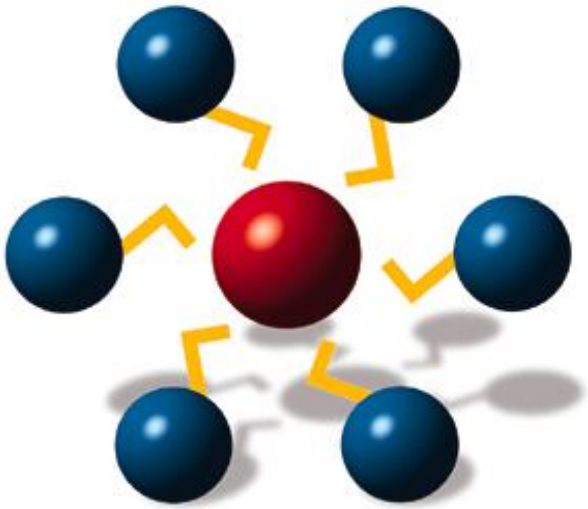
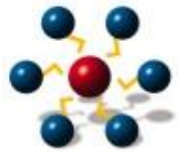
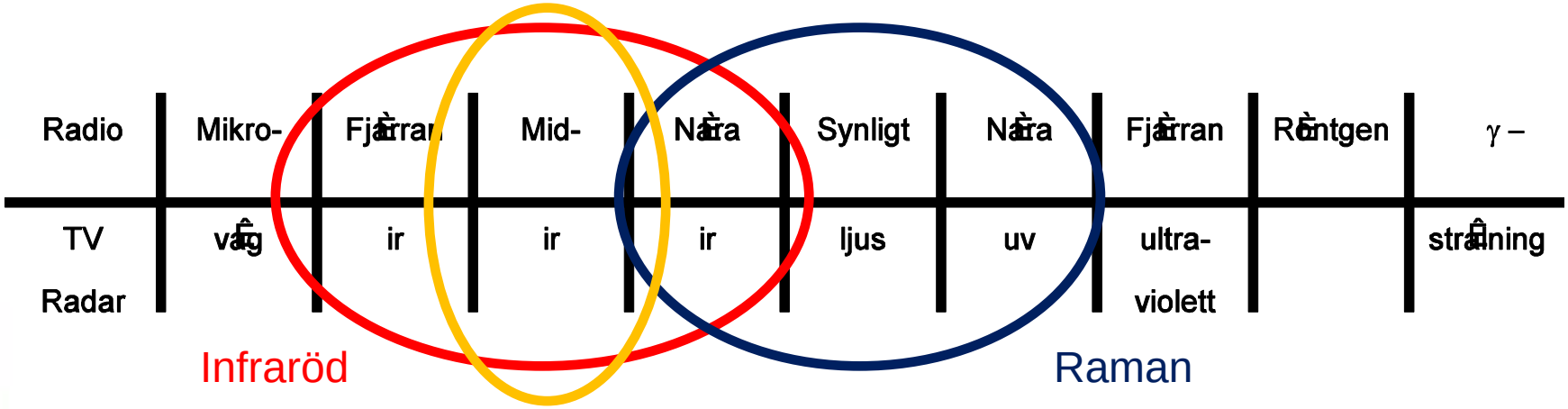
Vibrationspektrometri

Matti Hotokka

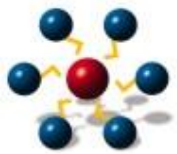




Elektromagnetiskt spektrum

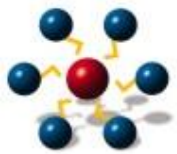


λ	3 cm	1 mm	25 μm	2.5 μm	770 nm	400 nm	200 nm	10 nm	0.2 nm
$\tilde{\nu}$ (cm^{-1})	0.3	10	400	4000	13,000	25,000	50,000		
E(eV)	$4x10^{-5}$	10^{-3}	$5x10^{-2}$	0.5	2	3	6	100	$6x10^{3}$
E(J)	$6x10^{-24}$	$2x10^{-22}$	$8x10^{-21}$	$8x10^{-20}$	$3x10^{-19}$	$5x10^{-19}$	10^{-18}	$2x10^{-17}$	10^{-15}
E(Hz)	$9x10^{9}$	$3x10^{11}$	10^{13}	10^{14}	$4x10^{14}$	$7x10^{14}$	10^{16}	$3x10^{16}$	10^{18}
E(K)	0.4	14	$6x10^{2}$	$6x10^{3}$	$2x10^{4}$	$4x10^{4}$	$7x10^{4}$	10^{6}	$7x10^{7}$
	NMR EPR	Rotations-spektra	Vibrations-spektra			Elektroniska övergångar	Fotoelektron-spektra	ESCA Auger	



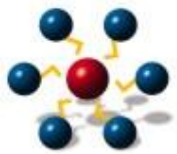
Energienheter

- ⇨Vågtal (cm^{-1}); det vanliga $\tilde{\nu}$
- ⇨Frekvens (Hz, cps); för teoretiker ν
- ⇨Vinkelhastighet (1/s); föråldrad ω
- ⇨Våglängd (μm); sällsynt λ
- ⇨Joule (J); opraktisk E



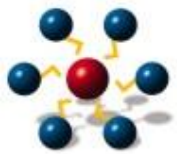
Infrarödområden

- Fjärran ir (FIR, far infrared)
  - 10 – 400 cm^{-1}
- Mid-ir (MIR)
  - 400 – 4000 cm^{-1}
- Nära ir (NIR, near infrared)
  - 4000 – 12 000 cm^{-1}
- Alla har användningar, Mid-ir viktigast

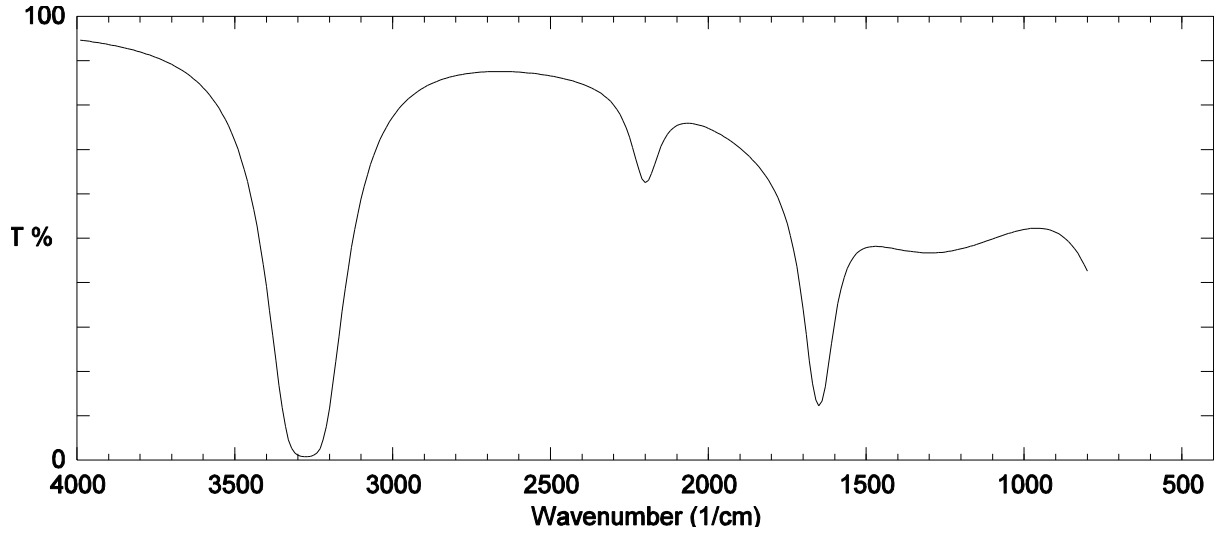


Mätmetoder

- ⇨Infraröd
  - Vanlig
  - Baserar sig på absorption
- ⇨Raman
  - Sällsynt (tyvärr)
  - Baserar sig på ljusspridning



Infraröd spektrum



Beer-Lambert

⇨Absorptionshastighet

$$dI(\lambda) = -I(\lambda)\gamma(\lambda)dx$$

⇨Intensitet efter provet

$$I(\lambda) = I_0(\lambda)e^{-\gamma(\lambda)\ell}$$

⇨Transmittans

$$T(\lambda) = I(\lambda)/I_0(\lambda) = e^{-\gamma(\lambda)\ell} = e^{-\varepsilon(\lambda)c\ell}$$

⇨Absorbans

$$A(\lambda) = \ln(I_0(\lambda)/I(\lambda)) = \varepsilon(\lambda)c\ell$$