

## IR spektroskopija

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### Infrardeče sevanje

$$\lambda = 2.5 \text{ to } 17 \mu\text{m}$$

$$\nu = 4000 \text{ to } 600 \text{ cm}^{-1}$$

V tem energijskem nivoju vzbujanja pride do vibracij kovalentnih vezi, zato se infrardeča spektroskopija uporablja za karakterizacijo kovalentnih vezi v molekulah.

IR se uporablja za:

1. ugotavljanja tipa kemijskih vezi
2. pridobivanje nekaterih strukturnih informacij

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## IR ABSORPCIJA

- Energija IR je premajhna za vzbujanja elektronov
- Absorpcija je omejena na **vibracijsko-rotacijske** nivoje
- Za tekočine in trdne snovi je molekulska rotacija omejena, zato so v tem primeru pogostejše vibracije

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### IR absorpcija

- Vibracije v molekuli določajo:
- Število atomov
- Vrste atomov
- Vrste vezi med atomi

**IR spektroskopija je učinkovito orodje za karakterizacijo čistih organskih in anorganskih spojin**

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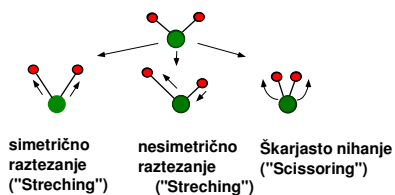
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### IR absorpcija-vrste vibracij




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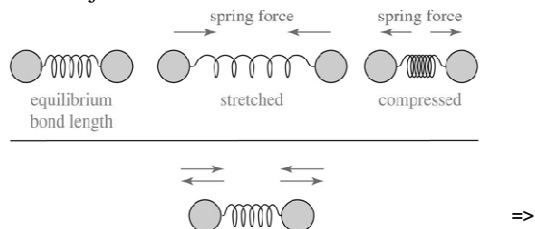
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### Molekulske vibracije

Kovalentana vez vibrira le pri določeni dovoljeni frekvenci.




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## Frekvence raztezanja

Bond	Bond Energy [kcal (kJ)]	Stretching Frequency (cm <sup>-1</sup> )
<i>Frequency dependence on atomic masses</i>		
C—H	100 (420)	3000
C—D	100 (420)	2100
C—C	83 (350)	1200
		↓ $\bar{\nu}$ decreases
<i>Frequency dependence on bond energies</i>		
C—C	83 (350)	1200
C=C	146 (611)	1660
C≡C	200 (840)	2200
	↓ stronger bond	↓ $\bar{\nu}$ increases

- Frekvenca se zmanjša pri težjih atomih.
- Frekvenca se poveča pri večji energiji vezi.

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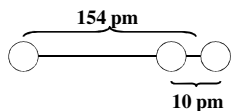
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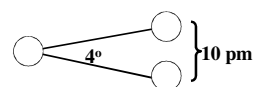
## Kakšne deformacije imamo pri C-C vezi?

### raztezanje



Za C-C vez z dolžino 154 pm predstavlja raztezanje odmik okoli 10 pm od ravnotežja.

### upogibanje



Pri C-C-C vezi se kot med vezmi spreminja za okoli 4°. To predstavlja premik C atomov za 10 pm.

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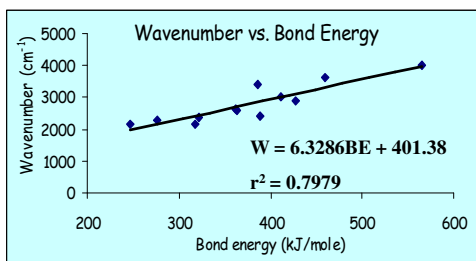
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## Ali je jakost vezi povezana s energijo vibracij?




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## Matematični opis vibracij

Velja Hookov zakon za harmonično nihalo

$$F = -ky$$

$$\Delta E = h \nu_m = \frac{h}{2\pi} \sqrt{\frac{k}{\mu}} \quad \mu = \frac{m_1 m_2}{m_1 + m_2}$$

$$\bar{\nu} = \frac{1}{2\pi c} \sqrt{\frac{k}{\mu}} = 5.3 \times 10^{-12} \sqrt{\frac{k}{\mu}}$$

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## Primer 1

Izračunajte valovno število za absorpcijo C=O vezi kot posledico raztezanja! (k=1000 N/m)

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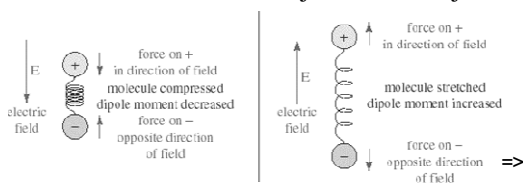
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## IR-aktivne in naaktivne vezi

- Polarne vezi so IR-aktivne.
- Nepolarne vezi in simetrične molekule le malo ali celo ne absorbirajo v IR območju.




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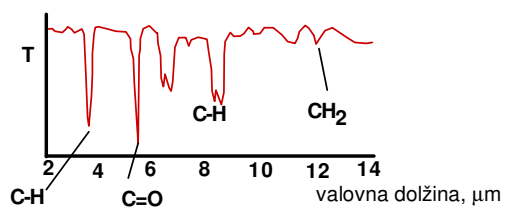
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## IR-spekter (primer)




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## IR absorpcija

Funkc.skupina	val število $\text{cm}^{-1}$	val. dolžina $\mu\text{m}$
C-H, alifatski	3000-2850	3,3-3,5
C-H, aromatski	3150-3000	3,2-3,3
O-H	3600-3000	2,8-3,3
C=O, aldehidi, ketoni	1740-1660	5,7-6,0
CH <sub>2</sub> Cl	1300-1200 850-890	7,6-8,2 13,2-14

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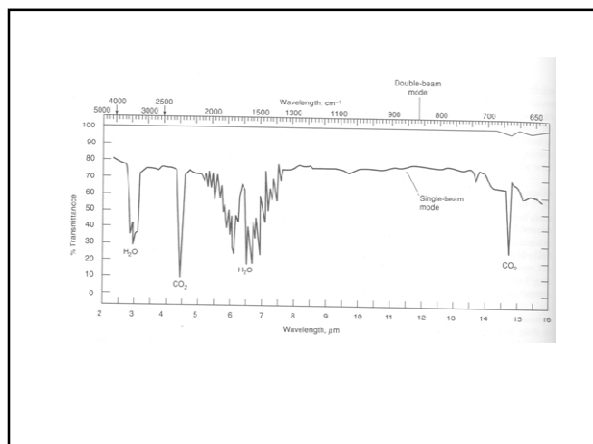
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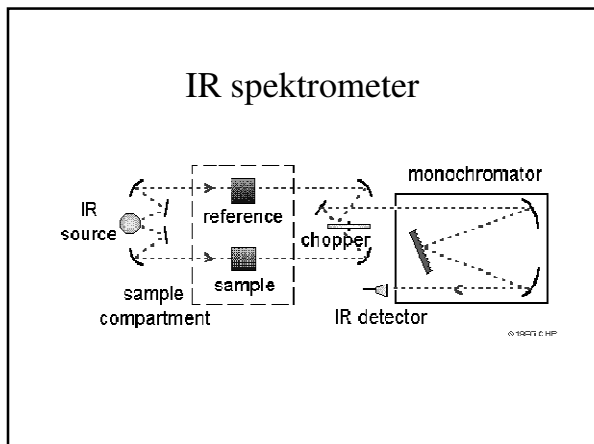
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### Izvori svetlobe

IR izvori:

Nernstov gorilec –cirkonijev oksid/itrijev oksid  
100-20 000 nm (negativen temperaturni koeficient upornosti)

Globar- SiC palica 1200-40 000 nm (pozitiven temperaturni koeficient upornosti)

Laserski izvori (CO<sub>2</sub> laser)  
Uporabljamo jih, če potrebujemo visoke intenzitete

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### Monokromatorji

Prizme:  
IR NaCl, KCl

**Prednosti:**  
Omogoča izbiro valovnih dolžin v širokem območju

**Slabosti:**  
Majhna disperzija (ločljivost)  
Svetloba prehaja skozi material, zato je omejeno območje valovnih dolžin (absorpcija!)

Uklonske mrežice  
IR 10-200 črt/mm  
Število vpliva na ločljivost!

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## Detektorji

Vrste detektorjev:	val. dolž.	Mejena količina	Področje
Termočleni	600-20000	tok	IR
termistorji	600-20000	upor	IR

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## Prstni odtis molekule (Fingerprint)

- Kvantiziramo vse vibracije v molekuli.
- Dve različni molekuli ne dajata enakih IR spektro (razen enantiomers).
- Enostavno raztezanje:  $1600-3500\text{ cm}^{-1}$ .
- Kompleksne vibracije:  $600-1600\text{ cm}^{-1}$ , imenujemo "fingerprint" območje.

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### IR spektri ALKANOV

C—H vez "nasičena"

( $\text{sp}^3$ )  $2850-2960\text{ cm}^{-1}$

+  $1350-1470\text{ cm}^{-1}$

-CH<sub>2</sub>- +  $1430-1470$

-CH<sub>3</sub> + " in  $1375$

-CH(CH<sub>3</sub>)<sub>2</sub> + " in  $1370, 1385$

-C(CH<sub>3</sub>)<sub>3</sub> + " in  $1370(\text{s}), 1395(\text{m})$

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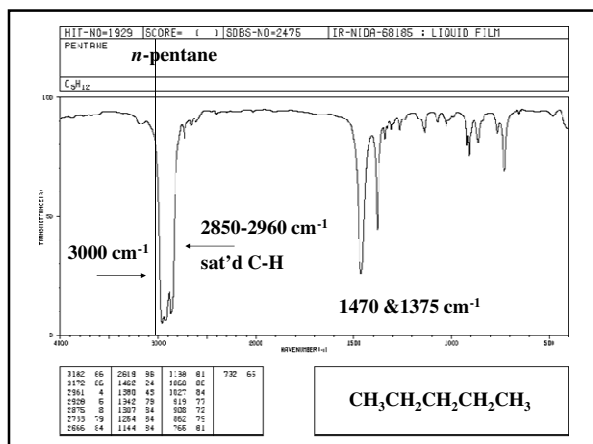
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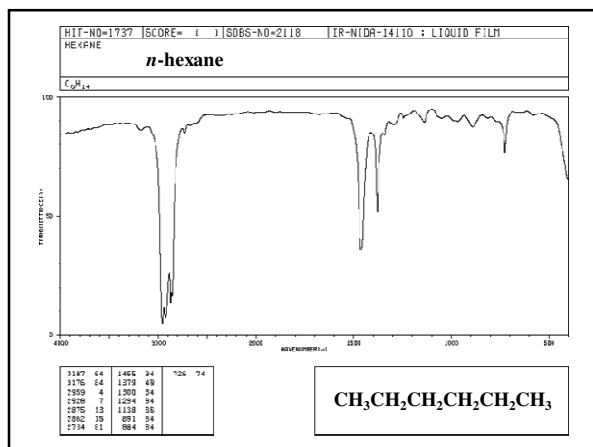
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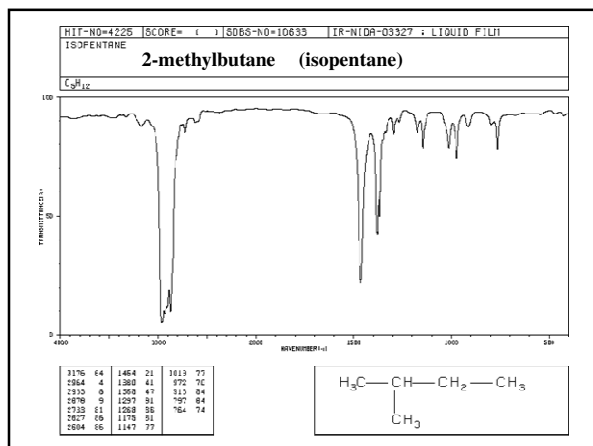
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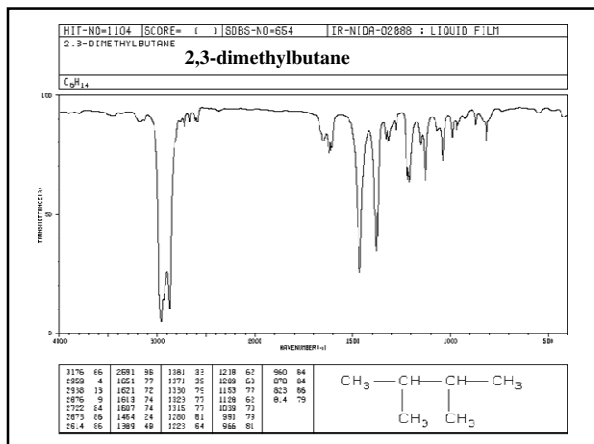
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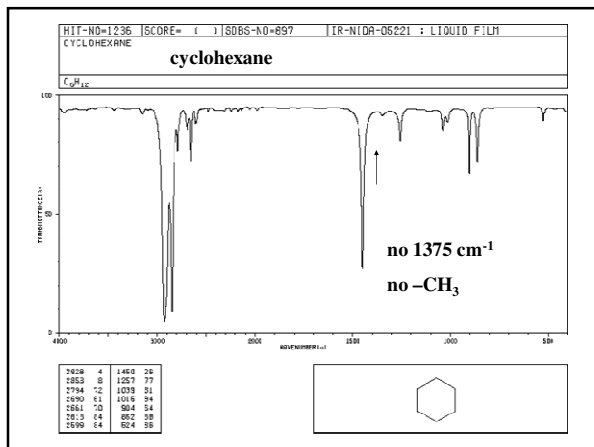
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**Novejše aplikacije IR spektroskopije**

- raziskave in kontrola materialov  
 (IR spektri se uporabljajo kot prstni odtis določenega materiala. Ob podobni kemijski sestavi dobimo podobne spektre)
- kvantitativno delo  
 (IR spektroskopija je nedestruktivna tehnika, ki se lahko uporablja tudi za kvantitativno delo. Kalibracijski modeli so vedno večfaktorski. Uporabljamo lahko multiplo-linearno regresijo (MLR), metodo delnih najmanjših kvadratov (PLS), umetne nevronske mreže (UNM),...

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