350-1150 cm⁻¹

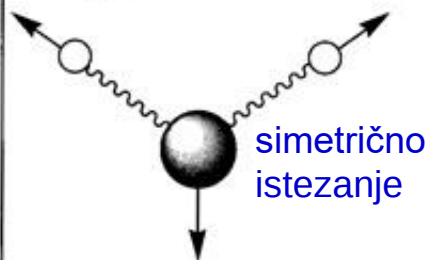


Out-of-plane bending or twisting (τ CH₂)
1350-1150 cm⁻¹

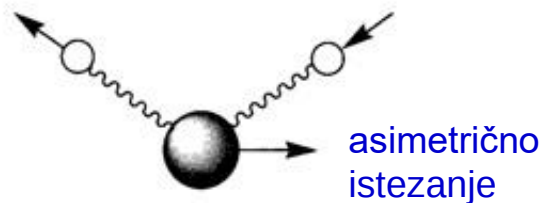


In-plane bending or rocking (ρ CH₂)
~720 cm⁻¹

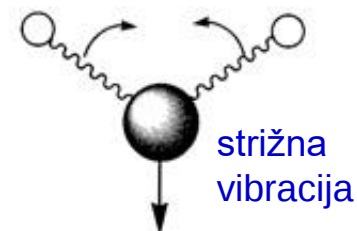
H₂O



Symmetrical stretching (ν_s OH)
3652 cm⁻¹



Asymmetrical stretching (ν_{as} OH)
3756 cm⁻¹



Scissoring (δ_s OH)
1596 cm⁻¹

CO₂

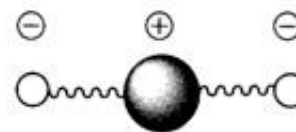


(1) Symmetrical stretching (ν_s CO₂)
1340 cm⁻¹

asimetrično istezanje
(2) Asymmetrical stretching (ν_{as} CO₂)
2350 cm⁻¹

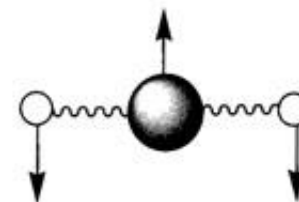


(3) Scissoring (bending) (δ_s CO₂)
665 cm⁻¹



strižna vibracija

(4) Scissoring (bending) (δ_s CO₂)
665 cm⁻¹

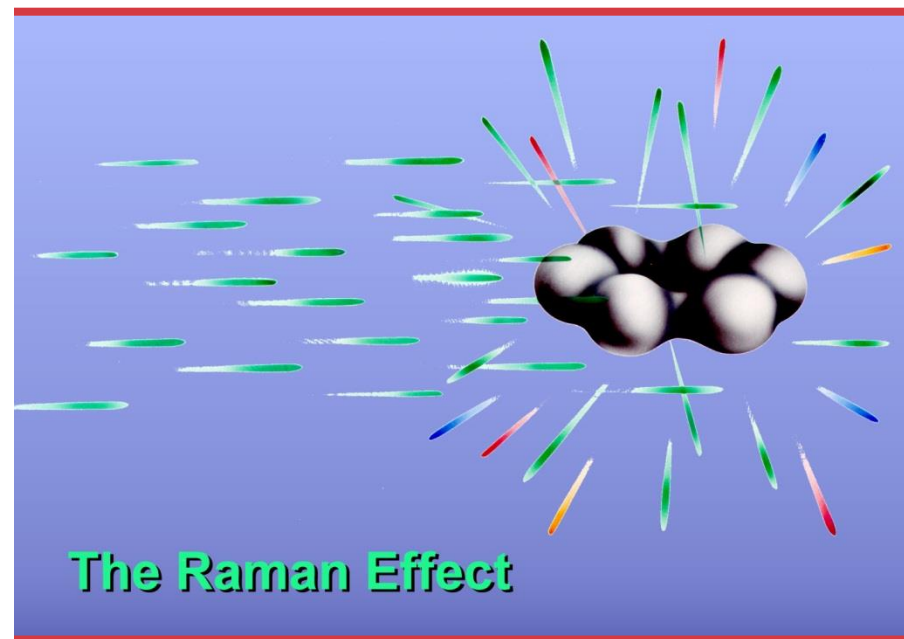


RAMANOV EFEKT

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

Promatrati sljedeće fizikalne efekte:

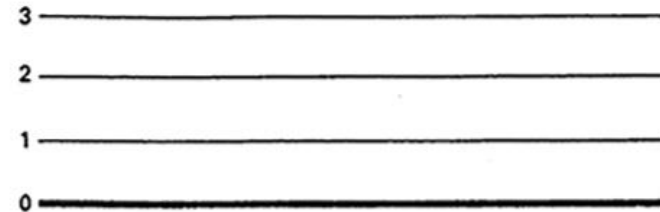
1. Glavni dio zračenja obasjava uzorak bez interakcije
2. Oko 10^{-4} zračenja raspršuje se elastično, tj. bez interakcije
– **Raleighovo zračenje**
3. Dio zračenja se putem elektronskih prijelaza apsorbira i emitira kao **fluorescencija**
4. Samo oko 10^{-8} upadnoga zračenja se raspršuje neelastično,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



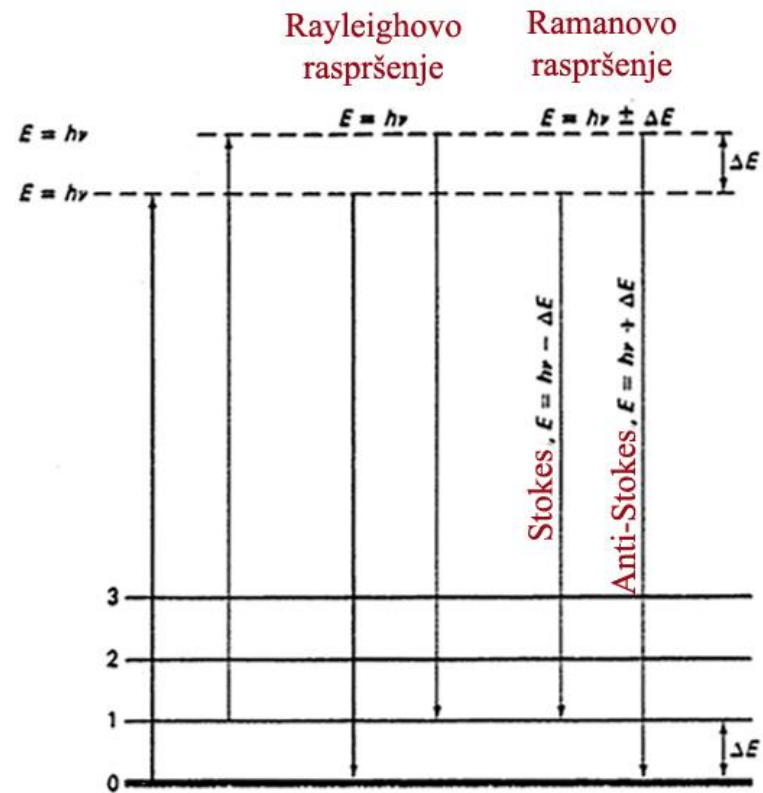
Ramanova spektroskopija

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

najniže
pobuđeno elektronsko
stanje



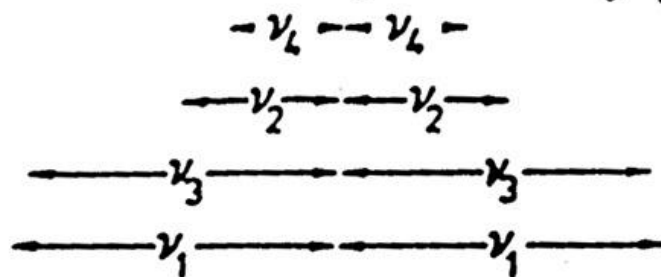
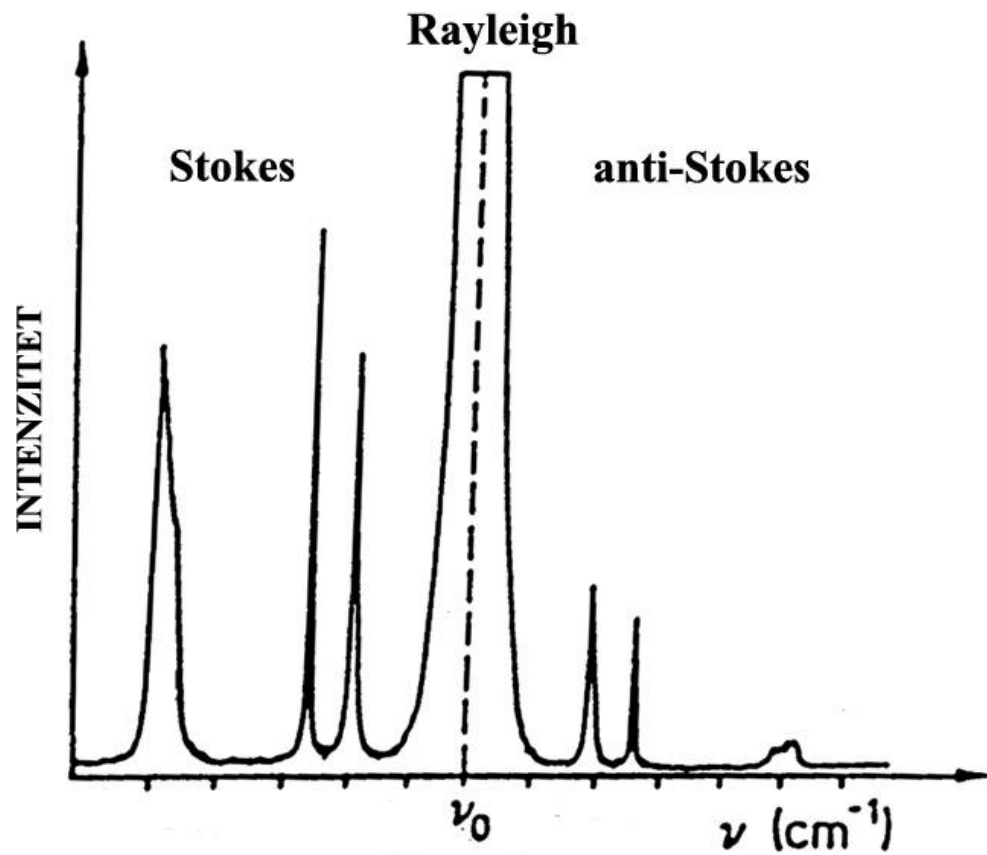
virtuelna stanja



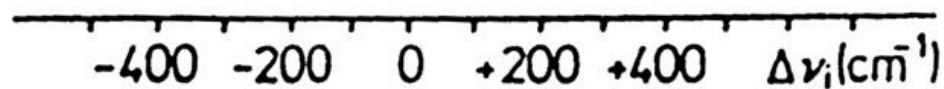
osnovno
elektronsko
stanje



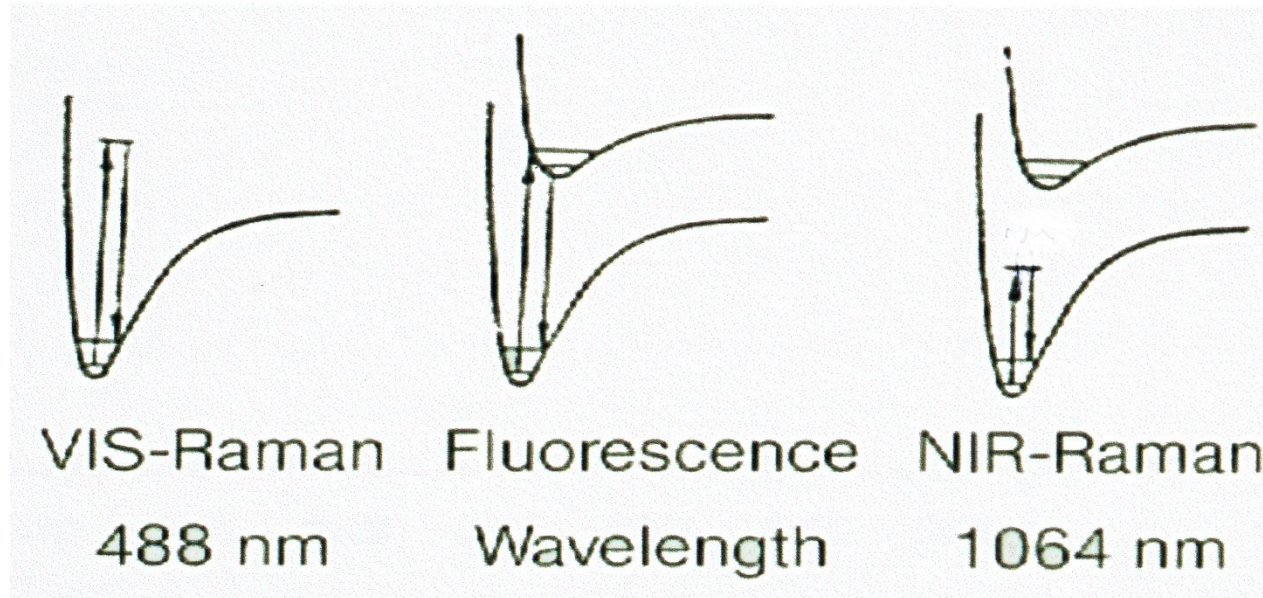
pobuda: $\lambda = 488 \text{ nm}$



Ramanov
pomak



Zašto NIR-Raman?



Nd-YAG laser
1064 nm

Ar 488 nm

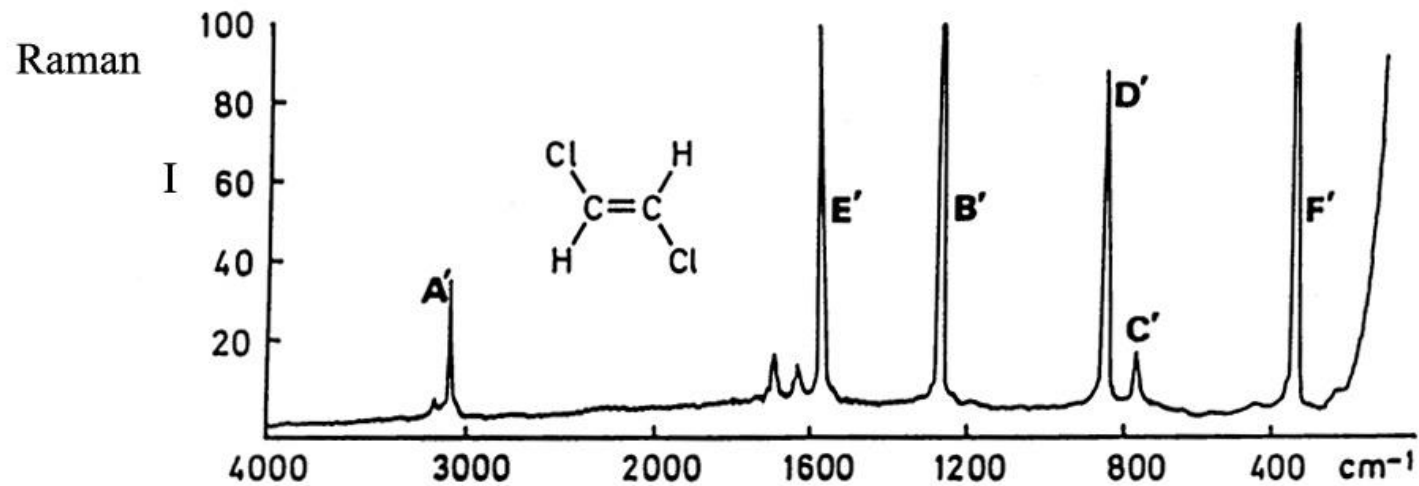
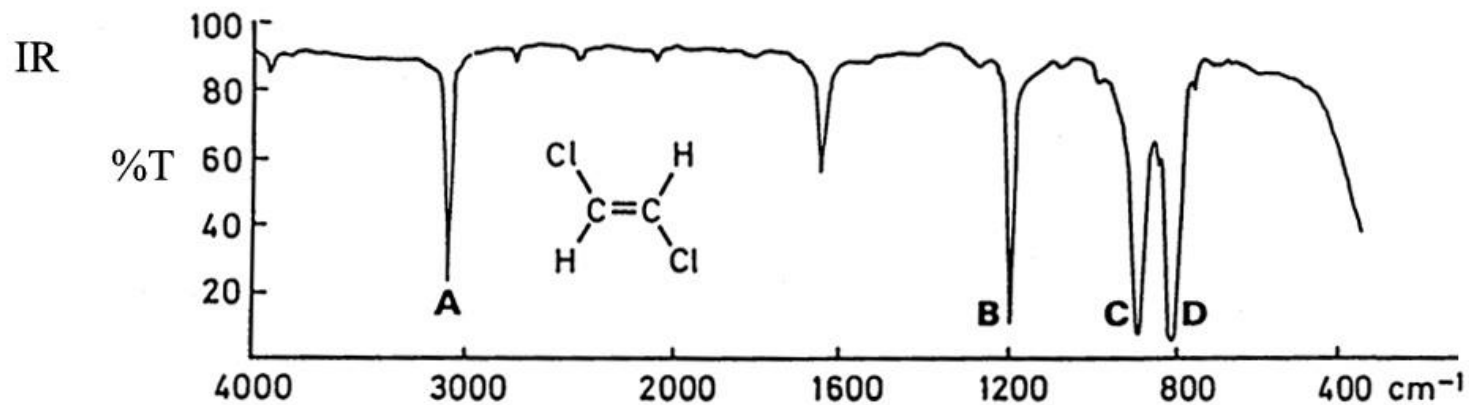
He-Ne 632 nm

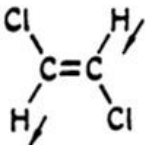
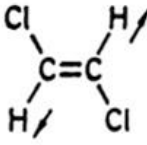
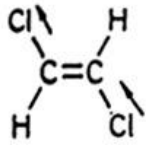
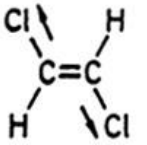
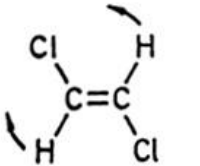
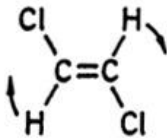
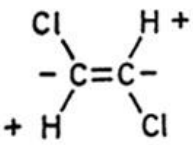
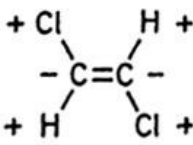
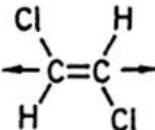
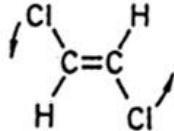
Diodni laseri 782 i 830 nm

Najčešće vrste Ramanove spektroskopije

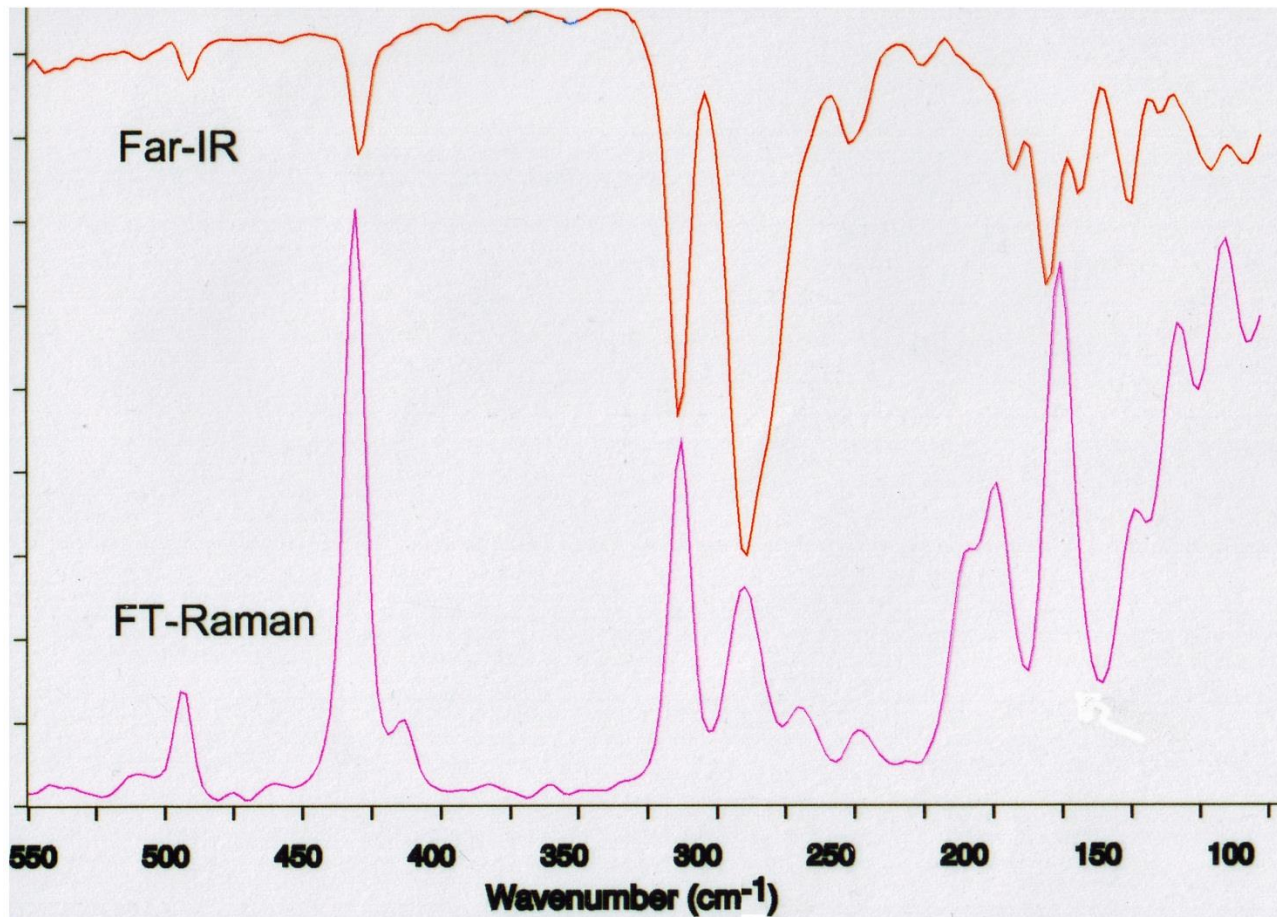
- FT Ramanova spektroskopija
- Disperzna Ramanova spektroskopija
- Rezonantna Ramanova spektroskopija
- Površinski pojačana Ramanova spektroskopija (SERS-Surface enhanced Raman spectroscopy)
- Površinski pojačana rezonantna Ramanova spektroskopija (SERRS)
- Nelinearna Ramanova spektroskopija- CARS (koherentna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

Pravilo isključenja



Način vibracije	asimetričan način vibracije (IR-aktivan)	IR-vrpca (cm ⁻¹)	simetričan način vibracije (Raman-aktivan)	Ramanova vrpca (cm ⁻¹)
ν (C—H)		3090 (A)		3070 (A')
ν (C—Cl)		817 (D)		844 (D')
δ (C—H)		1200 (B)		1270 (B')
γ (C—H)		895 (C)		760 (C')
ν (C=C)	—	—		1576 (E')
δ (C—Cl)	< 300 cm ⁻¹	—		350 (F')

Uzorak: kompleks bakra



Komplementarne informacije

VIBRACIJSKE FREKVENCije VEZA X-H/ cm^{-1}

ELEKTRONEGATIVNOST X					E L E K T R O N E G. X
BH 2500	CH 3000	NH 3400	OH 3600	FH 3960	
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 ₂ rast.
		C=S rast.	
		C-S rast.	
		S-S rast.	
		CH ₂ uv. ili njih.	

ALKANES

ALKENES

VINYL

TRANS

CIS

VINYLDIENE

TRISUBSTITUTED

TETRASUBSTITUTED

CONJUGATED

CUMULATED

CYCLIC

ALKYNES

MONOSUBSTITUTED

DISUBSTITUTED

MONONUCLEAR AROMATICS

BENZENE

MONOSUBSTITUTED

1,2-DISUBSTITUTED

1,3-DISUBSTITUTED

1,4-DISUBSTITUTED

1,2,4-TRISUBSTITUTED

1,2,3-TRISUBSTITUTED

1,3,5-TRISUBSTITUTED

ALCOHOLS AND PHENOLS

FREE OH

INTRAMOLECULAR BONDED (WEAK)

INTRAMOLECULAR BONDED (STRONG)

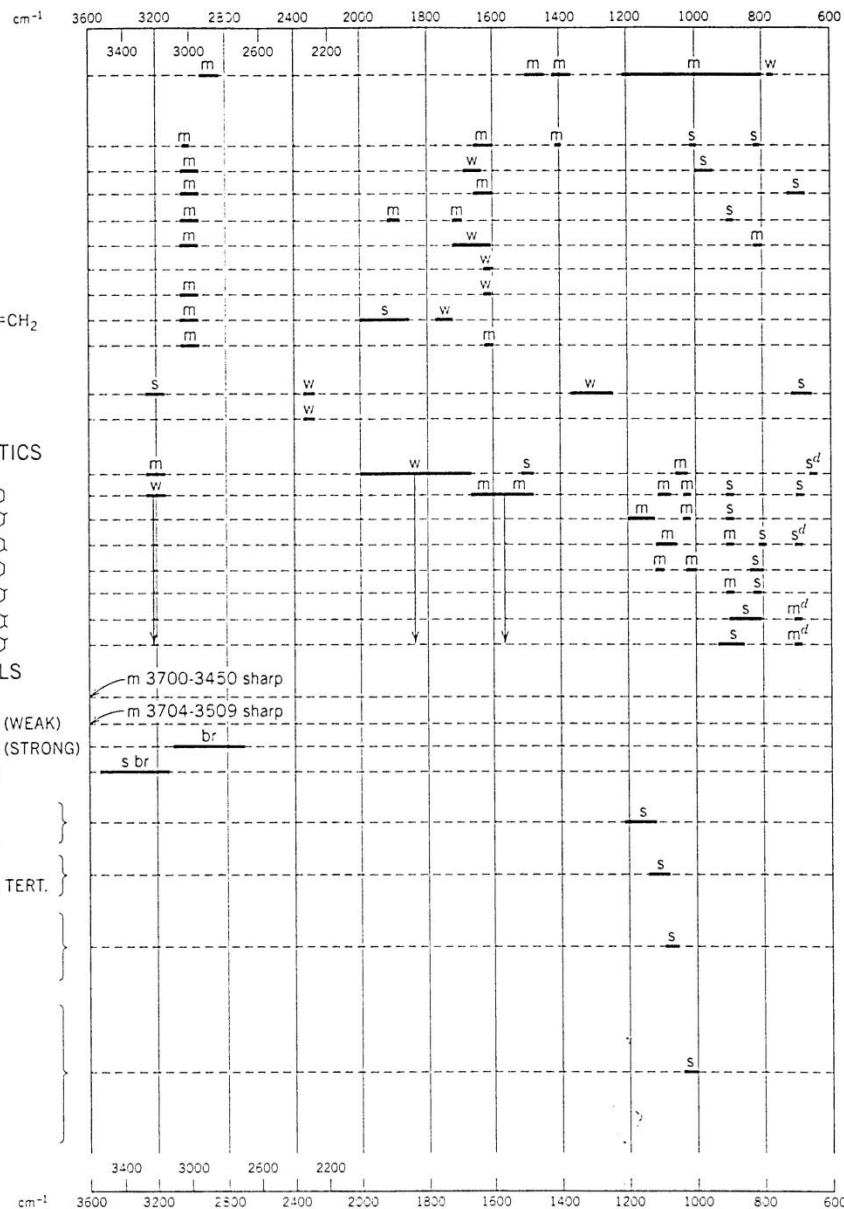
INTERMOLECULAR BONDED

SATURATED TERT.
HIGHLY SYMMETRICAL SEC.

SATURATED SEC.
 α -UNSATURATED OR CYCLIC TERT.

α -UNSATURATED SEC.
ALICYCLIC SEC. (5 OR 6-
MEMBERED RING)
SATURATED PRIMARY

α -UNSATURATED TERT.
 α -UNSATURATED AND
 α -BRANCHED SEC.
DI- α -UNSATURATED SEC.
ALICYCLIC SEC. (7 OR 8-
MEMBERED RING)
 α -BRANCHED AND/OR
 α -UNSATURATED PRIM.

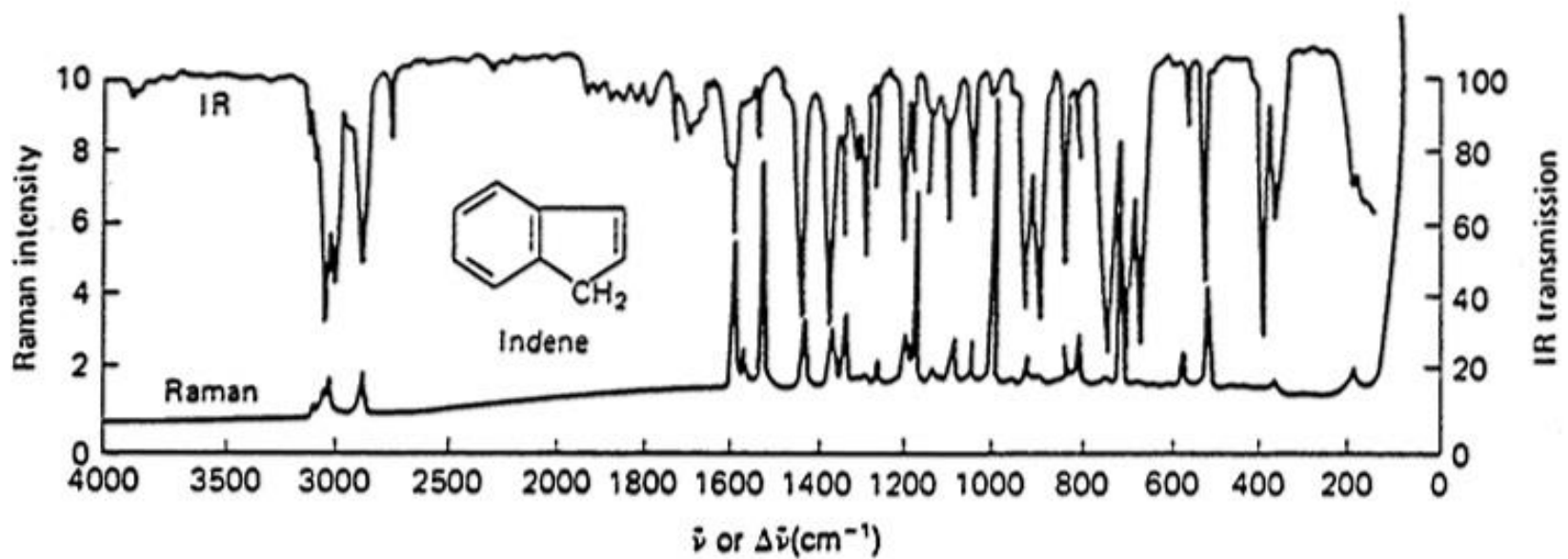
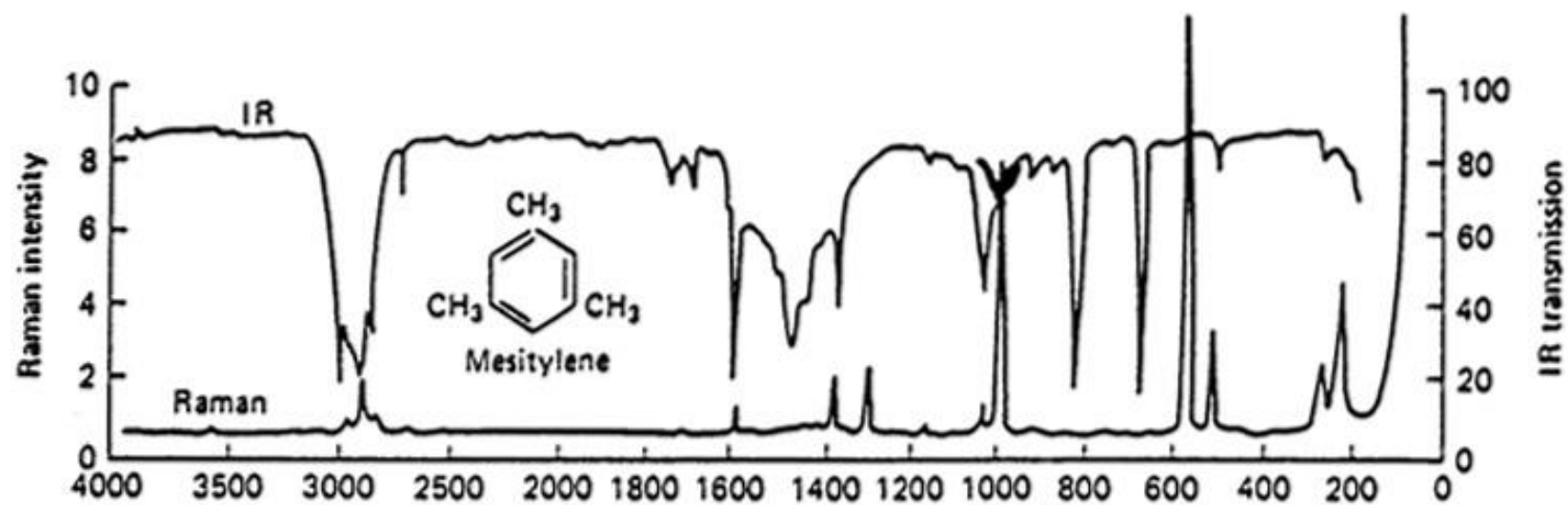


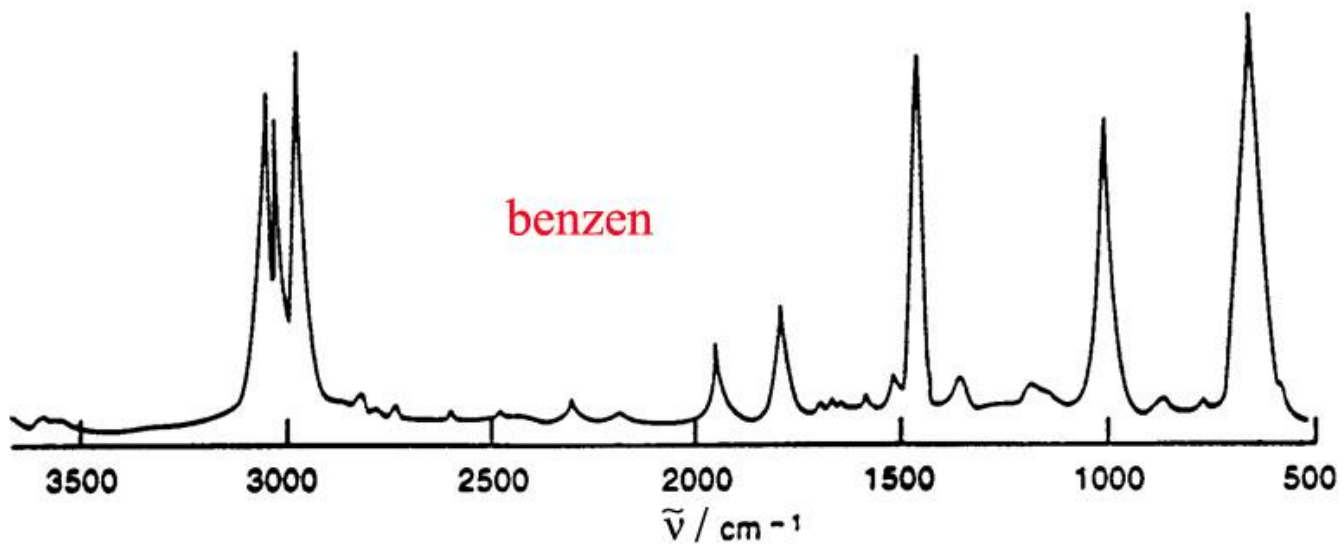
* Absorptions are shown by heavy bars. s = strong, m = medium, w = weak, sh = sharp, br = broad. Two intensity designations over a single bar indicate that two peaks may be present.

* May be absent.

* Frequently a doublet.

* Ring bending bands.





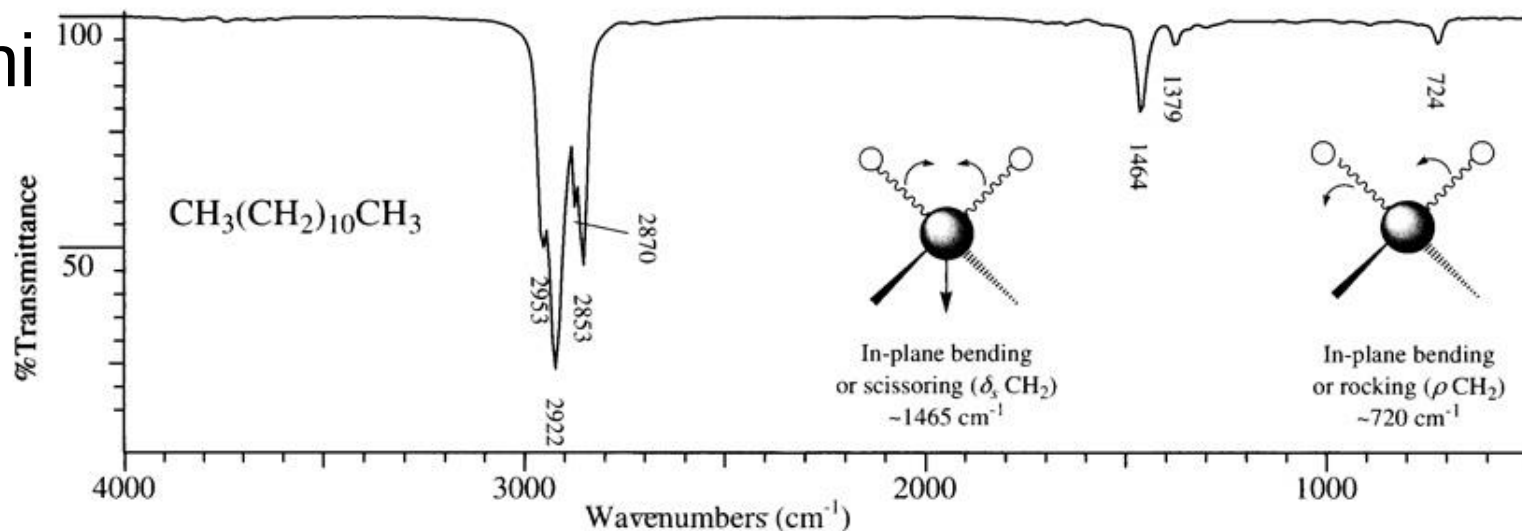
Primjena IR spektroskopije

- **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

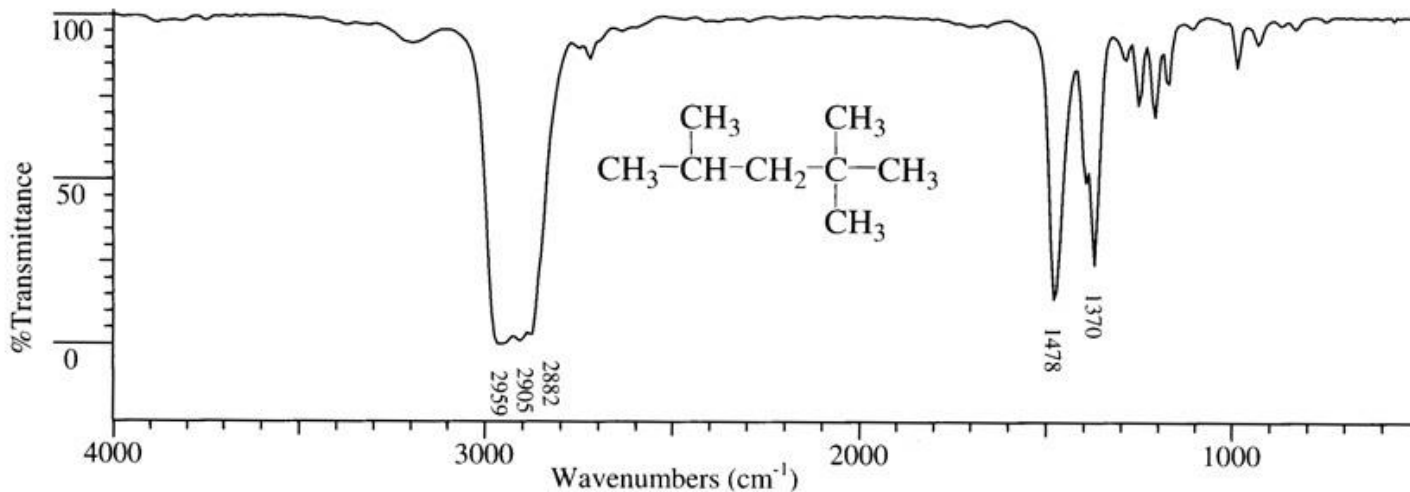
Primjena Ramanove spektroskopije

- Kvalitativna i kvantitativna analiza uzoraka u vodenoj otopini
- Analiza anorganskih spojeva: veze metal-ligand (100-700 cm^{-1}), koordinacijski spojevi ((halogenidni i oksikompleksi s metalima, npr. VO_4^{3-} , $\text{Al}(\text{OH})_4^-$))
- Analiza organskih spojeva: olefini, cikloalkani (veličina prstena)
- Analiza bioloških uzoraka

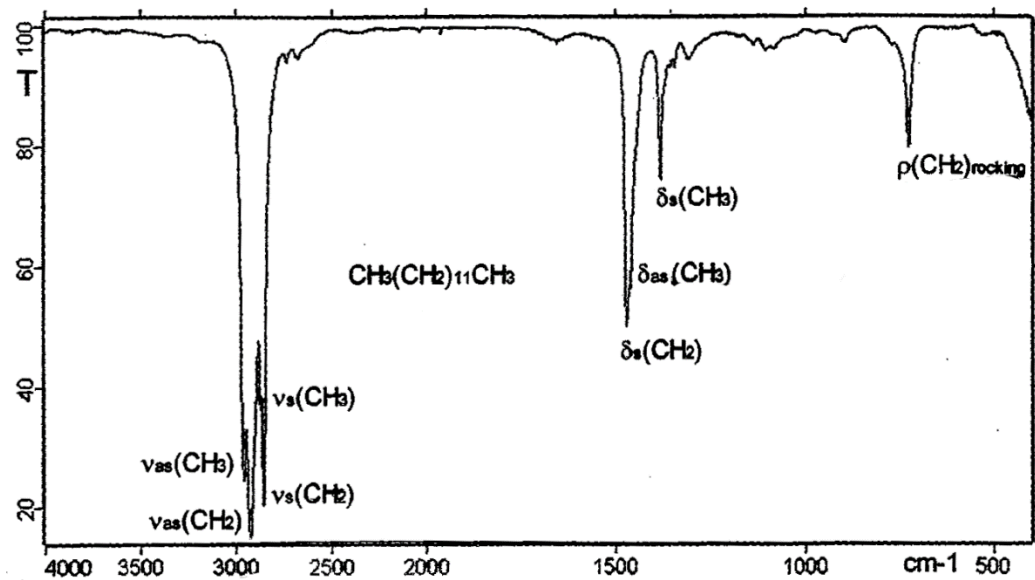
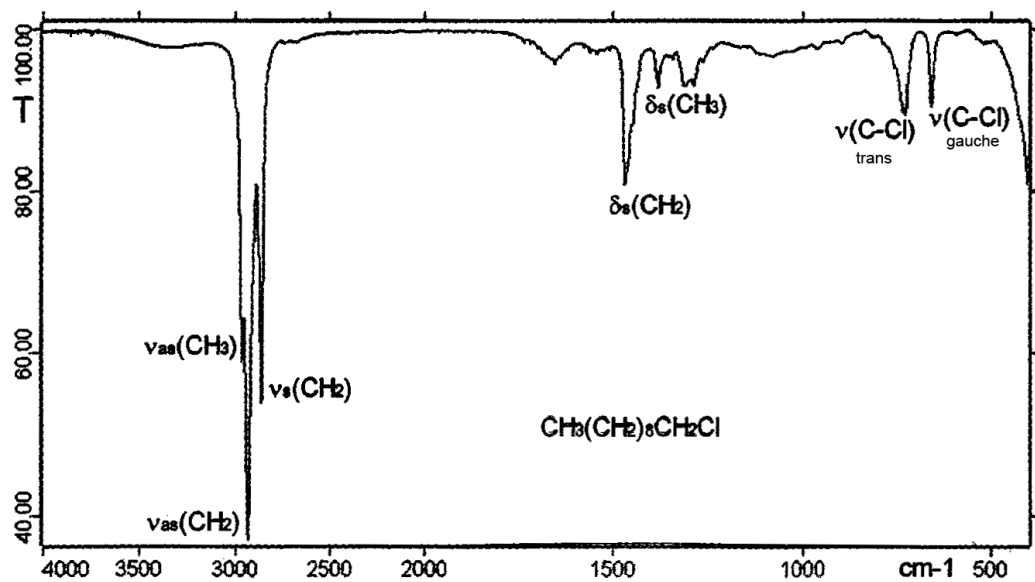
alkani



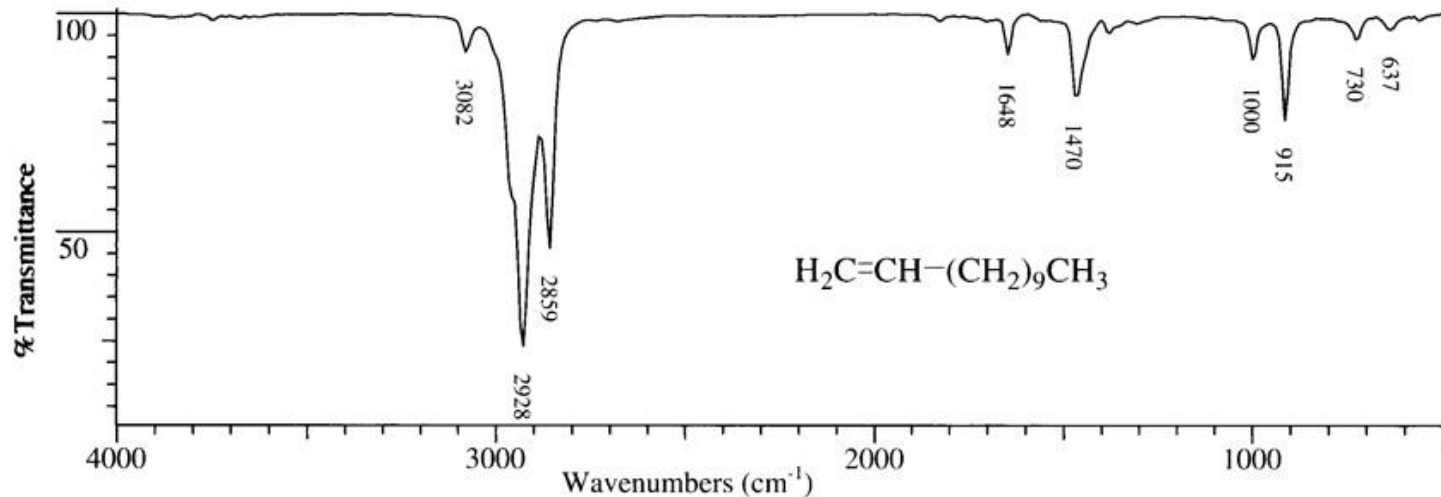
Dodecane. C—H stretch: $2953 \text{ cm}^{-1} \nu_{\text{as}} \text{CH}_3$, $2870 \text{ cm}^{-1} \nu_{\text{s}} \text{CH}_3$, $2922 \text{ cm}^{-1} \nu_{\text{as}} \text{CH}_2$, $2853 \text{ cm}^{-1} \nu_{\text{s}} \text{CH}_2$.
C—H bend: $1464 \text{ cm}^{-1} \delta_s \text{CH}_2$, $1450 \text{ cm}^{-1} \delta_{\text{as}} \text{CH}_3$, $1379 \text{ cm}^{-1} \delta_s \text{CH}_3$. CH_2 rock: $724 \text{ cm}^{-1} \rho \text{CH}_2$.



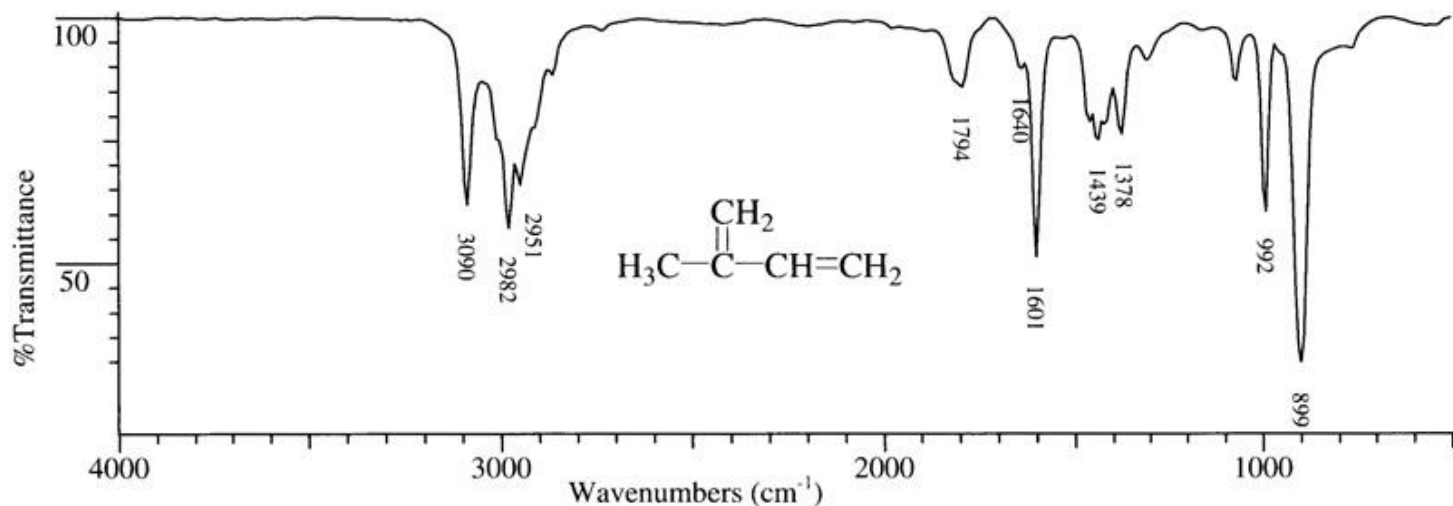
2,2,4-Trimethylpentane. C—H stretch. C—H bend. There are overlapping doublets for the *t*-butyl and the isopropyl groups at $1400\text{--}1340 \text{ cm}^{-1}$.



alkeni

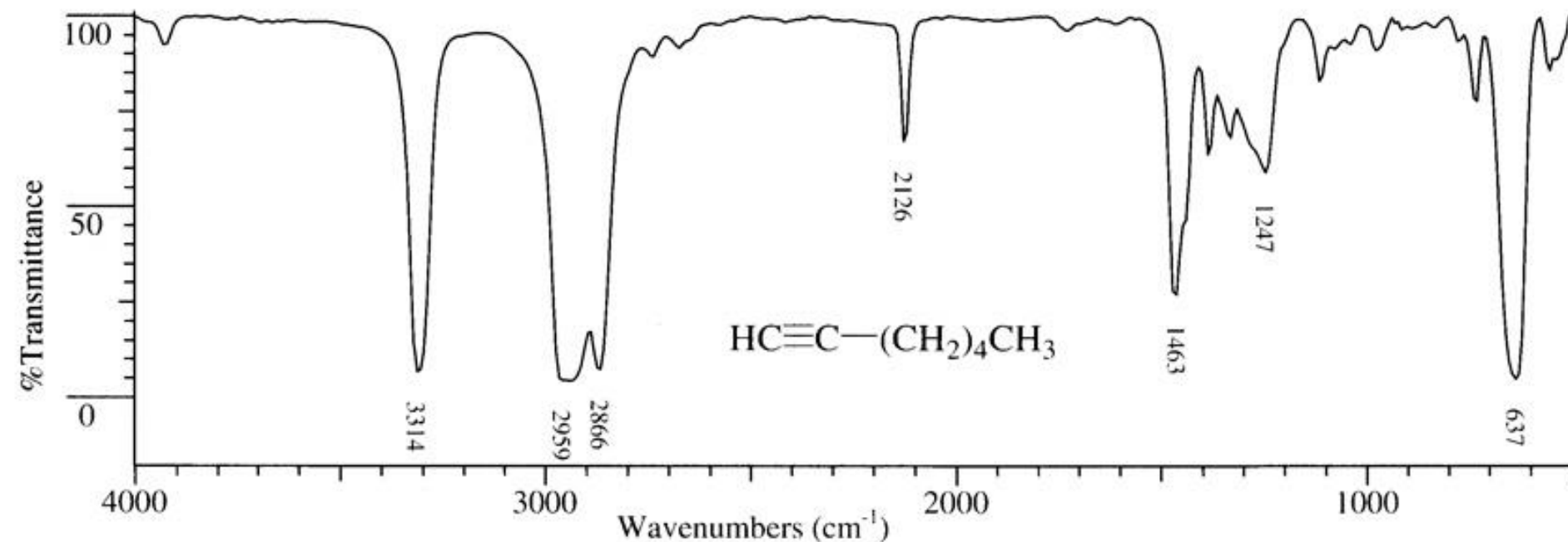


1-Dodecene. C—H stretch. Note alkene C—H stretch at 3082 cm^{-1} . C=C **stretch**, 1648 cm^{-1} . Out-of-plane C—H bend: 1000 cm^{-1} , (alkene) 915 cm^{-1} . Methylene **rock**: 730 cm^{-1} .

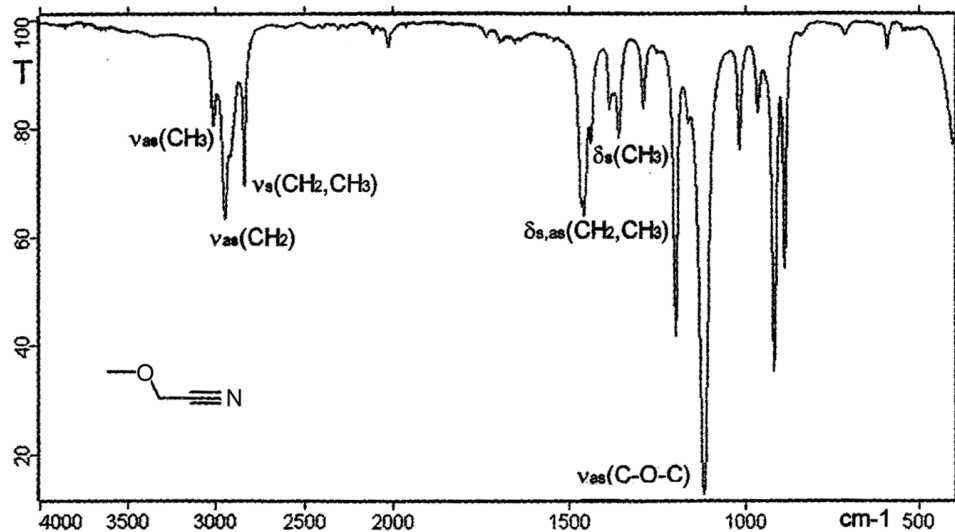
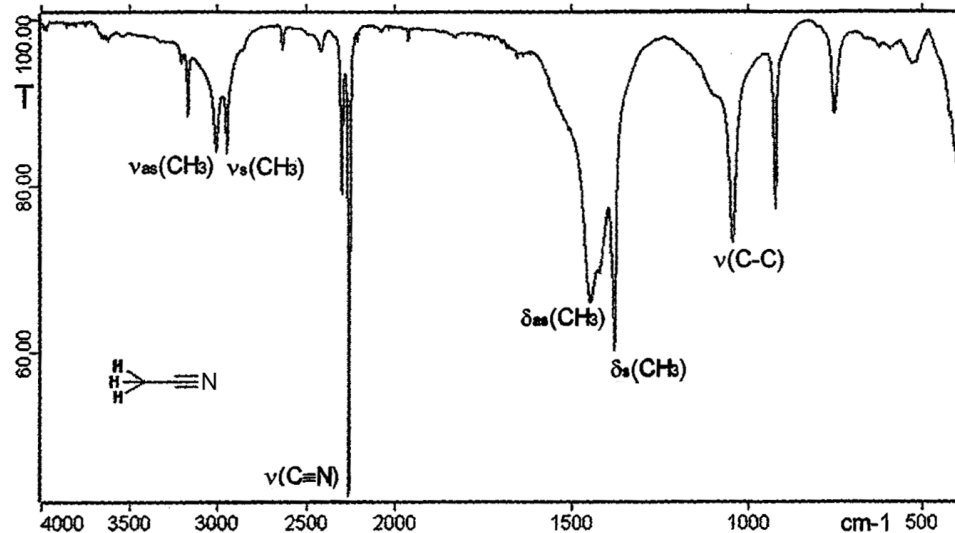
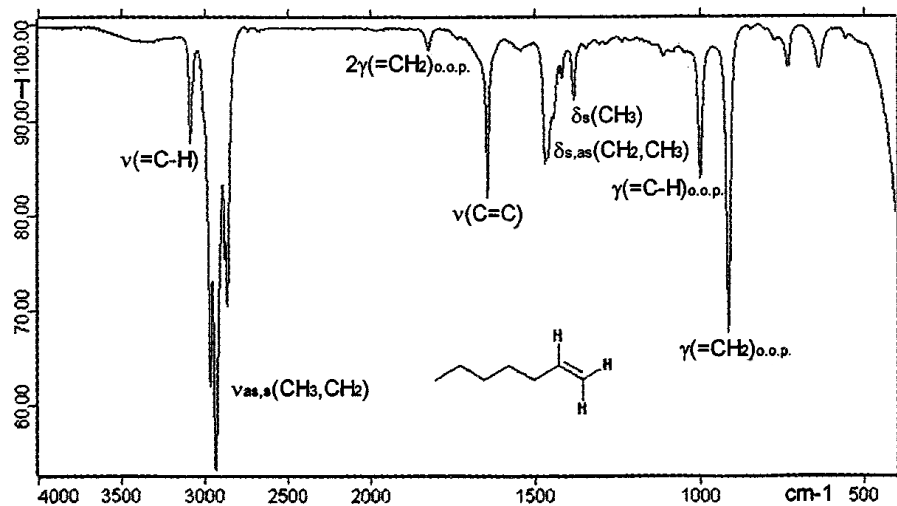


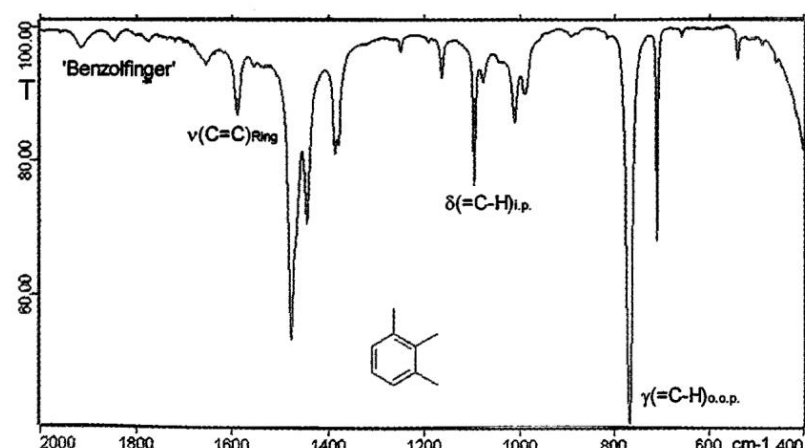
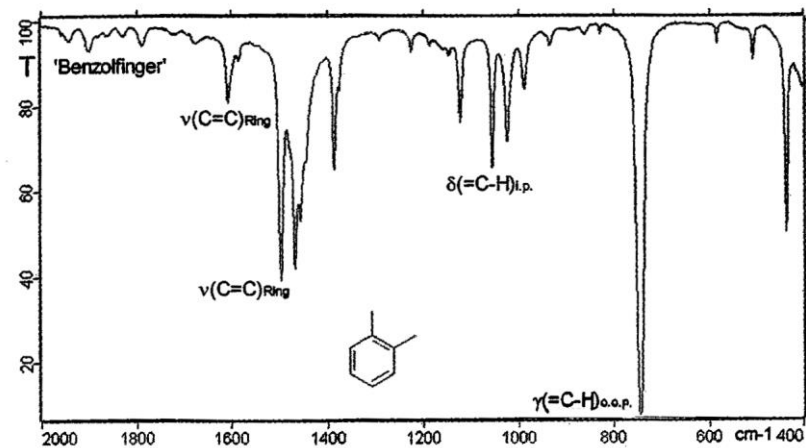
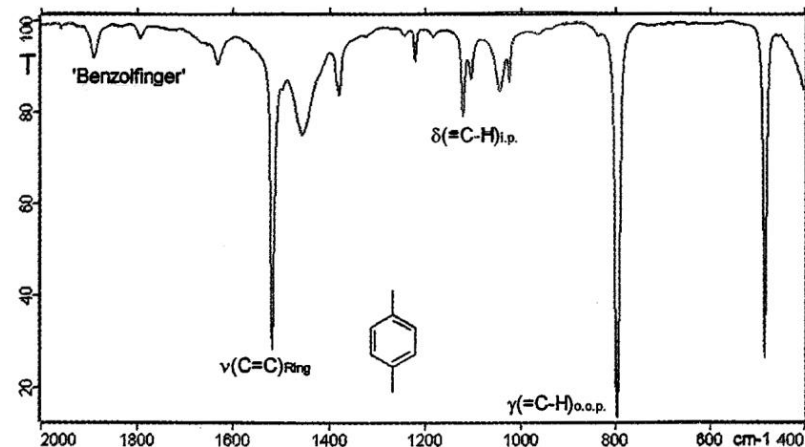
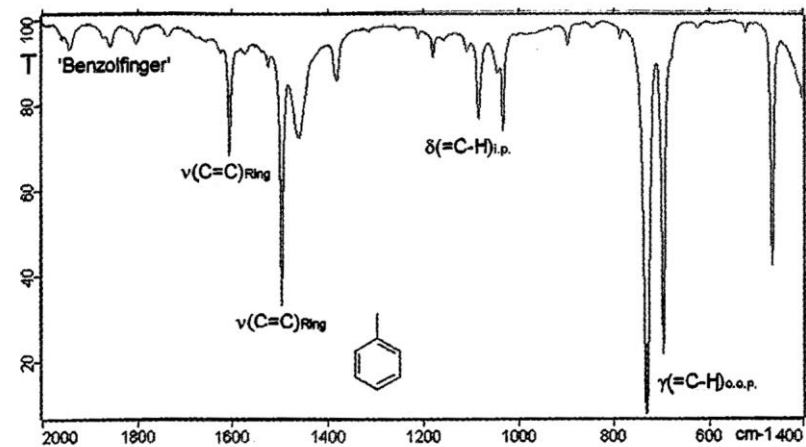
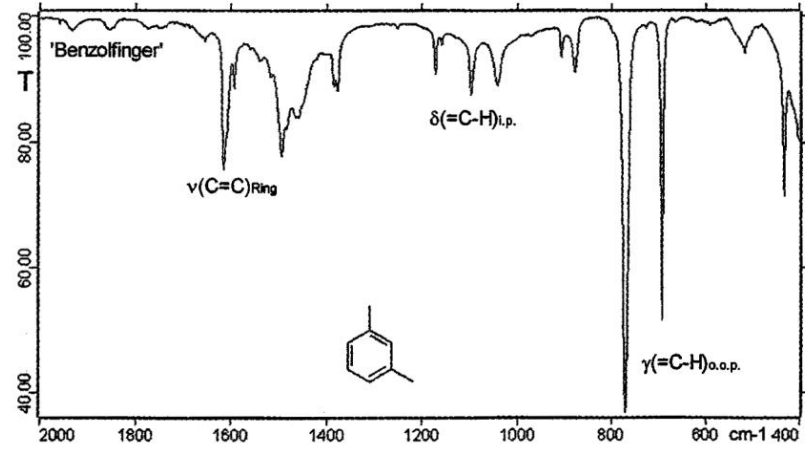
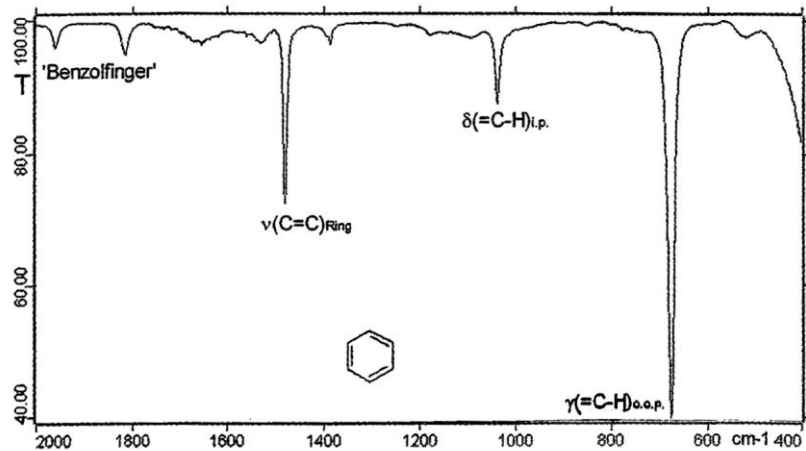
Isoprene. C—H stretch: $=\text{C}-\text{H}$ 3090 cm^{-1} . Coupled C=C—C=C stretch: symmetric 1640 cm^{-1} (weak), asymmetric 1601 cm^{-1} (strong). C—H bend (saturated, alkene in-plane). C—H out-of-plane bend: 992 cm^{-1} , 899 cm^{-1} .

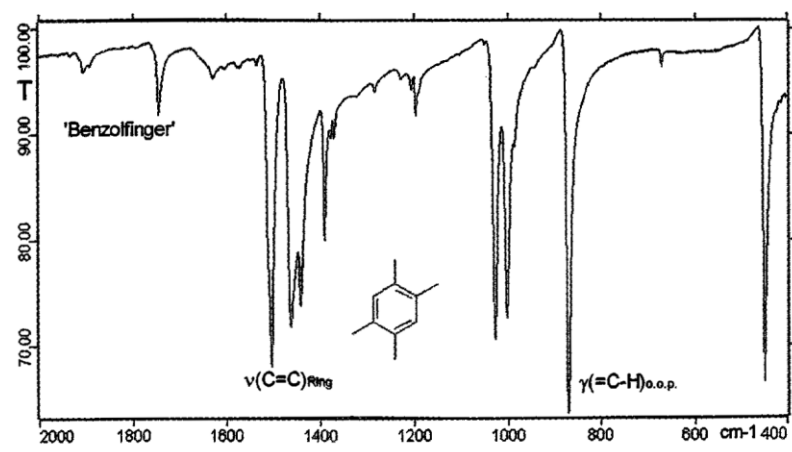
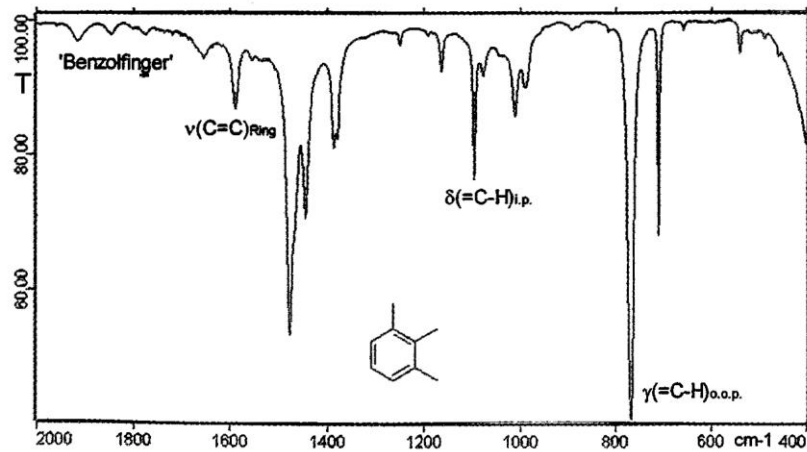
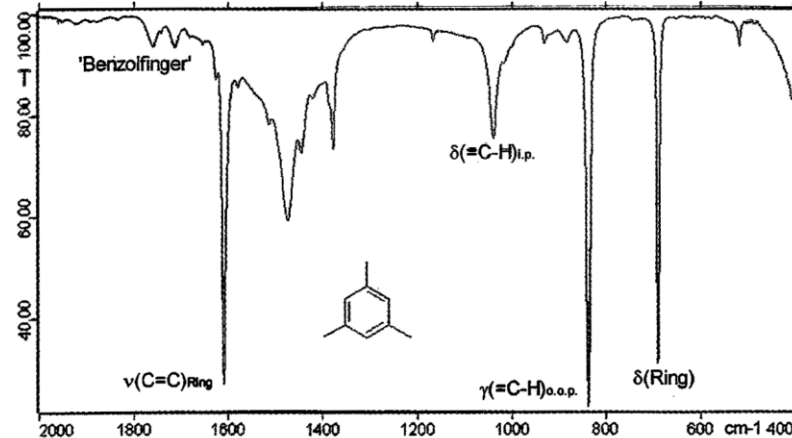
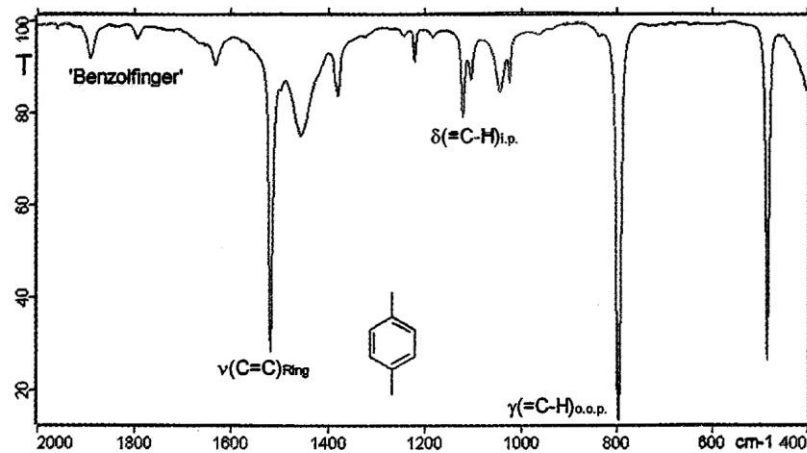
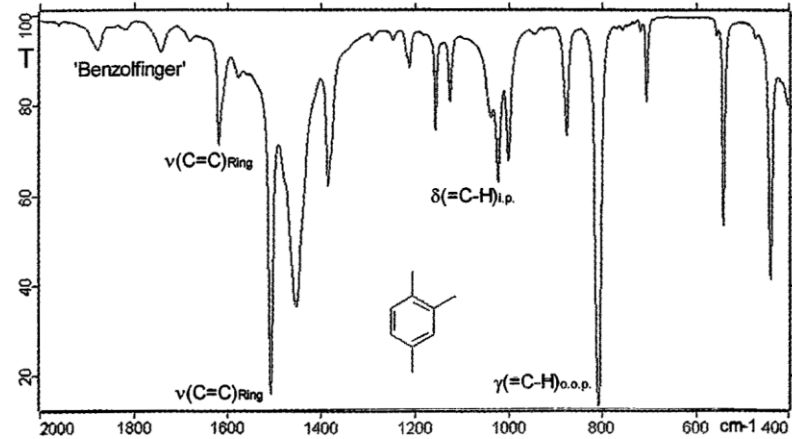
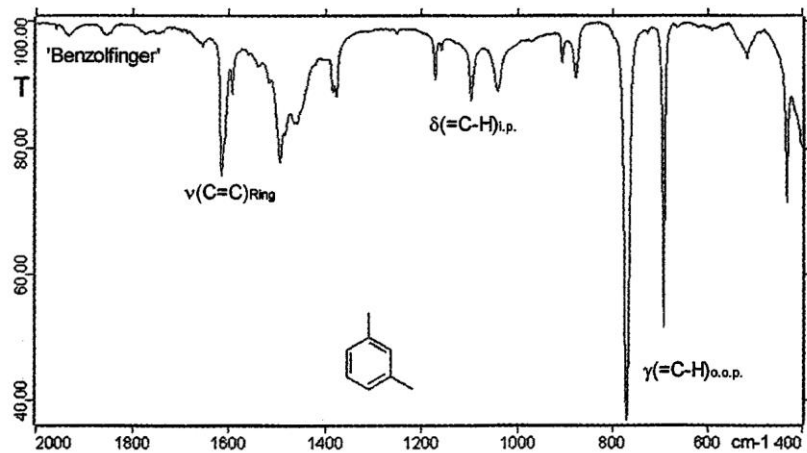
alkini

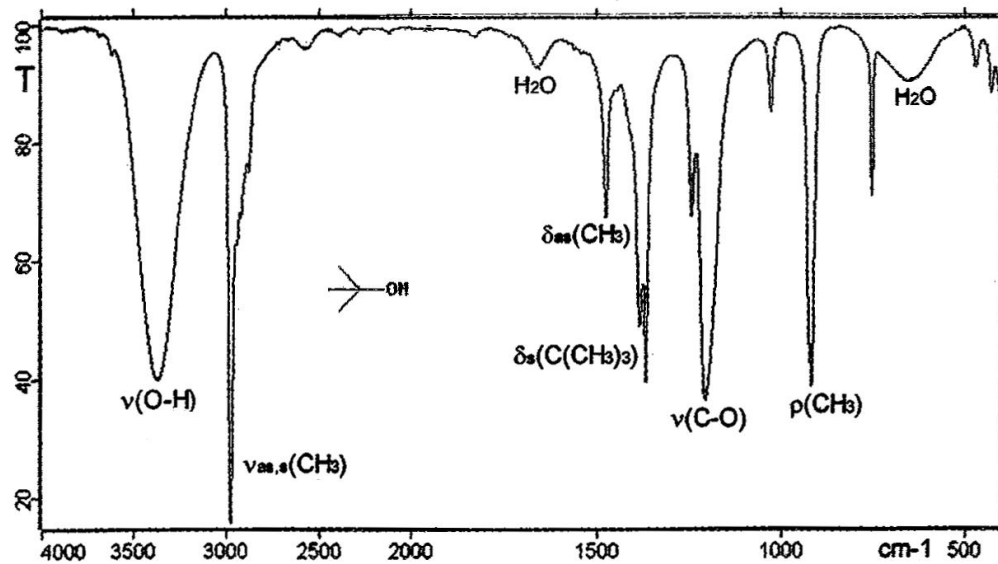
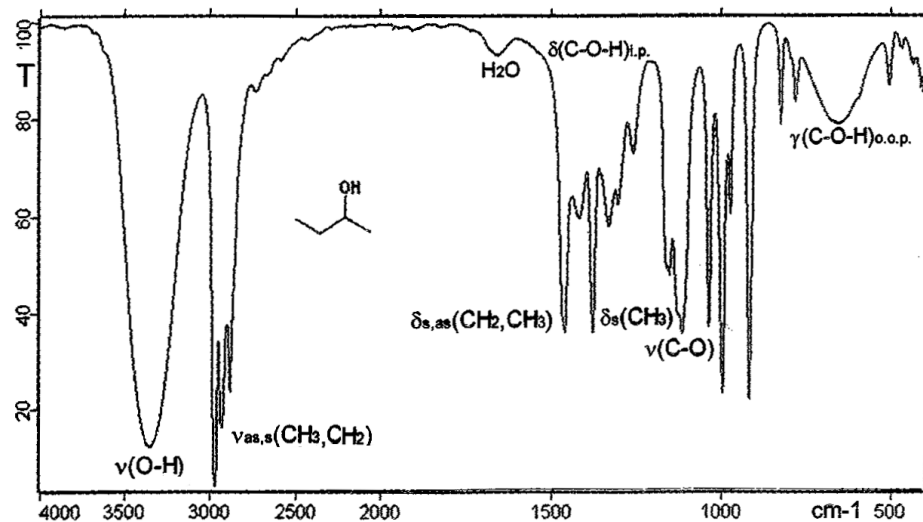
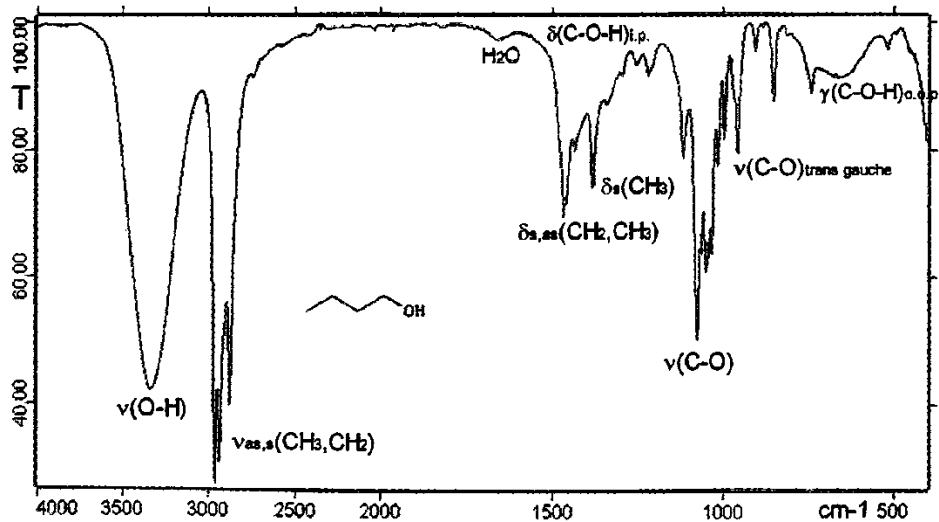


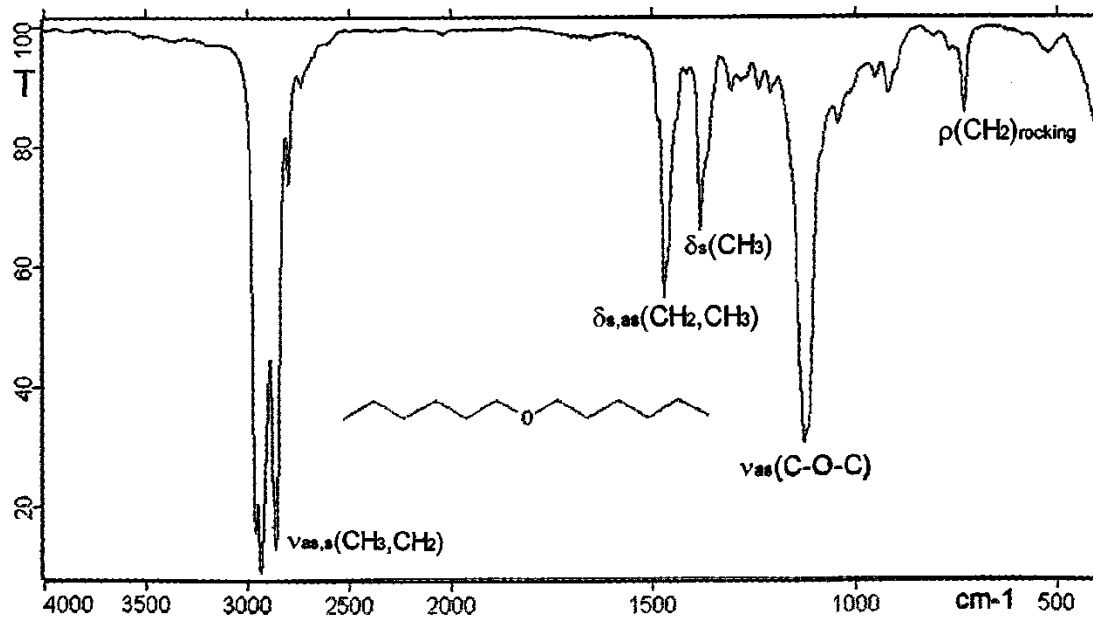
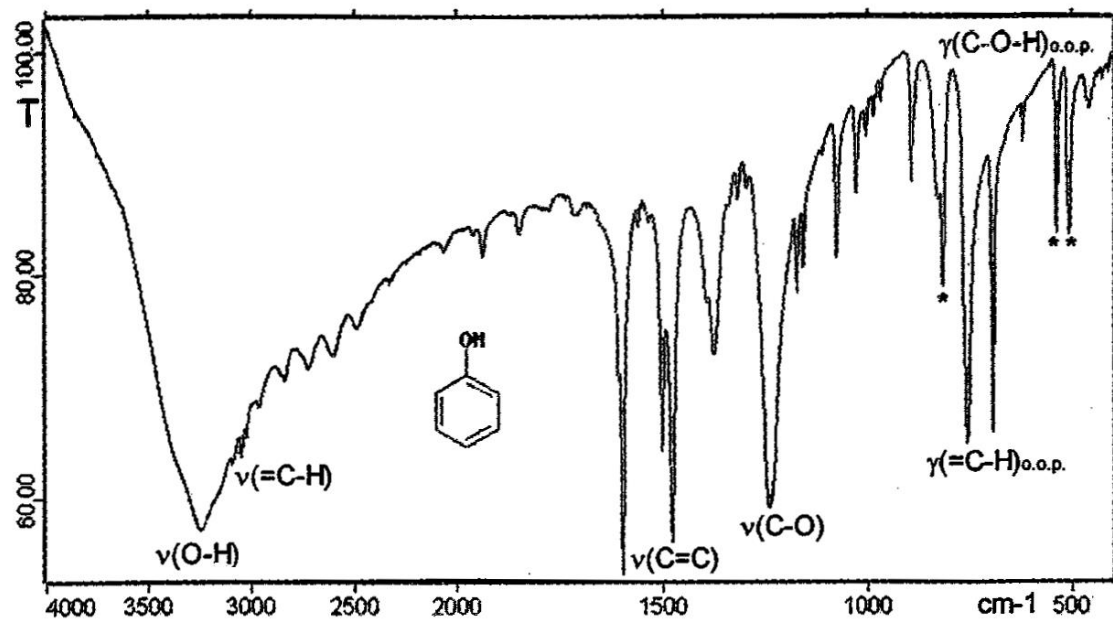
1-Heptyne, $\equiv\text{C}-\text{H}$ stretch, 3314 cm^{-1} . Alkyl $\text{C}-\text{H}$ stretch $1450-1360\text{ cm}^{-1}$, $2960-2860\text{ cm}^{-1}$. $\text{C}\equiv\text{C}$ stretch, 2126 cm^{-1} . $\text{C}-\text{H}$ bend: 1463 cm^{-1} $\delta_s\text{CH}_2$, 1450 cm^{-1} $\delta_{as}\text{CH}_3$.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

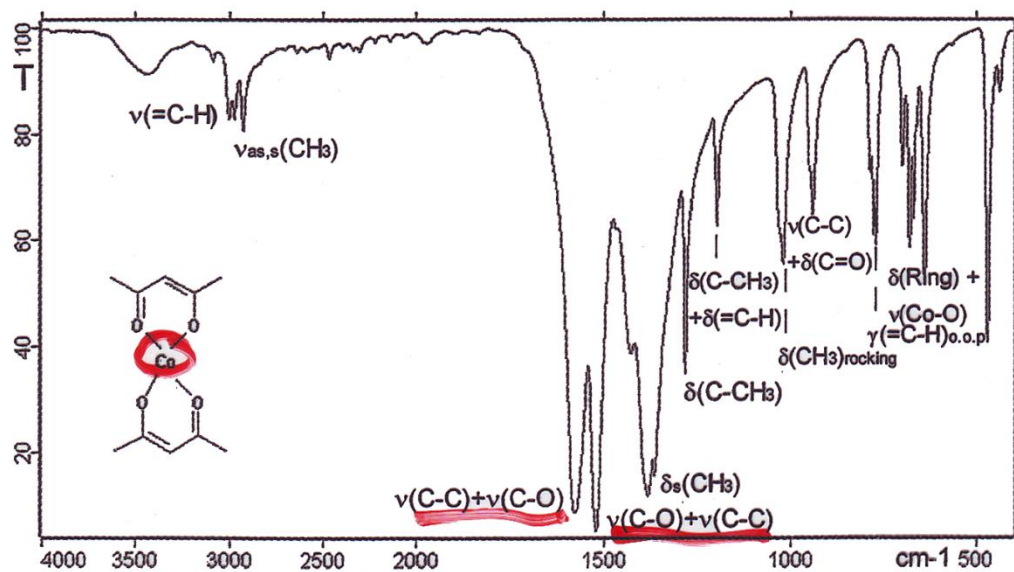
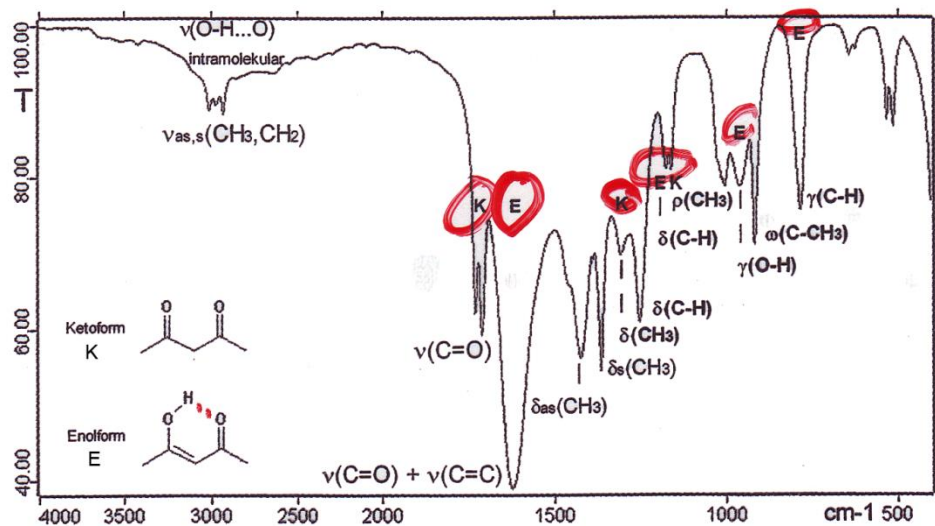
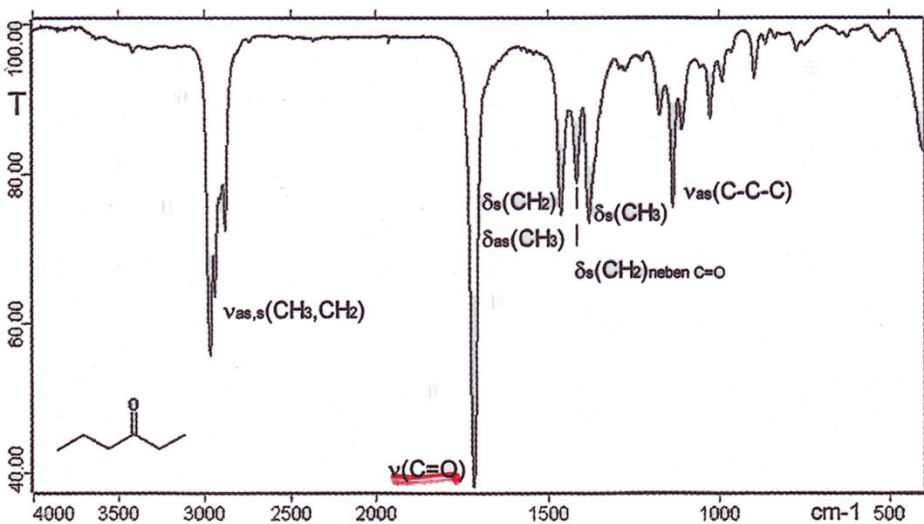


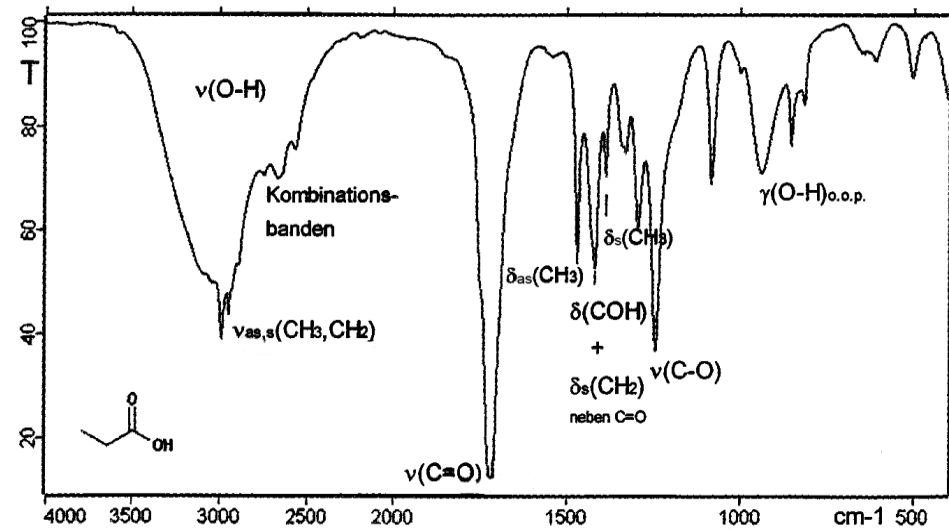
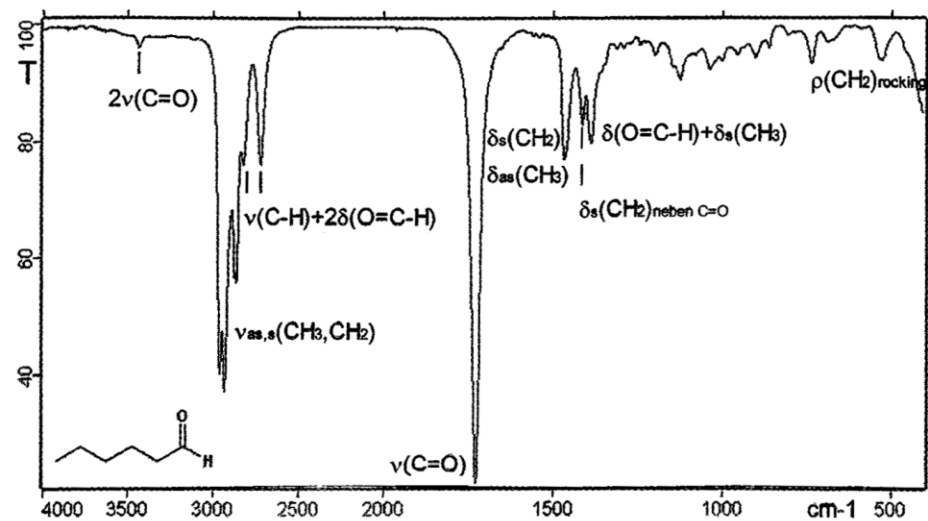


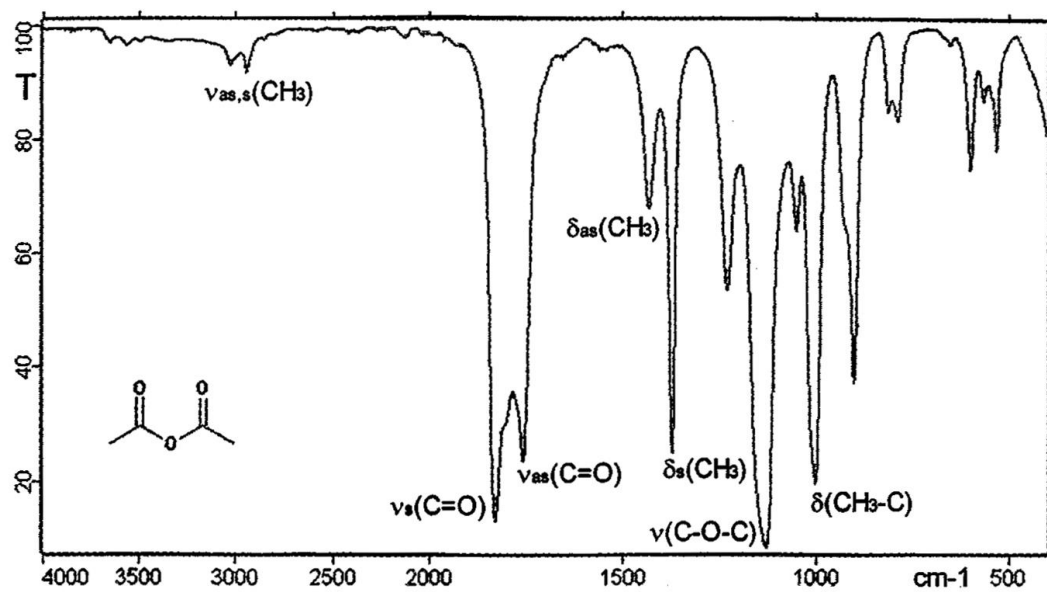
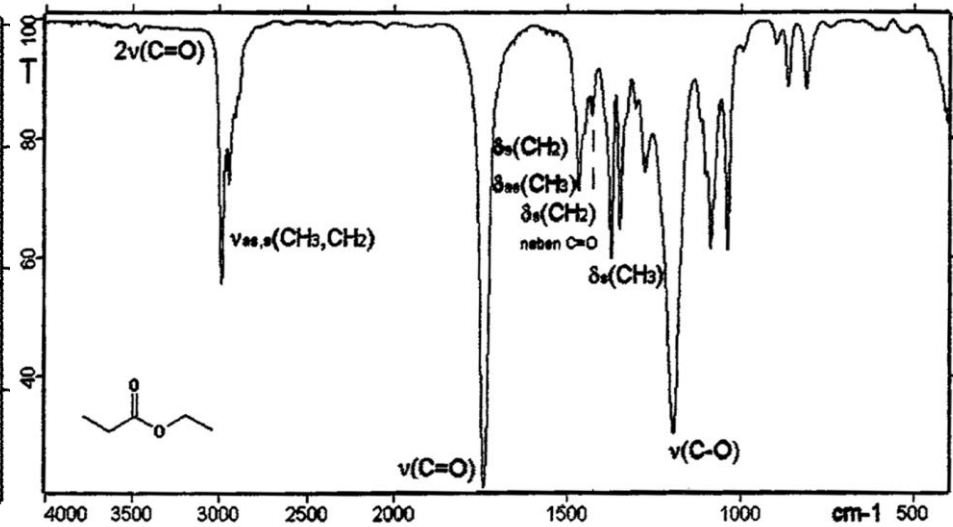
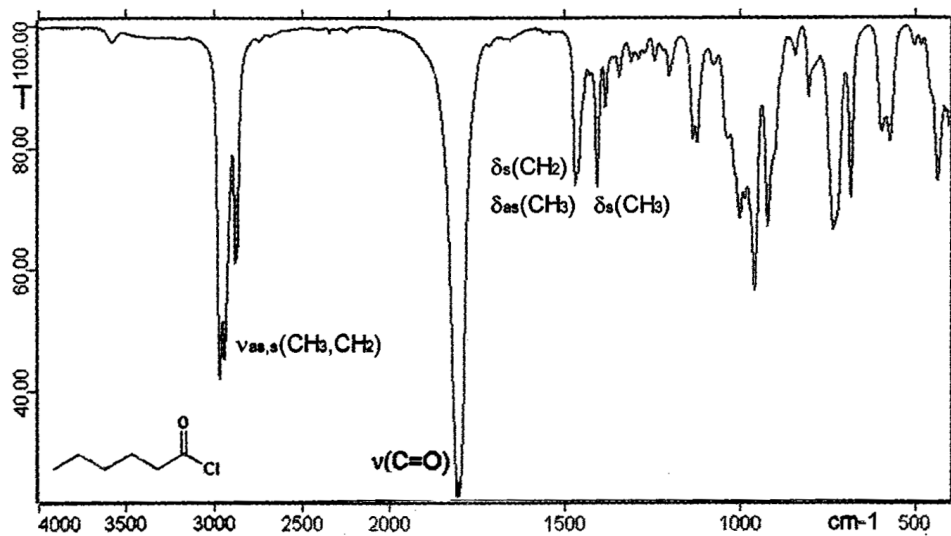


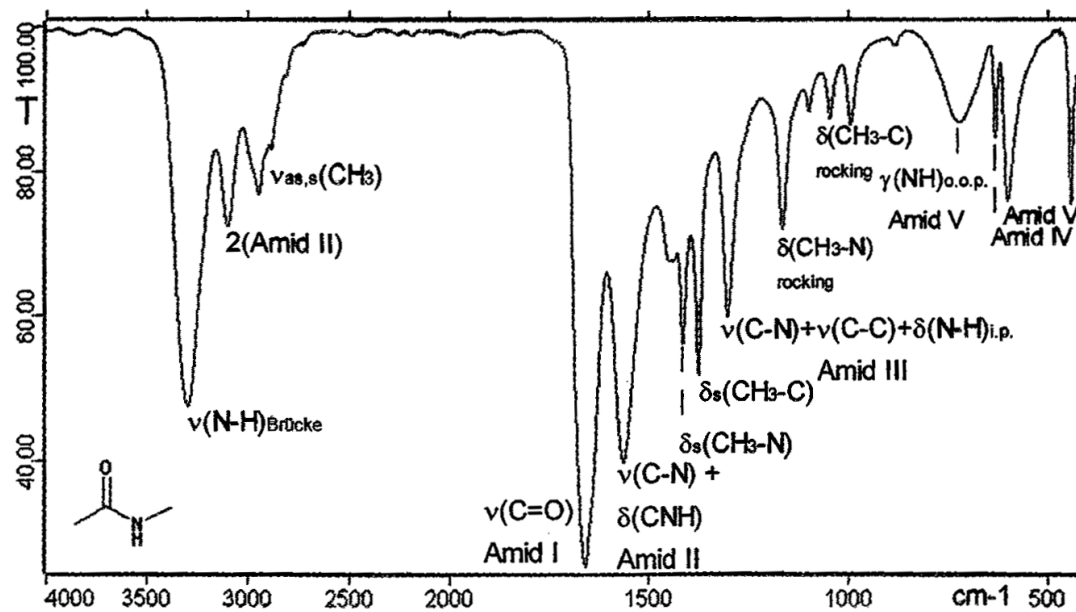
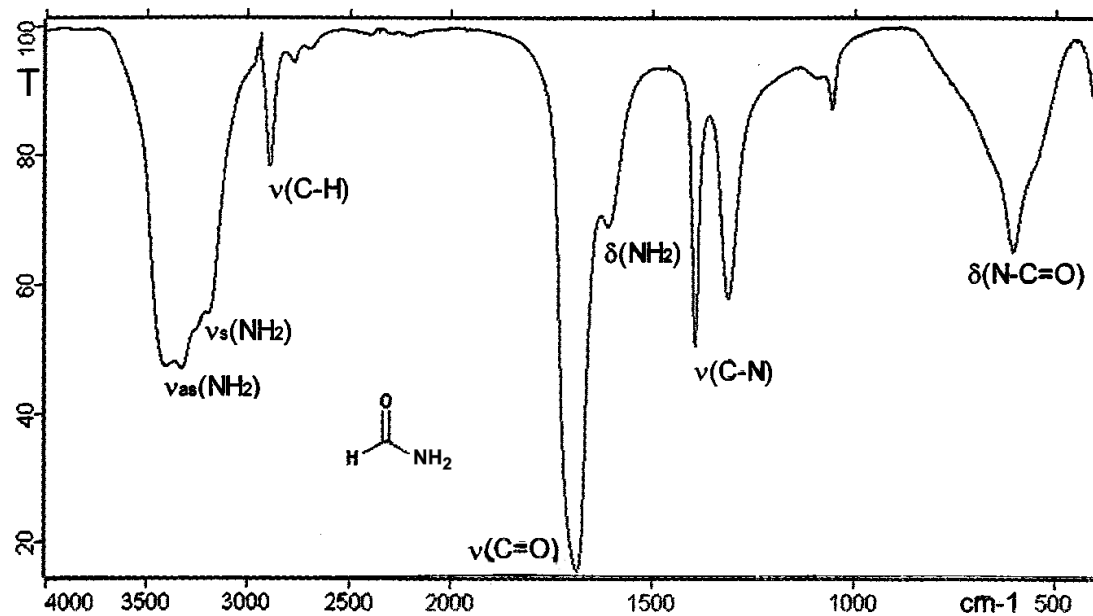


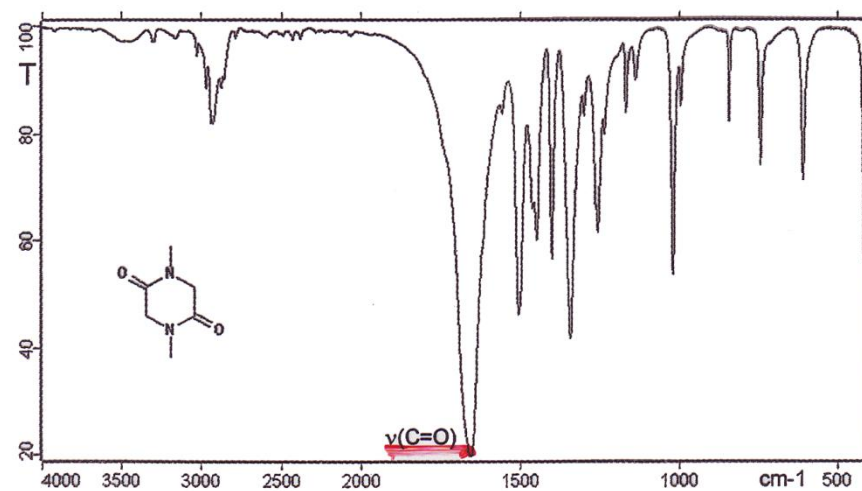
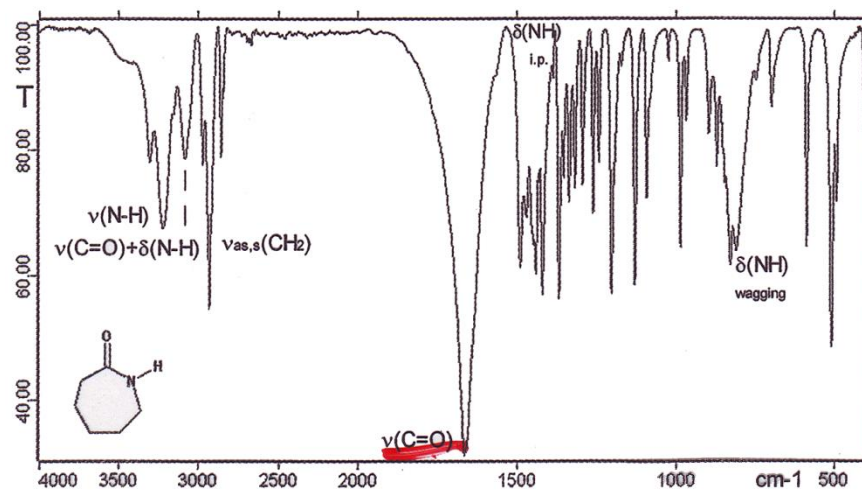


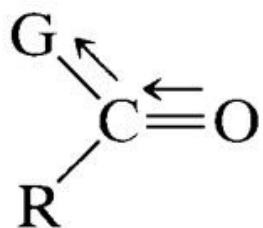






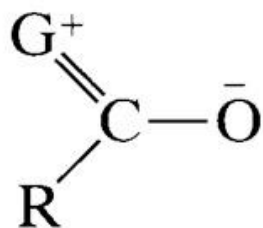






G Effect Predominantly Inductive

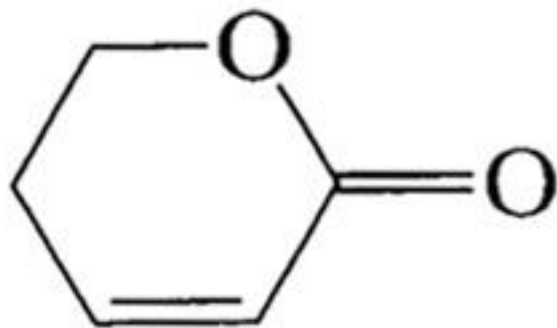
G	ν C=O (cm ⁻¹)
Cl	1815–1785
F	~1869
Br	1812
OH (monomer)	1760
OR	1750–1735



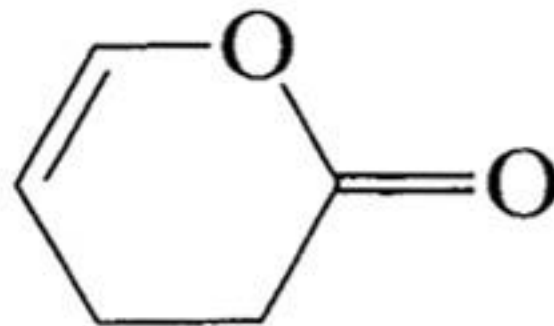
G Effect Predominantly Resonance

G	ν C=O (cm ⁻¹)
NH ₂	1695–1650
SR	1720–1690

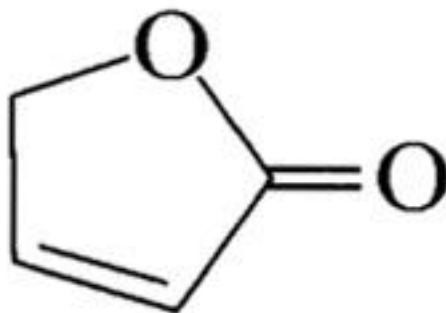
laktoni



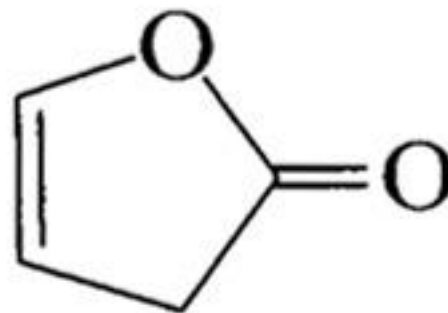
1720 cm^{-1}



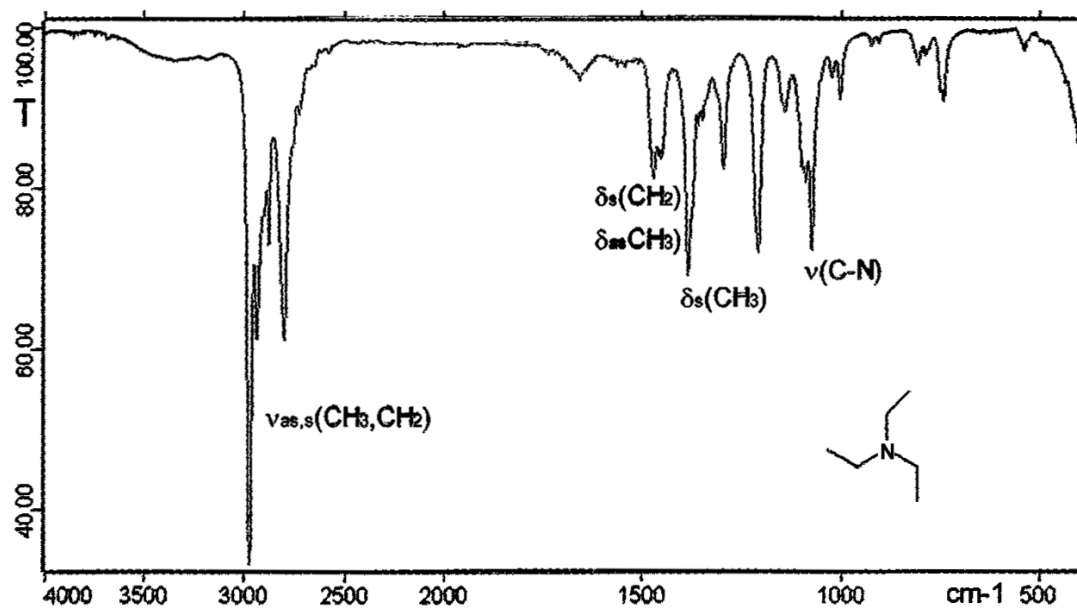
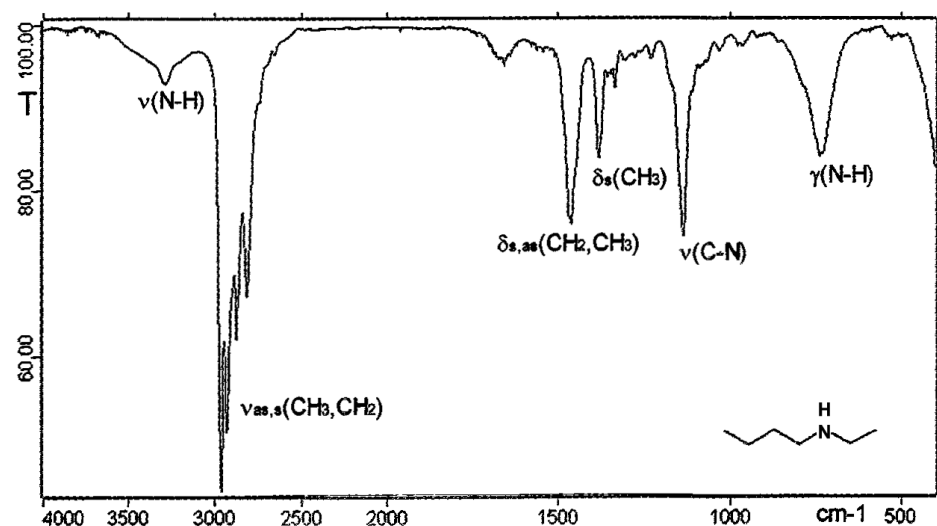
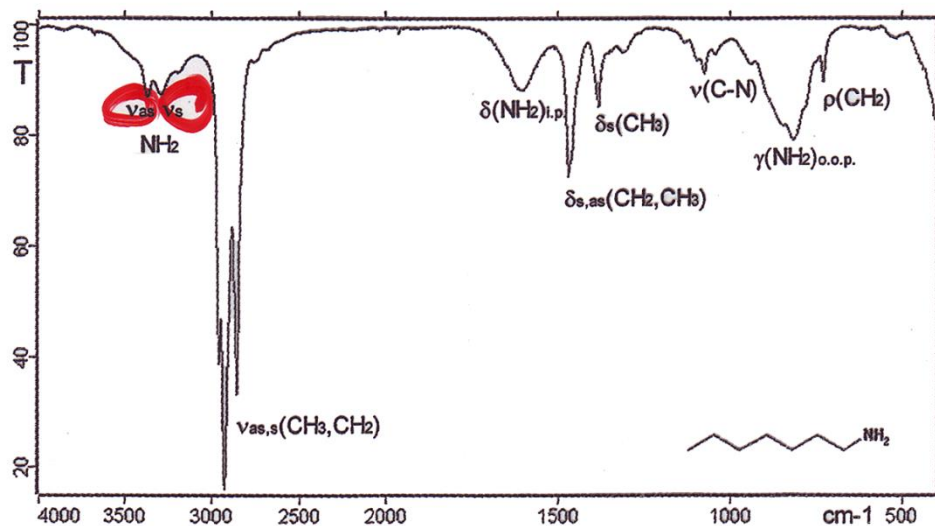
1760 cm^{-1}

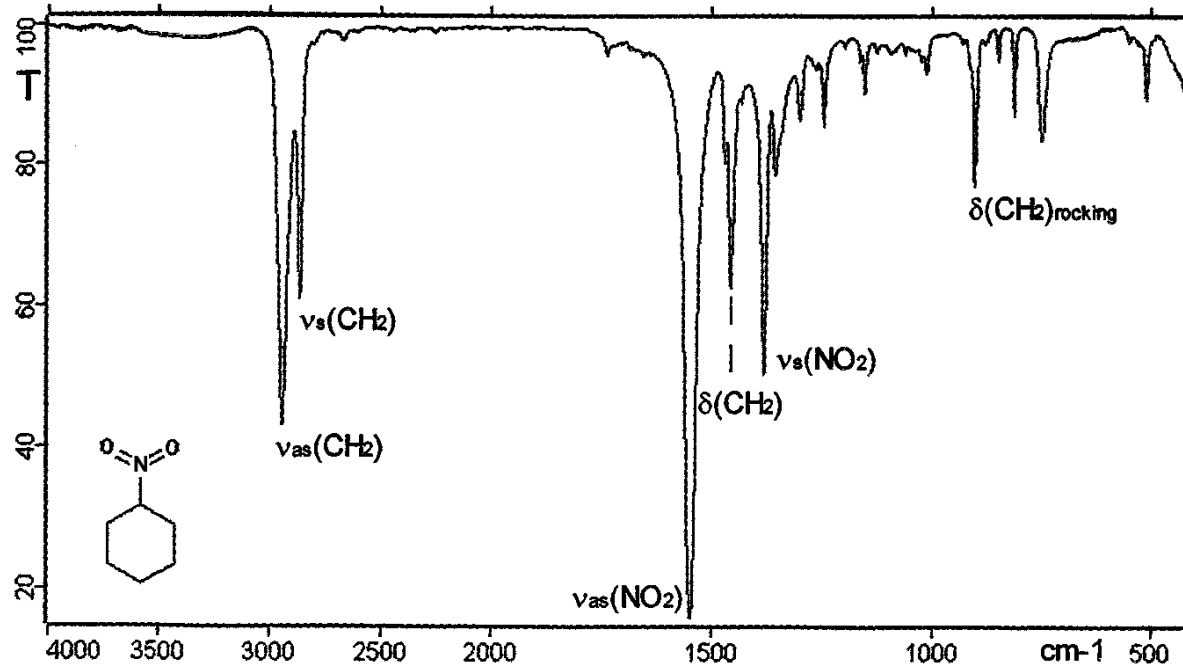
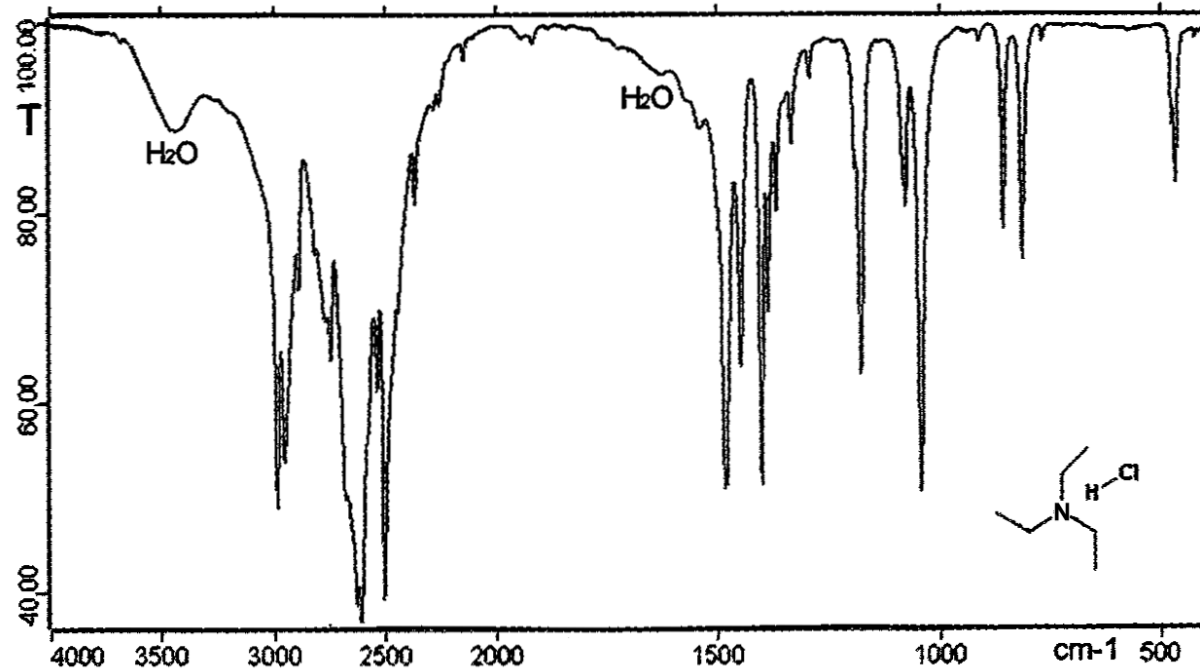


1750 cm^{-1}



1800 cm^{-1}

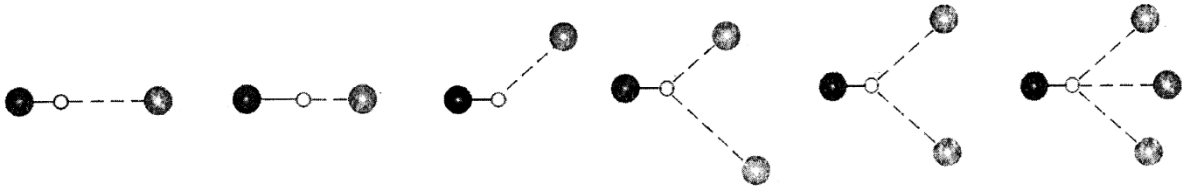




Vodikova veza

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 (σ -elektron-donor) ili π -orbitalu nezasićenog sustava.

Donori	C-H, P-H, S-H, Se-H	-O-H, =N-H, P-O-H	$[=O\cdots H]^+$, $[\equiv N\cdots H]^+$
Akceptori	C-Hal:, =S:, =Se:, π -veza	$=O:$, $\equiv N:$, $P=O:$	$[Hal]^-$, $[-O]^-$, $[P-O]^-$
Vodikove veze	C-H $\cdots$ O C-H $\cdots$ N C/O/N-H $\cdots$ Hal-C C/O/N-H $\cdots$ π -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 $\cdots$	$[H_2O\cdots H\cdots OH_2]^+$ $[\equiv N\cdots H\cdots N\equiv]^+$ $[F\cdots H\cdots F]^-$ $[RCOO\cdots H\cdots OOCR]^-$ $[O_3SO\cdots H\cdots OSO_3]^-$ $R_3N^+-H\cdots^-OOCR$ $\cdots O=C-C=C-OH\cdots$ $\cdots O=C-C=C-N(R)H\cdots$

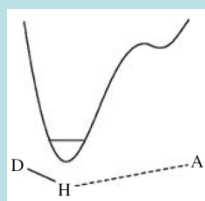


Strukture vodikovih veza: **a)** asimetrična linearna, **b)** simetrična linearna, **c)** svijena, **d)** asimetrična bifurkatna, **e)** simetrična bifurkatna, **f)** trifurkatna

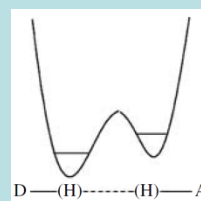
	Vodikova veza D–H…A		
Obilježja veze	Slaba	Umjereno jaka	Jaka
Tip interakcije	elektrostatska	elektrostatsko-kovalentna	pretežno kovalentna
Duljine veza	$d(\text{D–H}) \ll d(\text{H}\cdots\text{A})$	$d(\text{D–H}) < d(\text{H}\cdots\text{A})$	$d(\text{D–H}) \approx d(\text{H}\cdots\text{A})$
$d(\text{H}\cdots\text{A})$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

**Kvalitativna krivulja
potencijalne energije**

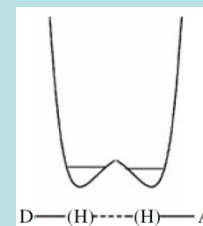
**asimetrična krivulja s
jednostrukim minimumom i
visokom energijskom
barijerom**



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



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



ili



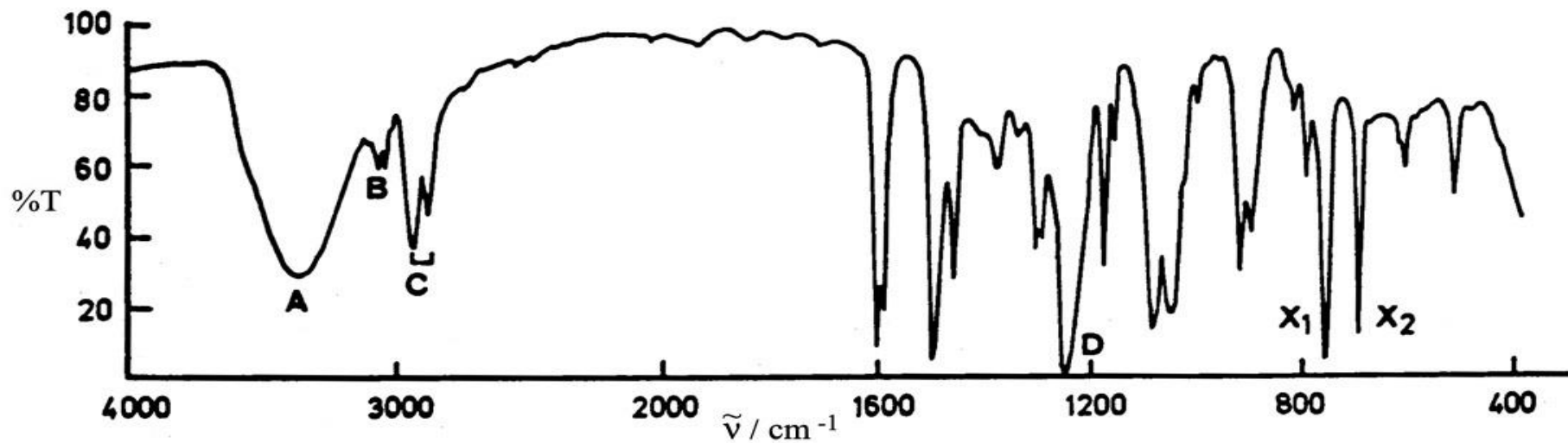
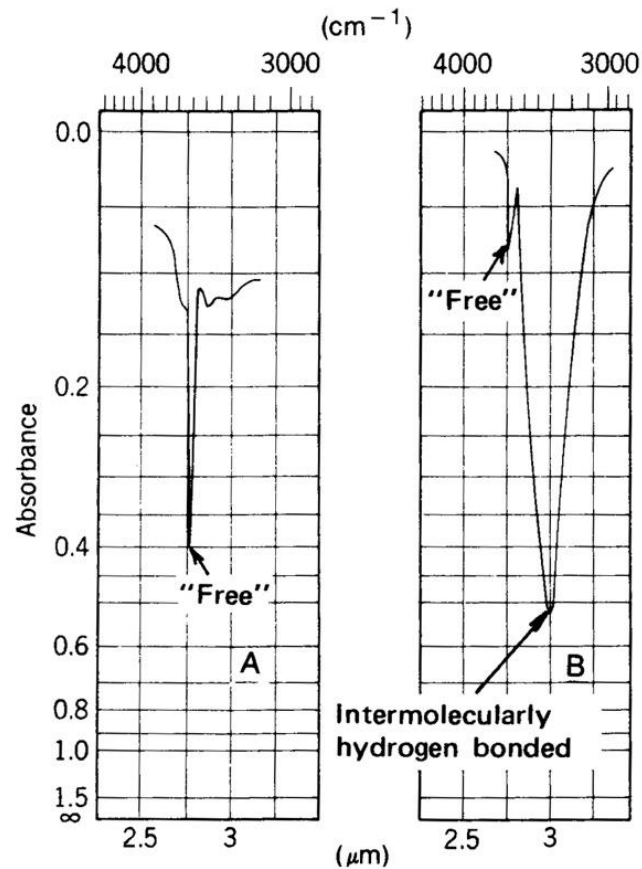
simetrična krivulja s jednostrukim
minimumom

Načini vibriranja sustava D-H···A.

IR područje / cm ⁻¹	Način vibracije		Opis vibracije
3500 – 2500	$\begin{array}{c} \leftarrow \quad \rightarrow \quad \rightarrow \\ \text{D}-\text{H}\cdots\text{A} \end{array}$	ν_s	D-H istezanje
1700 – 1000	$\begin{array}{c} \uparrow \\ \text{D}-\text{H}\cdots\text{A} \\ \downarrow \end{array}$	ν_b	D-H svijanje u ravnini
900 – 300	$\begin{array}{c} \pm \\ \text{D}-\text{H}\cdots\text{A} \end{array}$	ν_t	svijanje izvan ravnine
250 – 100	$\text{D}-\text{H}\cdots\leftarrow\text{A}\rightarrow$	ν_σ	H···D istezanje
< 200	$\begin{array}{c} \uparrow \\ \text{D}-\text{H}\cdots\text{A} \\ \downarrow \end{array}$	ν_β, ν_γ	H···D svijanje

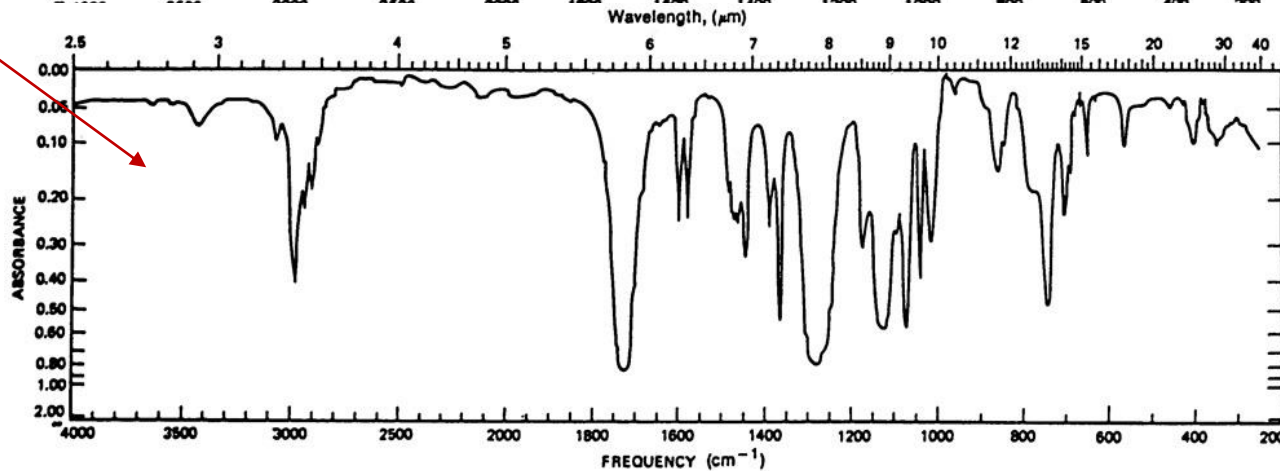
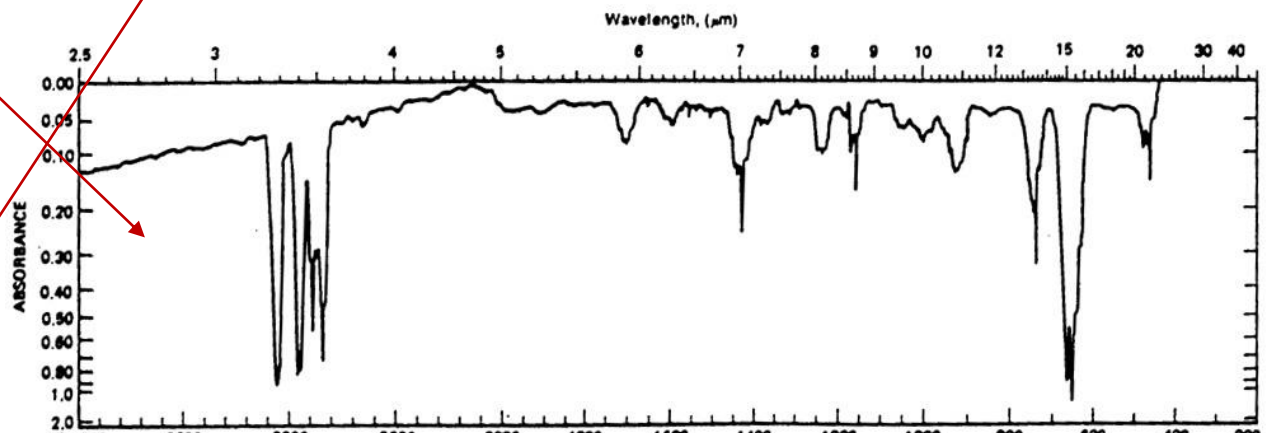
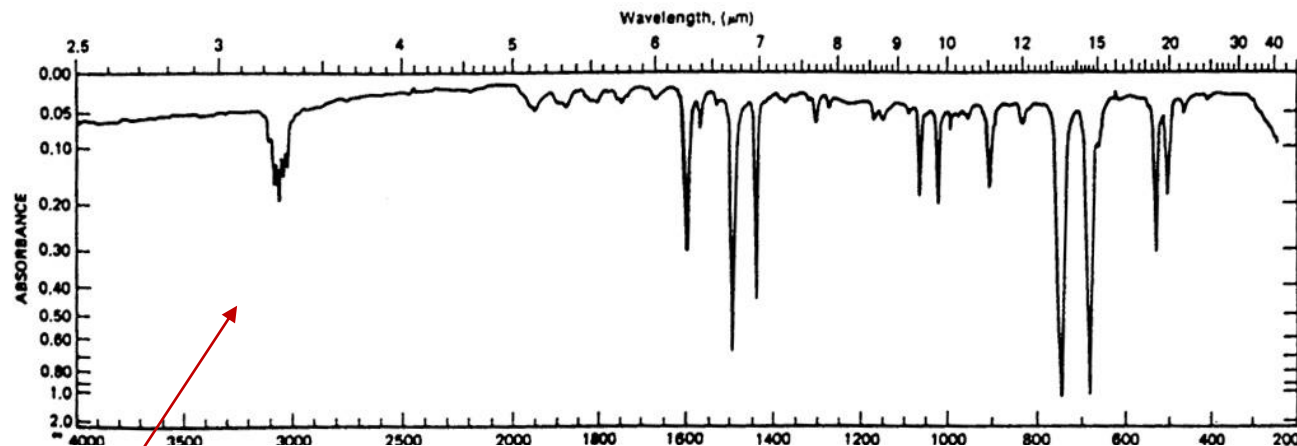
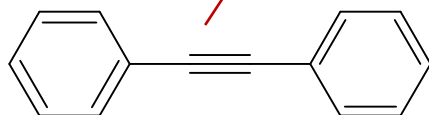
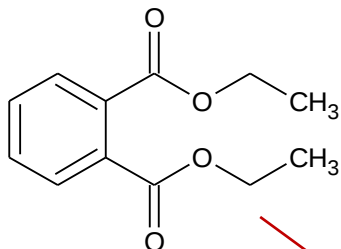
Vodikove veze

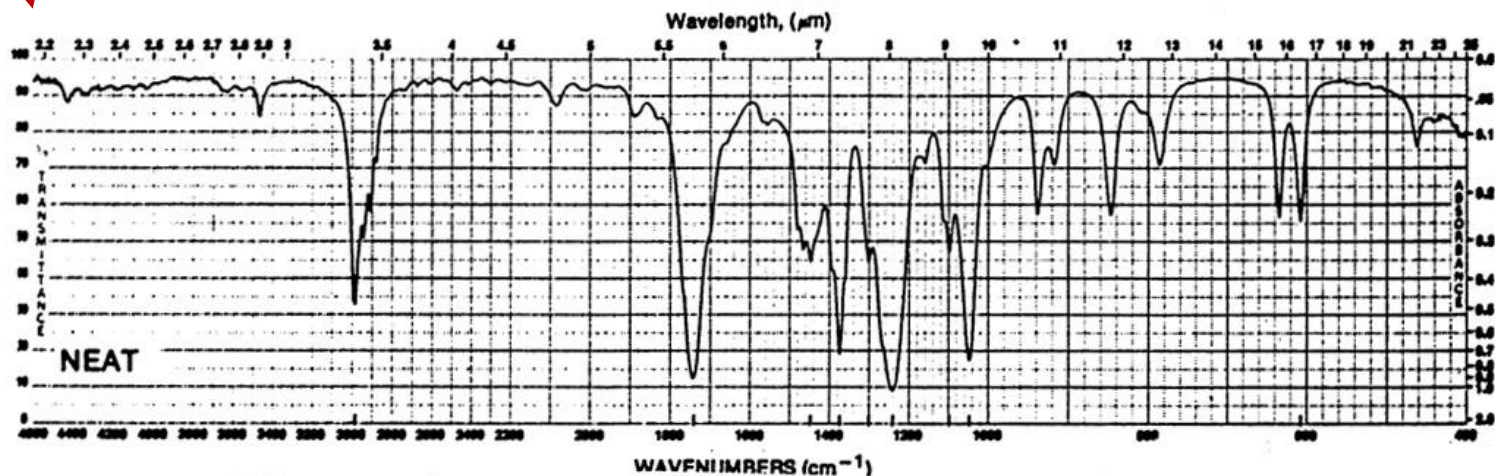
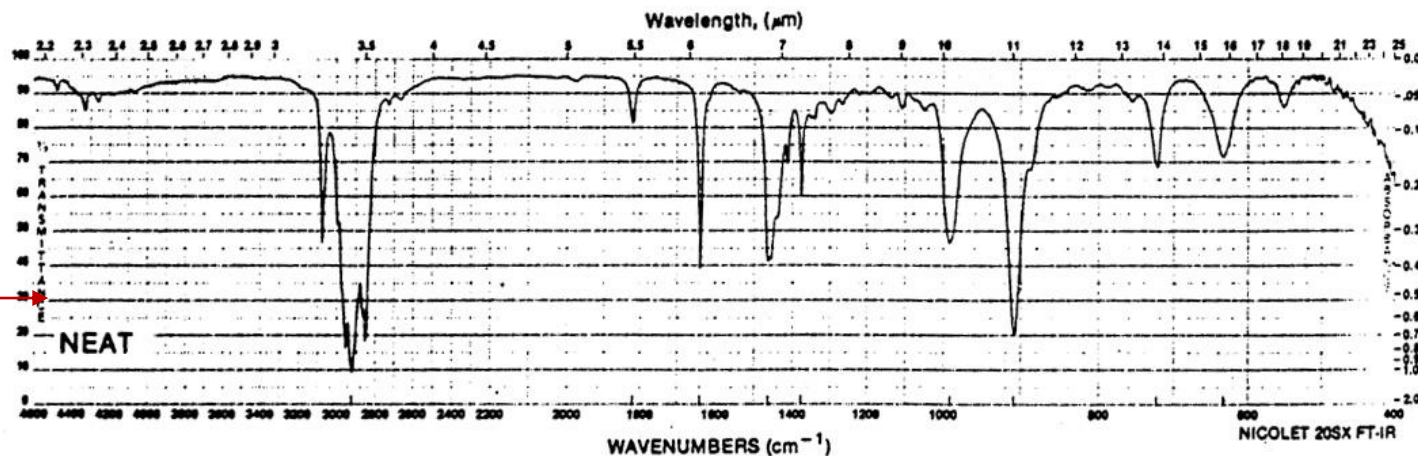
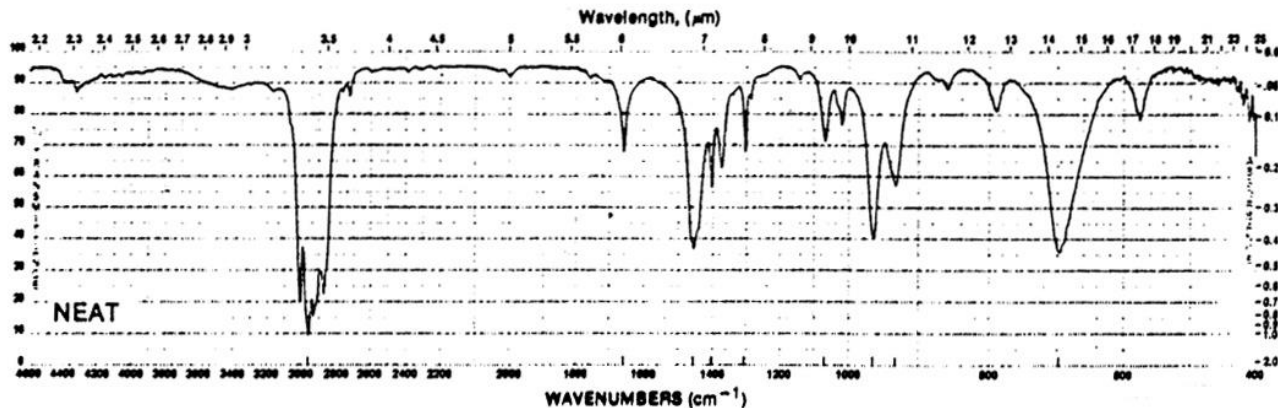
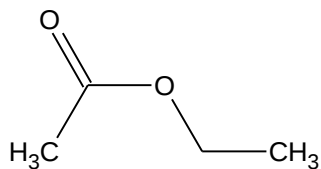
fenoksietanol



Koji spektar IR
odgovara ovim
spojevima?

1-okten





1,3-cikloheksa
dien

2-penten