

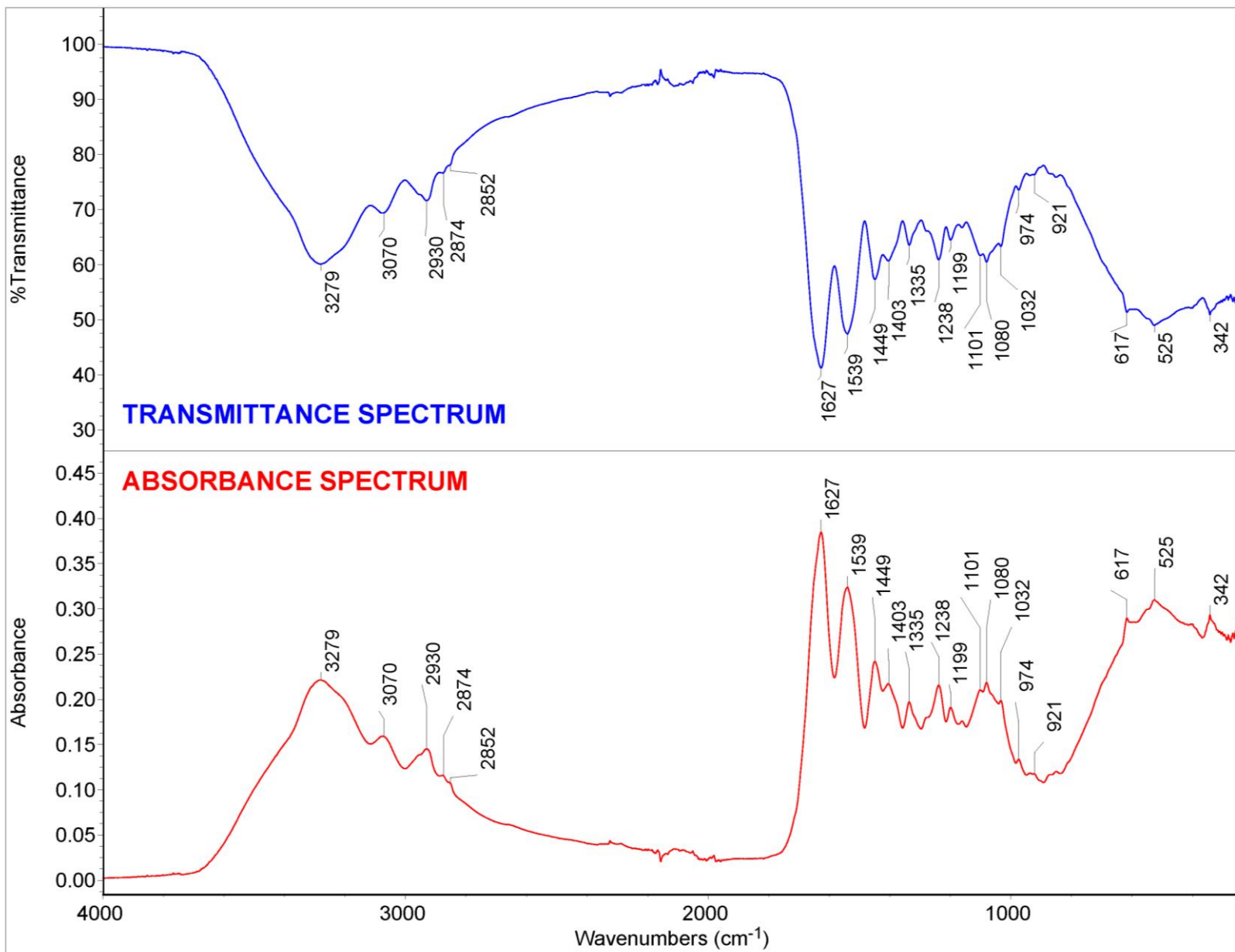
Infrared (IR) spectroscopy: fundamentals

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Infrared (IR) spectral range

	Near-IR (NIR)	Mid-IR (IR)	Far-IR
Radiation:			
Wavenumber:	14000 - 4000 cm^{-1}	4000 - 400 cm^{-1}	400 - 10 cm^{-1}
Wavelength:	0.7 - 2.5 μm	2.5 - 25 μm	25 - 1000 μm
	<ul style="list-style-type: none">• Analysis of organic compounds• Liquids, solids• Mostly quantitative analysis of well-known objects	<ul style="list-style-type: none">• Analysis of organic, inorganic and polymeric compounds• Liquids, solids, gases• Qualitative and quantitative analysis• Often very characteristic• Semi-non-destructive	<ul style="list-style-type: none">• Analysis of inorganic compounds• Mostly solids• Qualitative (and semi-quantitative analysis)• Semi-non-destructive

Spectra of rabbitskin glue



Transmittance and absorbance

- At every wavenumber the signal intensity can be expressed as **transmittance (%T)** or **absorbance (A)**:

$$T = \frac{I}{I_0} \cdot 100\%$$

I_0 – Intensity of radiation entering a sample
 I – Intensity transmitted (or absorbed) by the sample

$$A = \log \frac{I_0}{I}$$



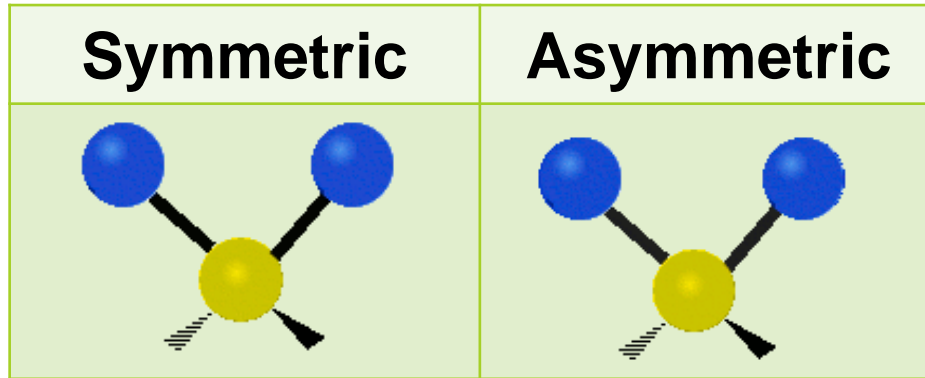
Lambert-Beer's Law

$$A = \epsilon l c$$

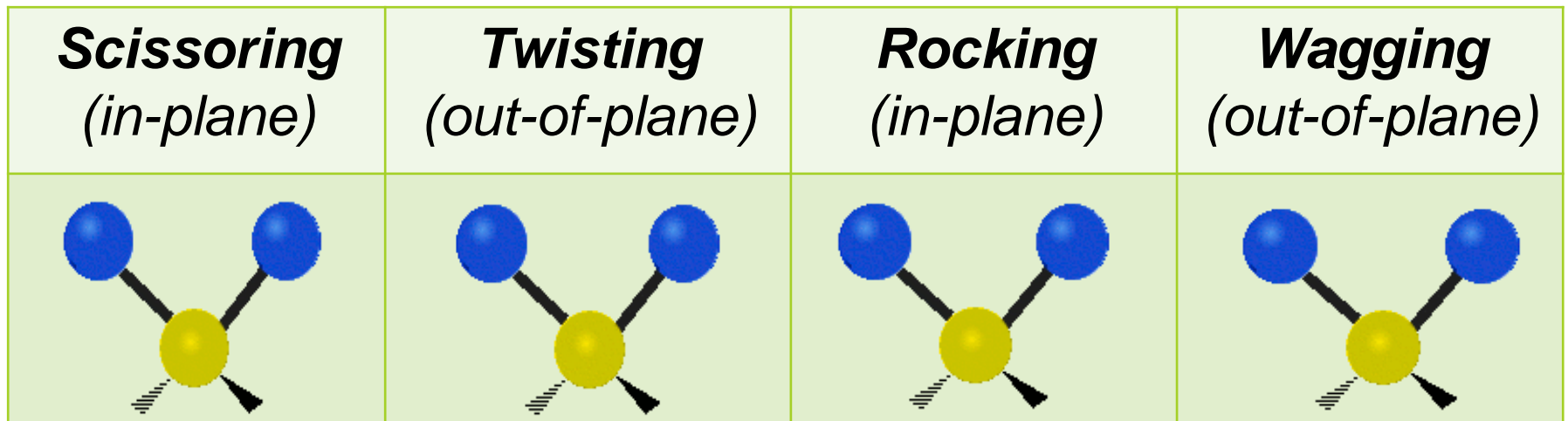
ϵ = absorptivity, l = path length, c = concentration

Vibrations

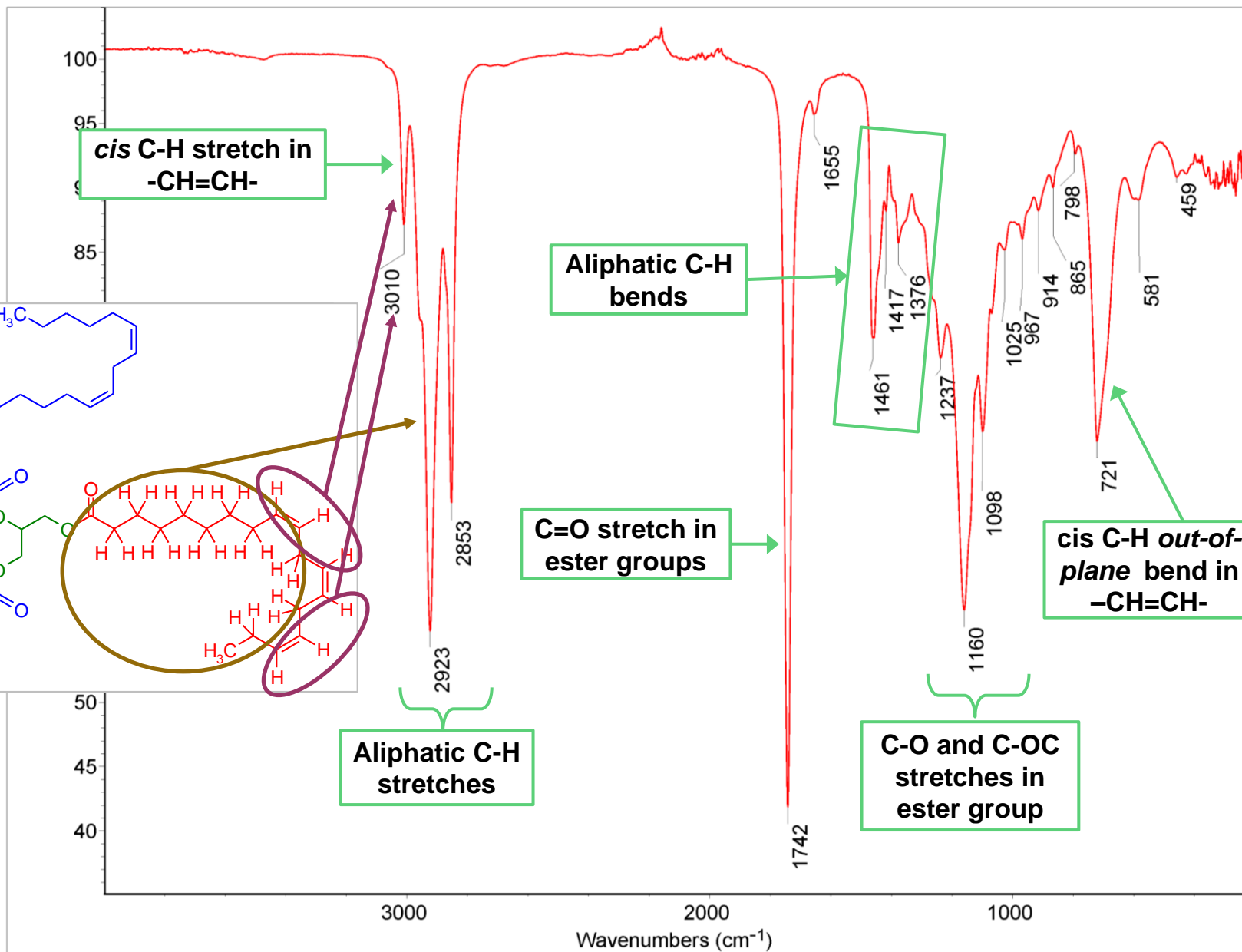
- **Stretching vibrations** – bond length changes



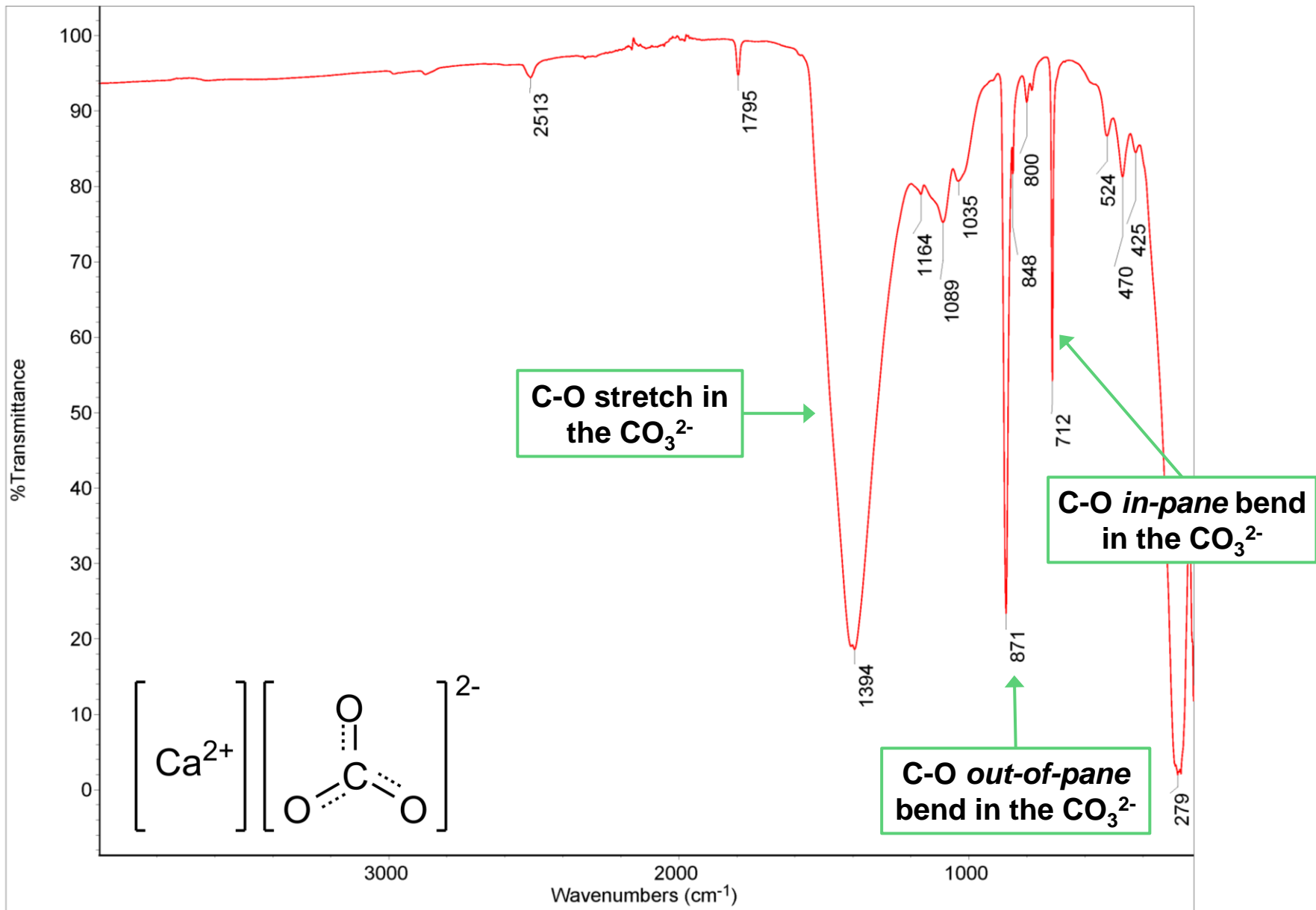
- **Bending (deformation) vibrations** – bond angle changes



IR spectrum of linseed oil

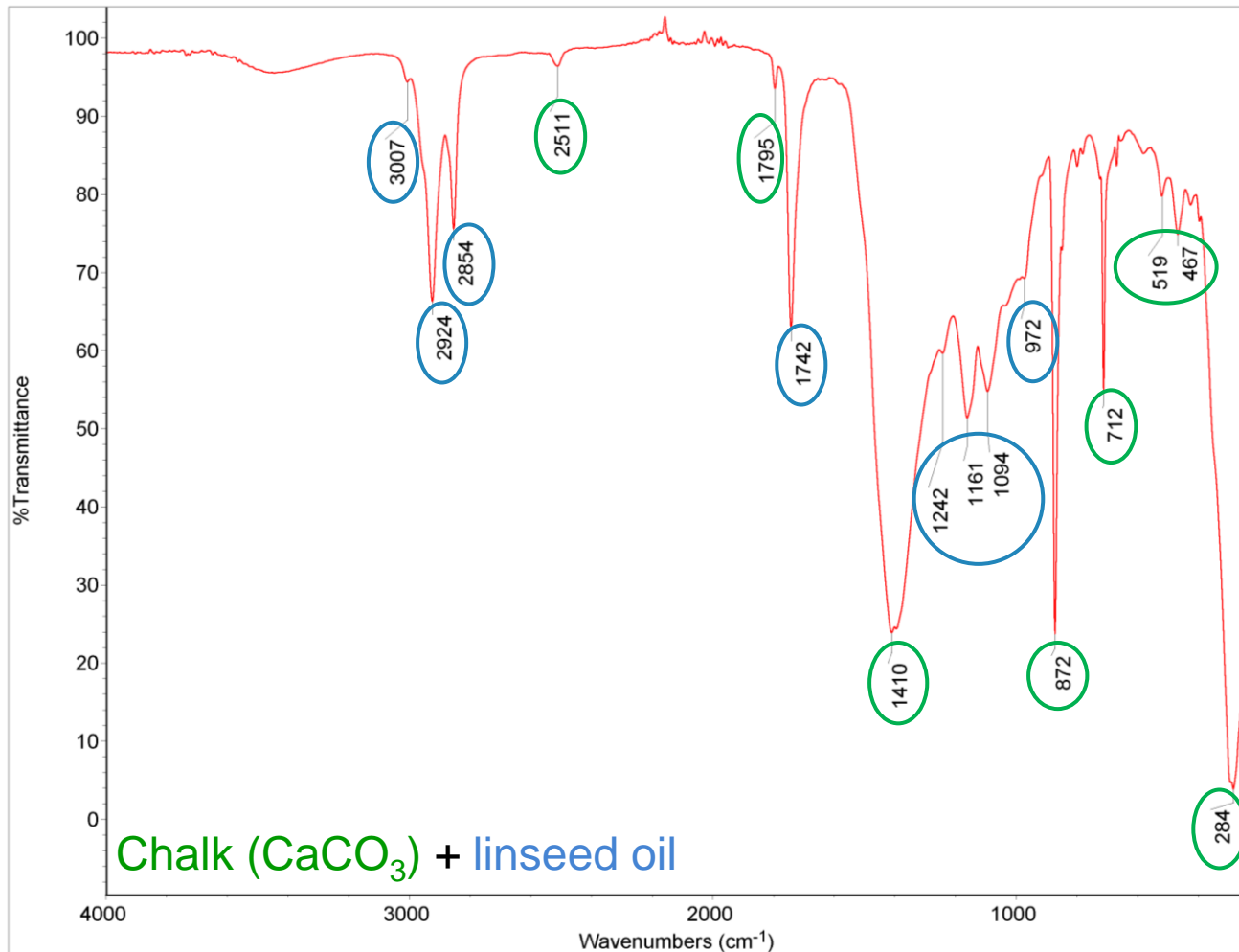


IR spectrum of chalk (CaCO_3)



IR spectra of complex mixtures

- In the IR spectrum of the mixtures often bands overlap
- For the interpretation IR spectra of the pure compounds are needed



Summary

- It is **molecular** and **vibrational spectroscopy**
 - Bands in the IR spectrum belong to the vibrations of specific fragments in molecules
- Useful for the identification of various **organic**, **inorganic** and **polymeric** materials
 - Gives **first general info** about composition of the material
- Enables **qualitative** and **quantitative** analysis
- For the interpretation of IR spectra of complex materials **reference IR spectra** of pure compounds are needed.