

General aspects of ATR-FT- IR spectroscopy

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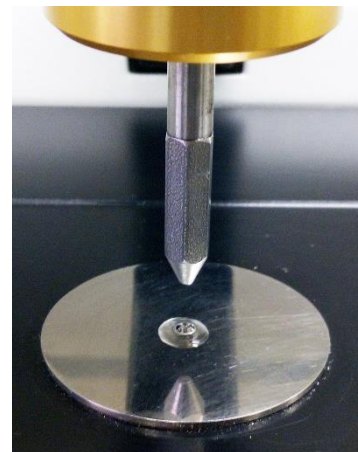
ATR - Attenuated Total Reflectance

(Internal reflection spectroscopy technique)

- Is **contact** technique
- Almost **non-destructive**
- Easy, fast and convenient
- Requires minimal or no sample preparation
- Can work with **very small samples**
- Spectra are recorded from sample surface that is in good contact with the **ATR crystal surface**
- Enables analysis of **solids** and **liquids**
- Qualitative and quantitative analysis



Diamond micro-ATR accessory

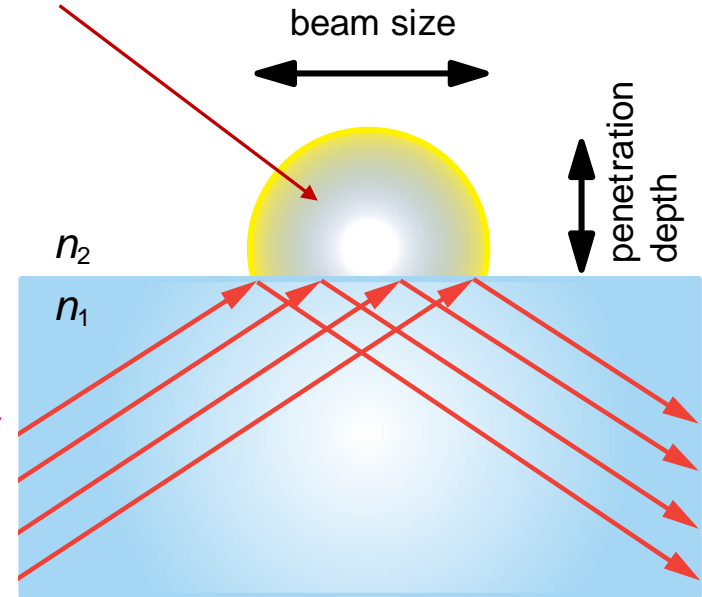


Principle of ATR

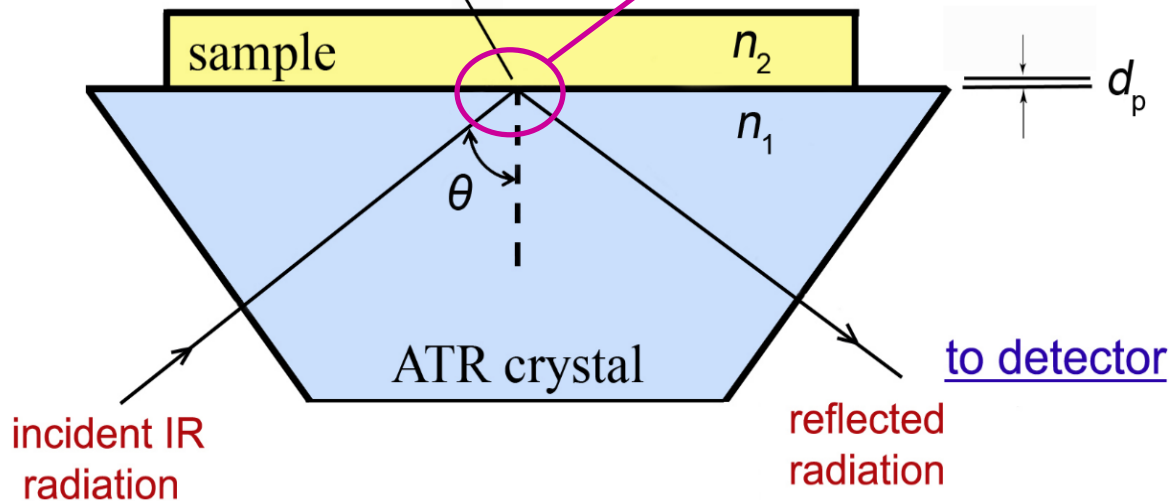
$$d_p = \frac{\lambda_1}{2\pi n_1 \sqrt{\sin^2 \theta - (n_2 / n_1)^2}}$$

Important:
 $n_1 > n_2!$

evanescent wave



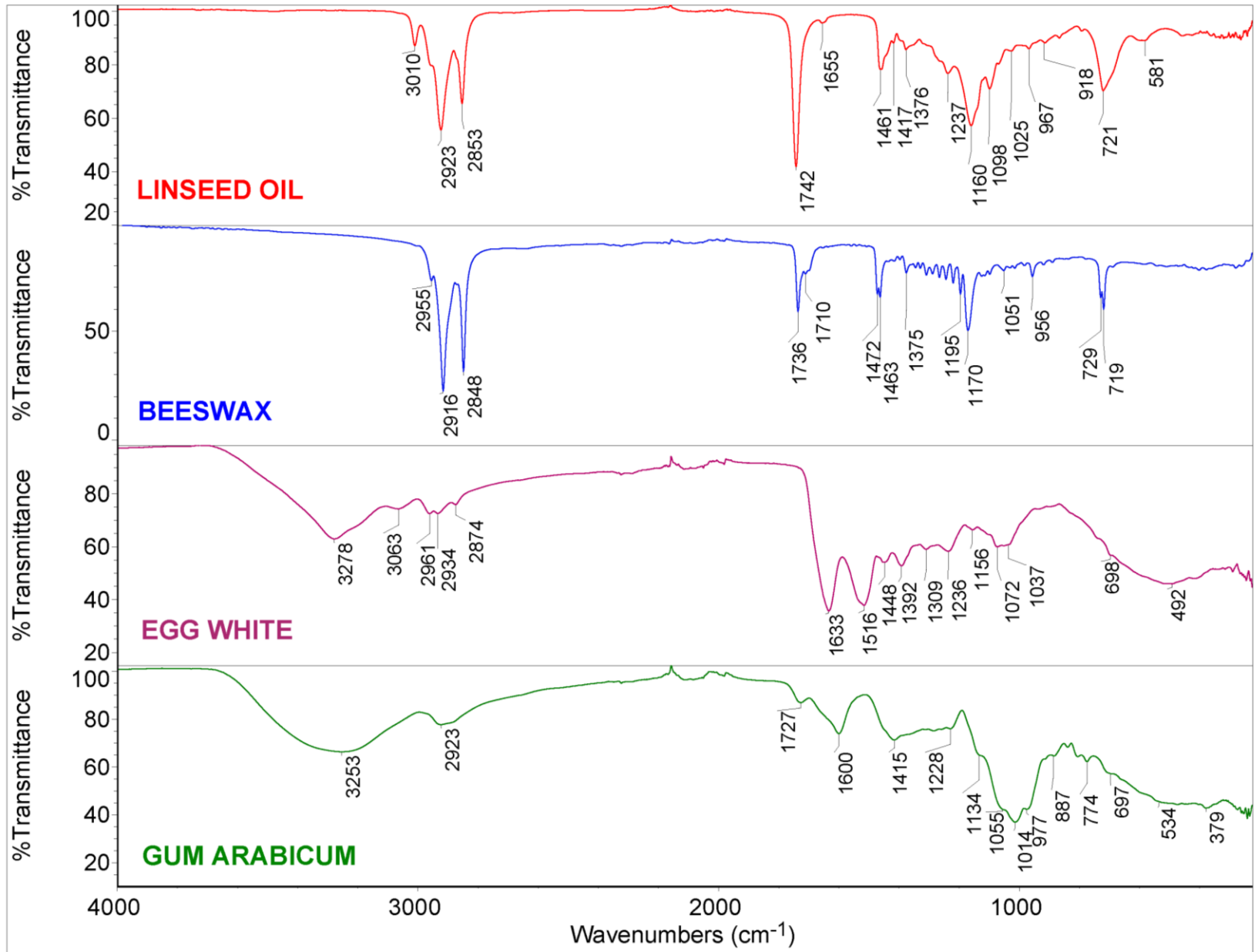
evanescent wave



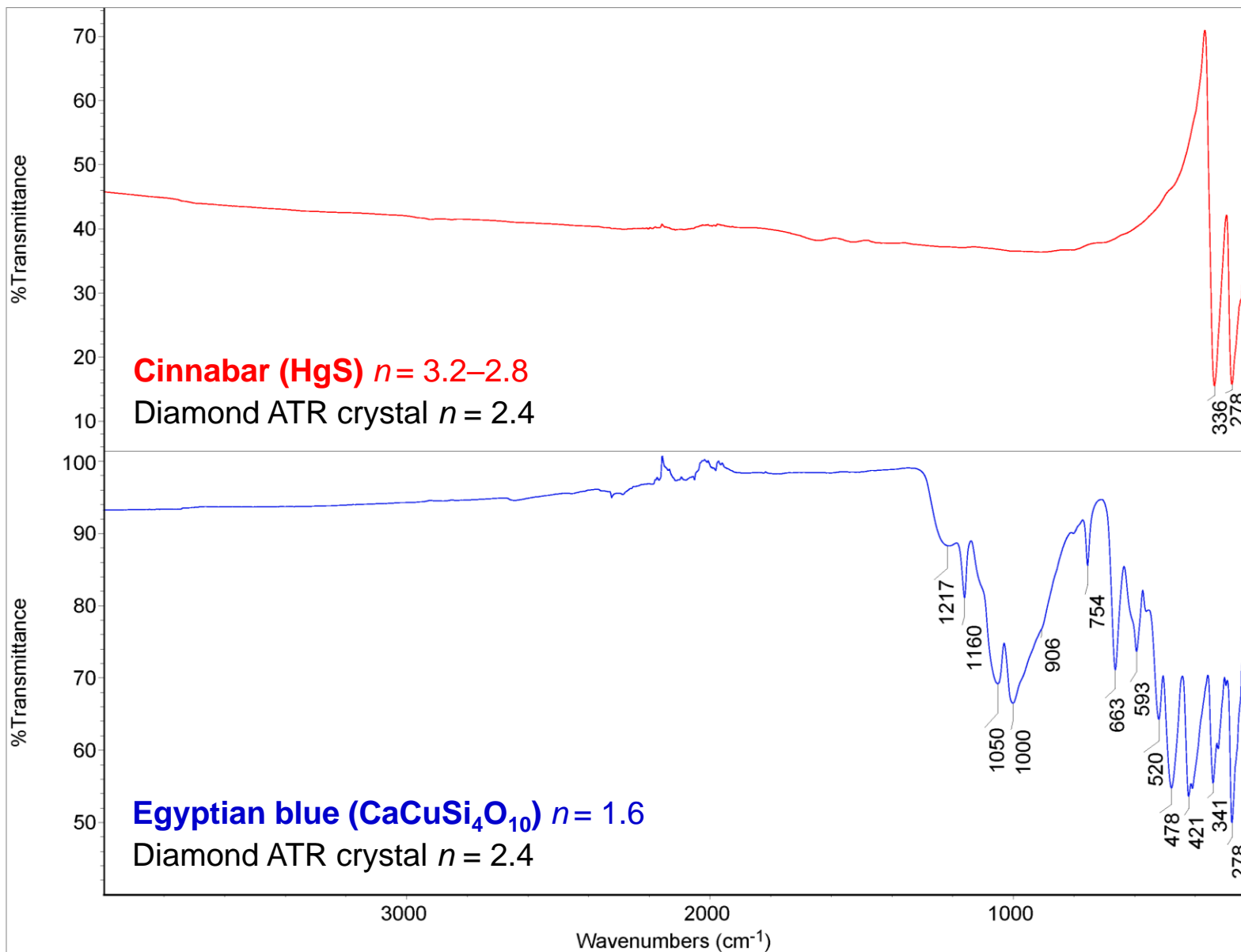
ATR crystals n :

- Diamond: $n = 2.4$
 - ZnSe: $n = 2.4$
 - Ge: $n = 4.0$
 - KRS-5: $n = 2.37$
- (all n correspond to n_D)

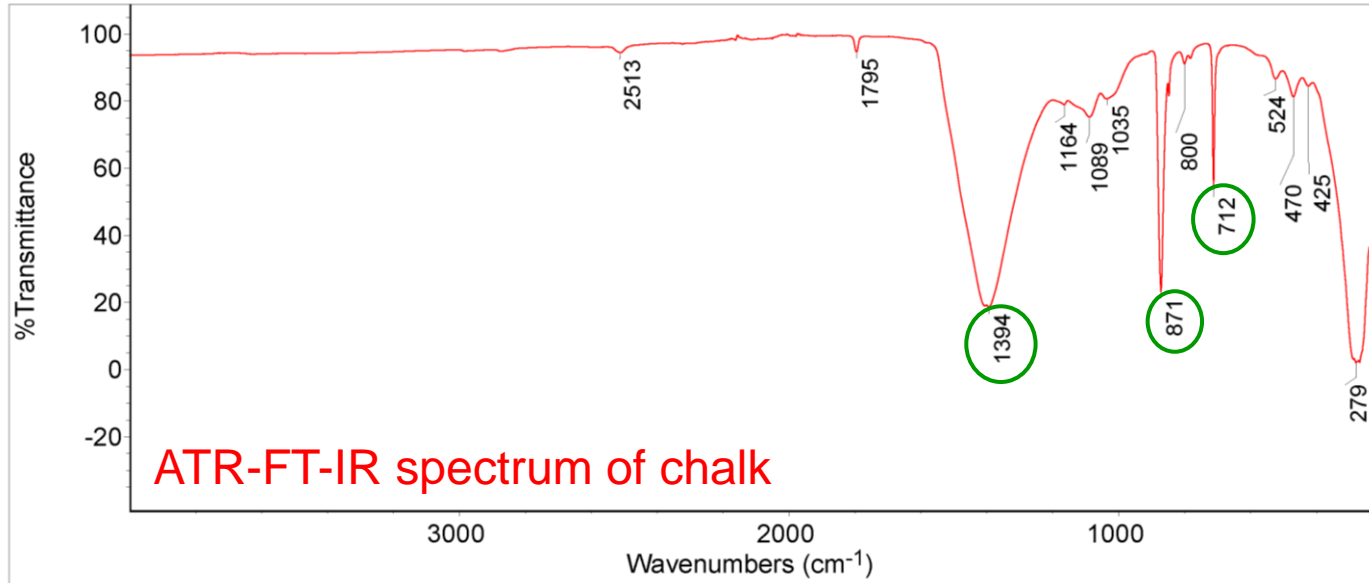
ATR-FT-IR spectra of different binders



Sometimes distorted spectra are observed



ATR and transmission mode IR spectra

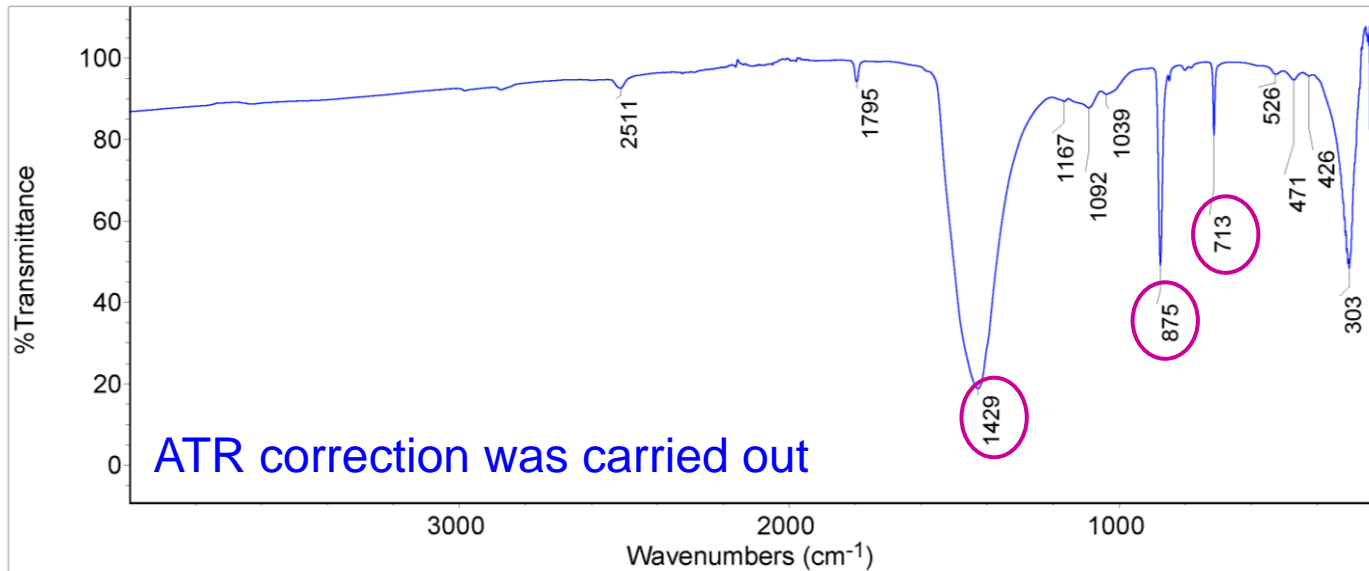


Transmission mode IR spectra (cm⁻¹):

1427

876

712



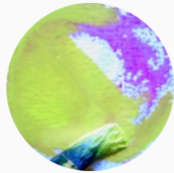
Reference IR spectra

http://tera.chem.ut.ee/IR_spectra/

Database of ATR-FT-IR spectra of various materials

ATR-FT-IR spectra of conservation-related materials in the MID-IR and FAR-IR region

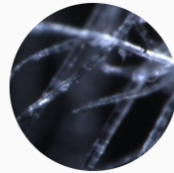
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Paint components

Selection of ATR-FT-IR spectra of various PIGMENTS, BINDERS and FILLERS in the MID-IR and FAR-IR region.

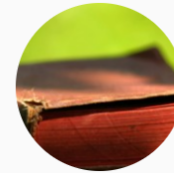
[Read more](#)



Textile fibres

Selection of ATR-FT-IR spectra of different single- and two-component textile fibres.

[Read more](#)



Publications

List of main publications of our work group related to the analysis of cultural heritage objects with different analytical methods.

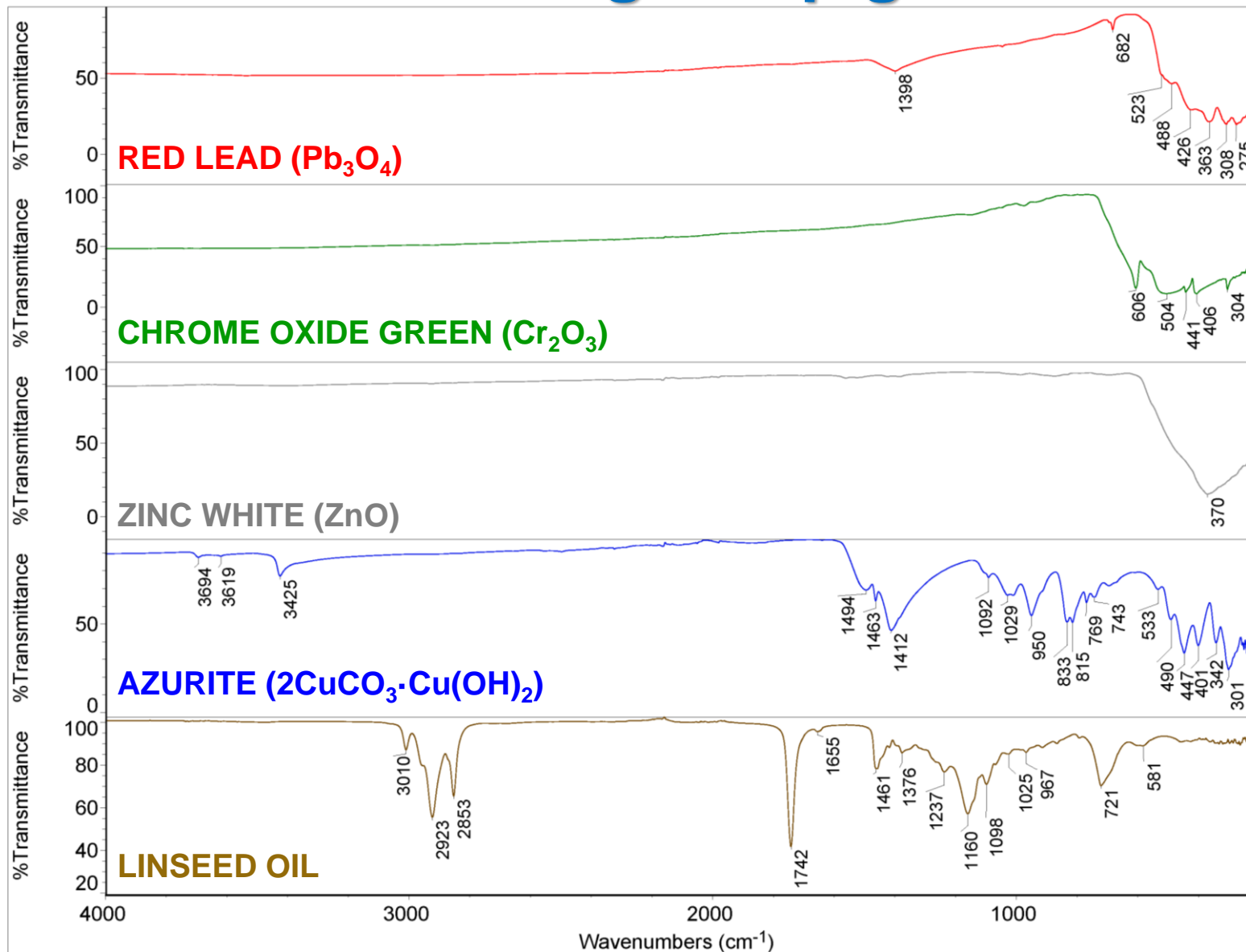
[Read more](#)

This database has been described in the article "ATR-FT-IR spectral collection of conservation materials in the extended region of 4000–80 cm^{-1} " *Analytical and Bioanalytical Chemistry*, 2016, 408 (13), pp 3373–3379. If you need to cite this database then please cite this article.

Some other IR spectral databases (Transmission and/or ATR spectra):

- IRUG - <http://www.irug.org/search-spectral-database>
- SDBS - http://sdb.sdb.aist.go.jp/sdb/cgi-bin/direct_frame_top.cgi

Different inorganic pigments



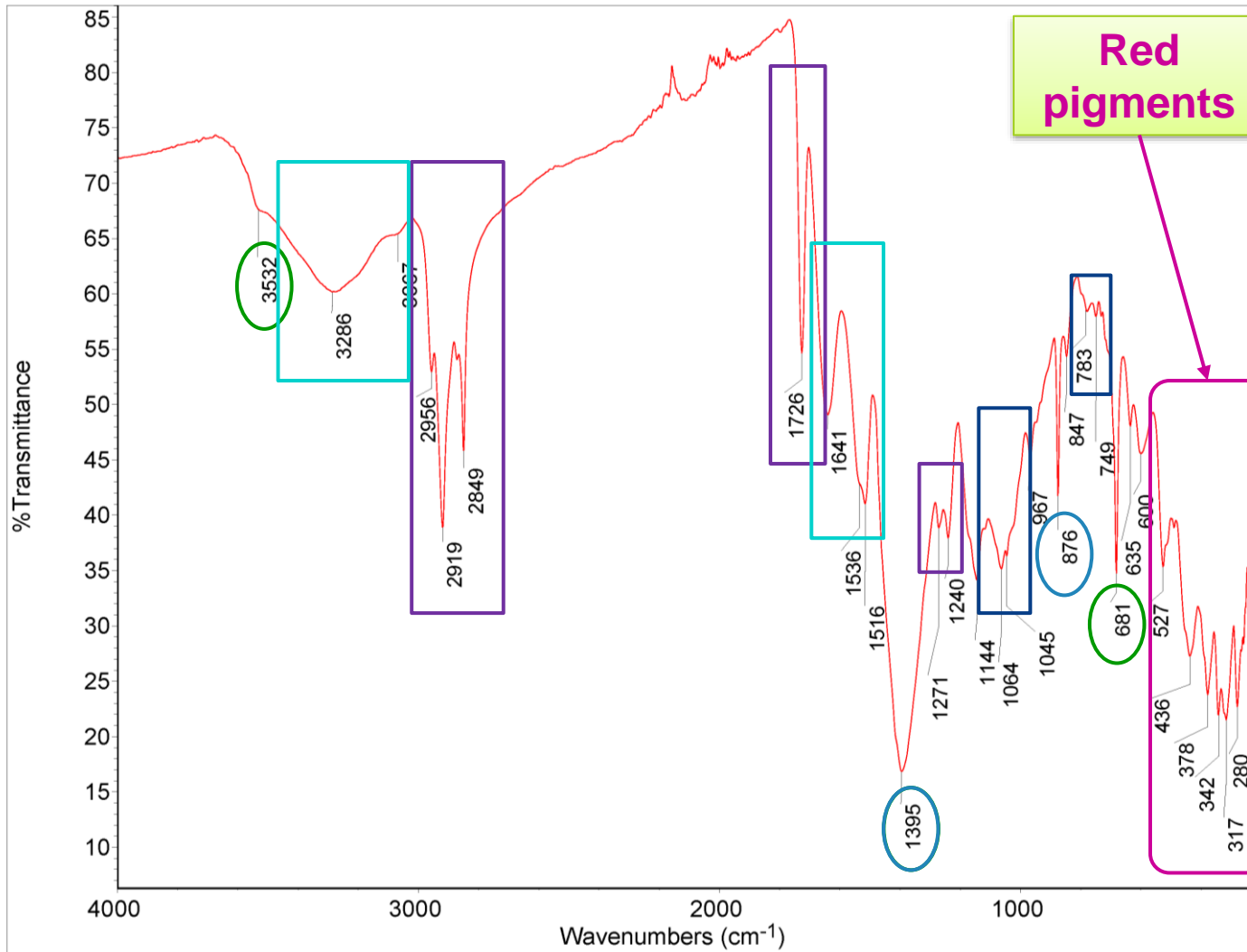
S. Vahur, A. Teearu, I. Leito. *Spectrochimica Acta Part A*, **2010**, 75, 1061 – 1072.

S. Vahur, U. Knuutinen, I. Leito. *Spectrochimica Acta Part A*, **2009**, 73, 764 – 771.

Red paint sample from the coat of arms of Bengt Hinrich von Biestram (18th century) from the Dome church in Tallinn



Photo: Conservation and Digitization Centre Kanut

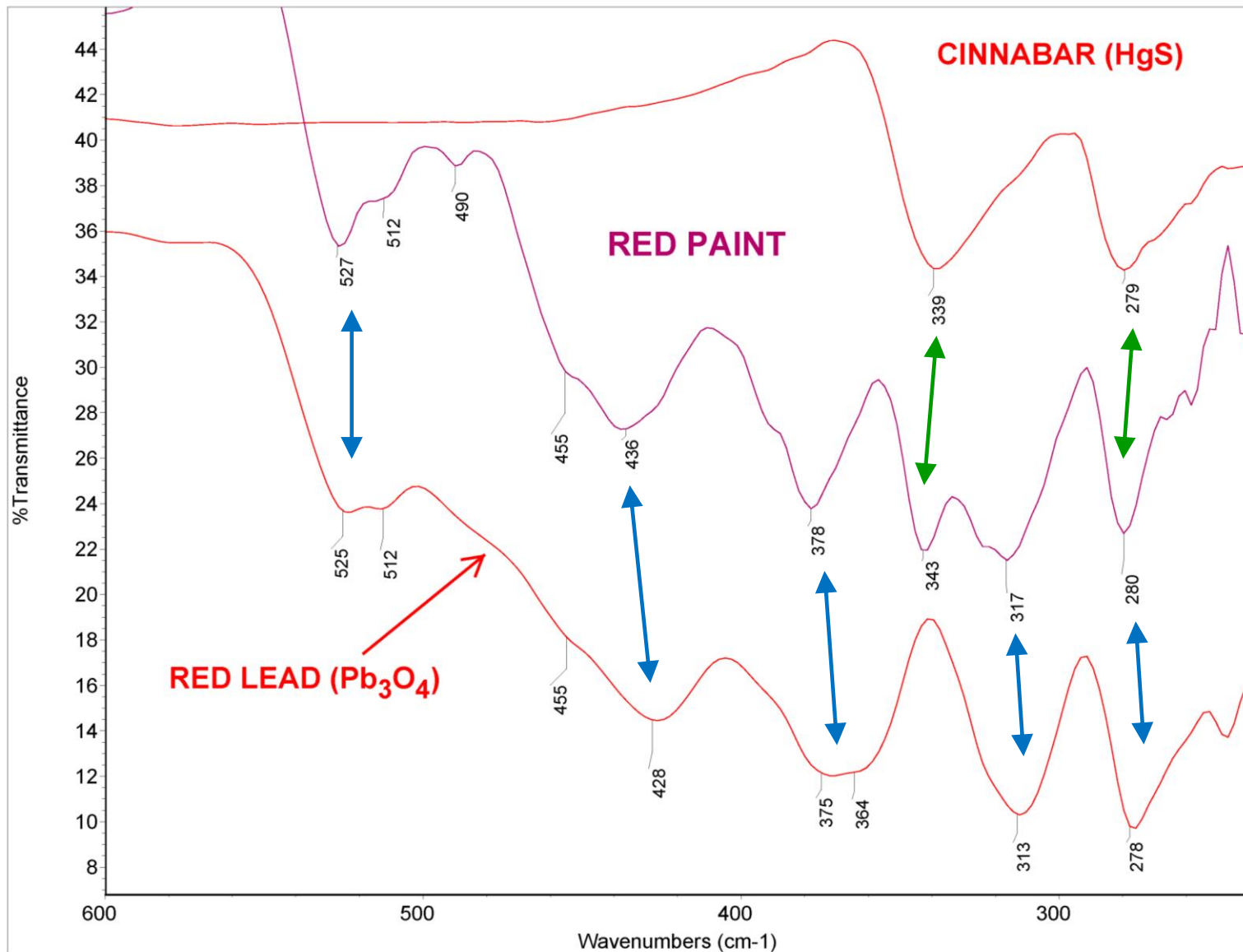


Fillers:

- Lead white
- Chalk
- Silicates

Binders:

- Protein
- Oil or possibly acrylic resin



Red pigments: **Cinnabar** and **Red lead**

Summary

- ATR is the most popular sampling technique for FT-IR spectroscopy.
- Enables to acquire high-quality IR spectra from easy and from difficult samples.
 - Refractive indices are important!
- Different materials (**paints, varnishes, textiles, clays, archeological residues, glues**, etc) can be analysed.
- Spectral maxima are slightly shifted compared to transmittance spectra
 - Compare against ATR spectra if possible
 - ATR correction can be applied