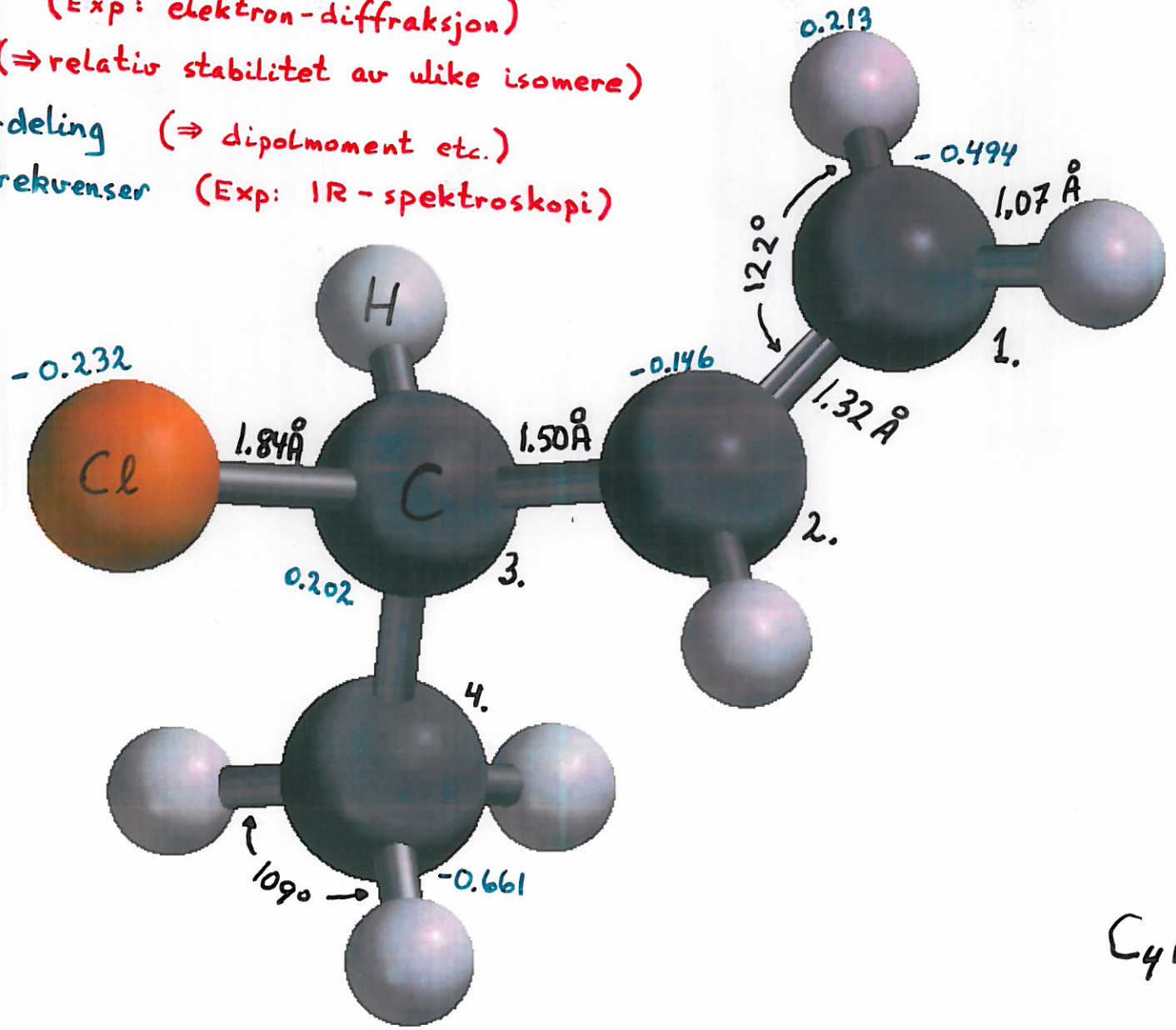
QM beregning ⇒

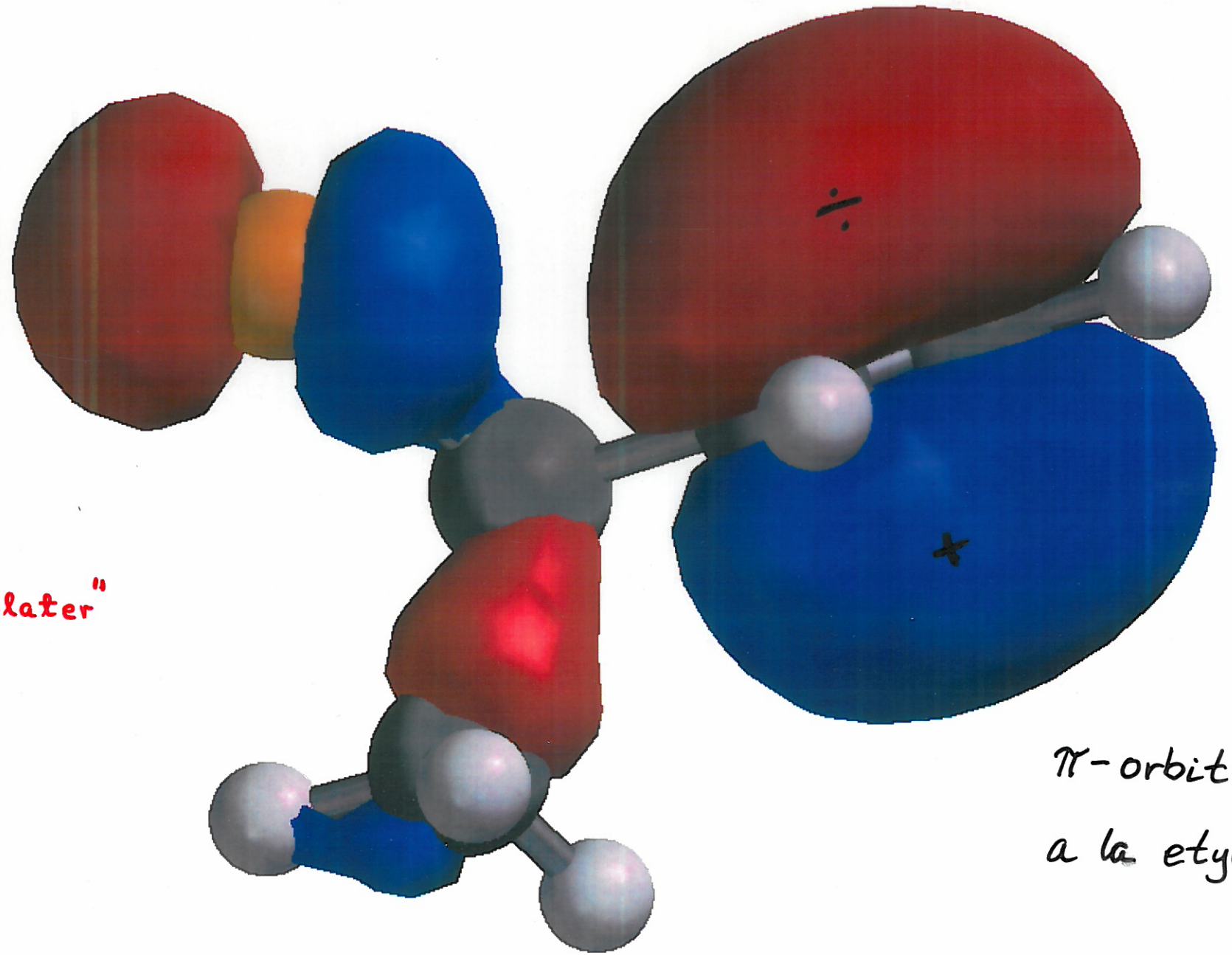
- geometri (Exp: elektron-diffraksjon)
- energi (⇒ relativ stabilitet av ulike isomere)
- ladningsfordeling (⇒ dipolmoment etc.)
- vibrasjons frekvenser (Exp: IR-spektroskopi)



C_4H_7Cl

Navn: 3-kloro-1-buten

Molekylorbital

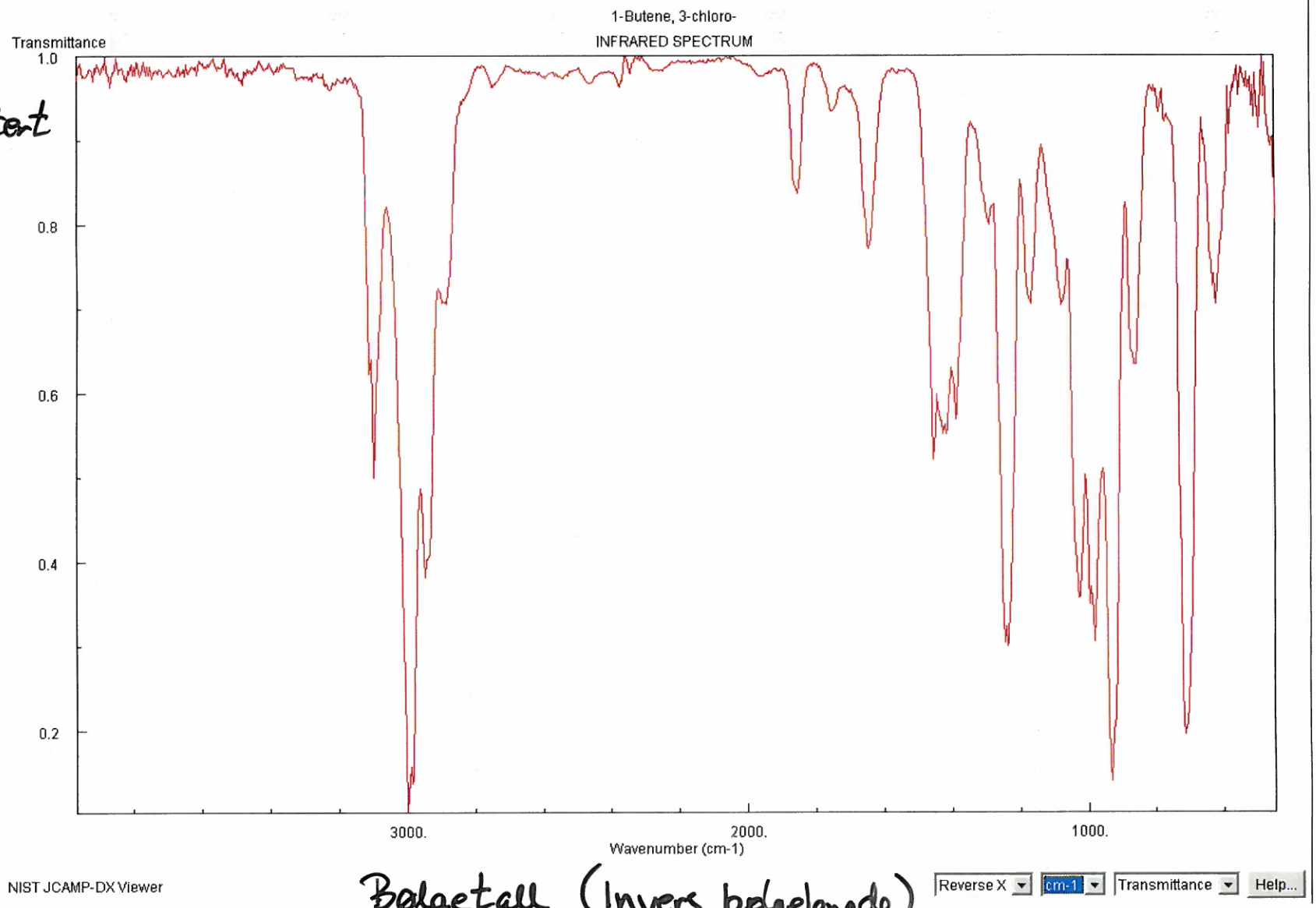


"ekvi-Ψ-flater"

π-orbital
a la etylen

Absorbere lys med bestemte bølgelengder:

3.

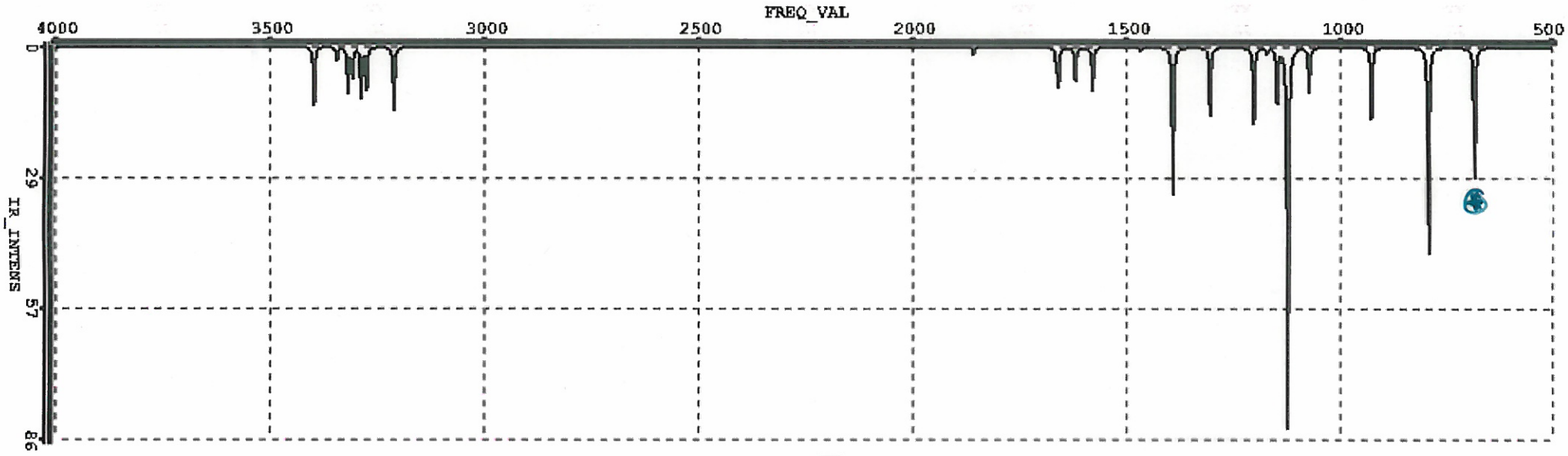


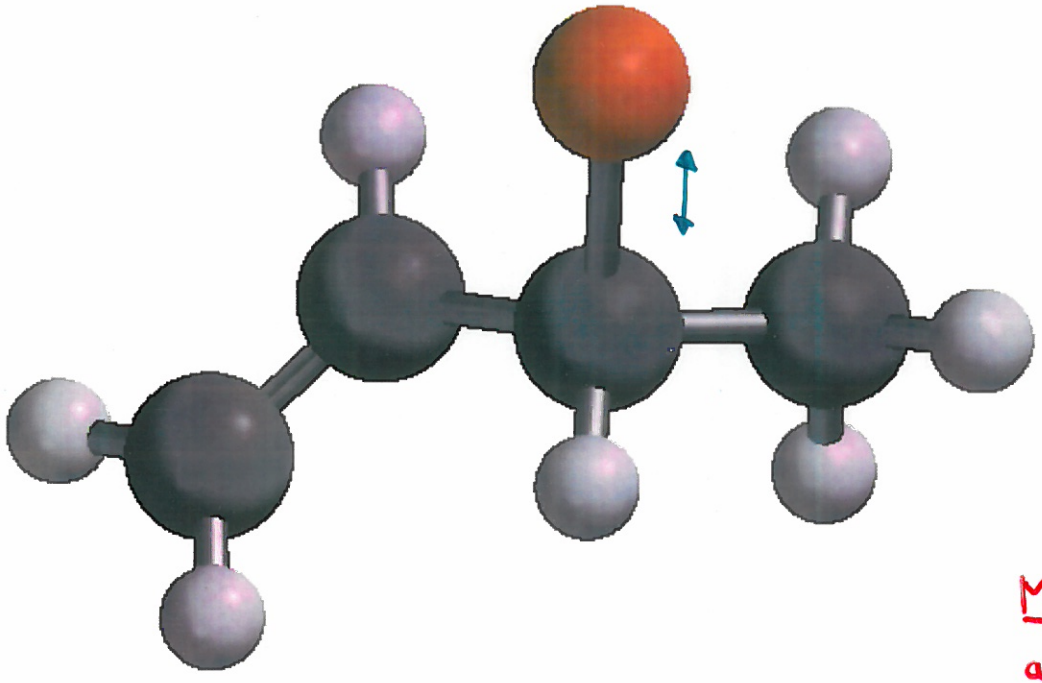
Transmittert lys

Bølgetall (Invers bølgelengde)

Notice: Concentration information is not available for this spectrum and, therefore, molar absorptivity values cannot be derived.

Beregnet transmisjonsspektrum



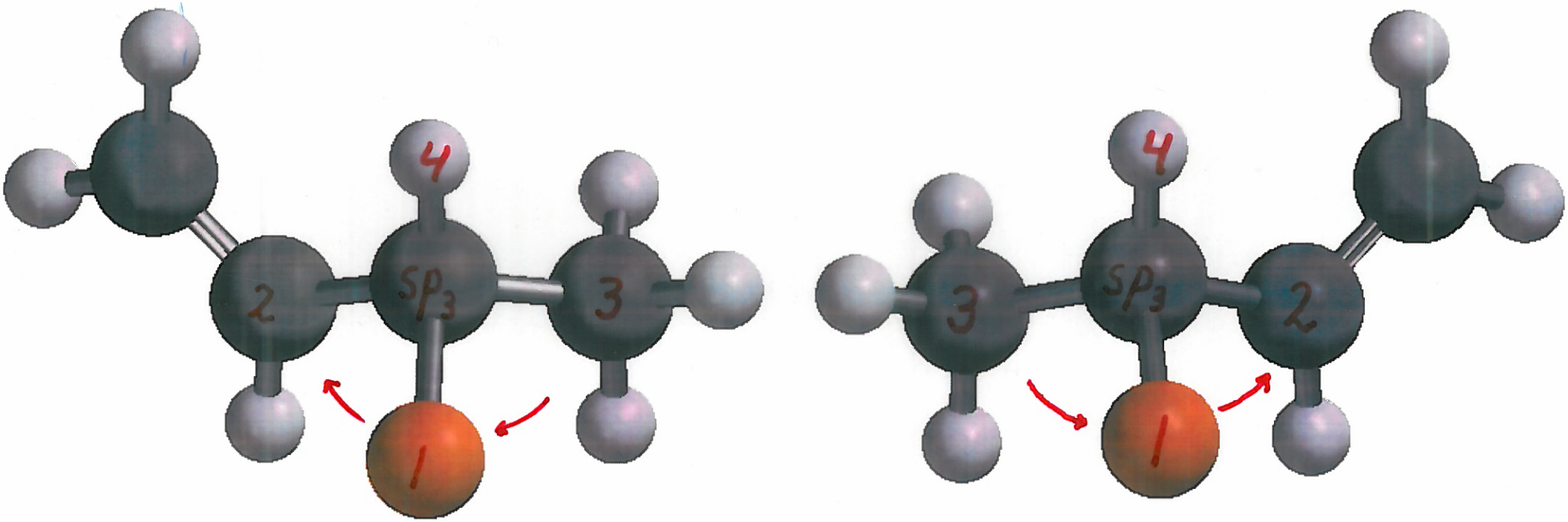


④ C-Cl strekk

Matematisk: Diagonalisering av matrise; egenverdiene gir frekvensene, egenvektorene gir vibrasjonsbevegelsene

Isomere

(= samme formel, ulike molekyler)



Hverandres speilbilde!

Ikke identiske egenskaper!

(Roterer polarisasjonsplanet til lineærpolarisert lys i hver sin retning ⇒ "optiske isomere")