

Infrared spectroscopy for fuel fraud detection – building reproducible data analysis protocol

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Introduction

- infrared spectroscopy - workhorse for many forensic (and not only) labs
- relatively simple, fast, well-established, inexpensive, safe (no x-rays, isotopes, chemicals)
- limitations: sample thickness, concentration, presence of water
- for fuel research: detection of contaminants, monitoring degradation, quantifying additives

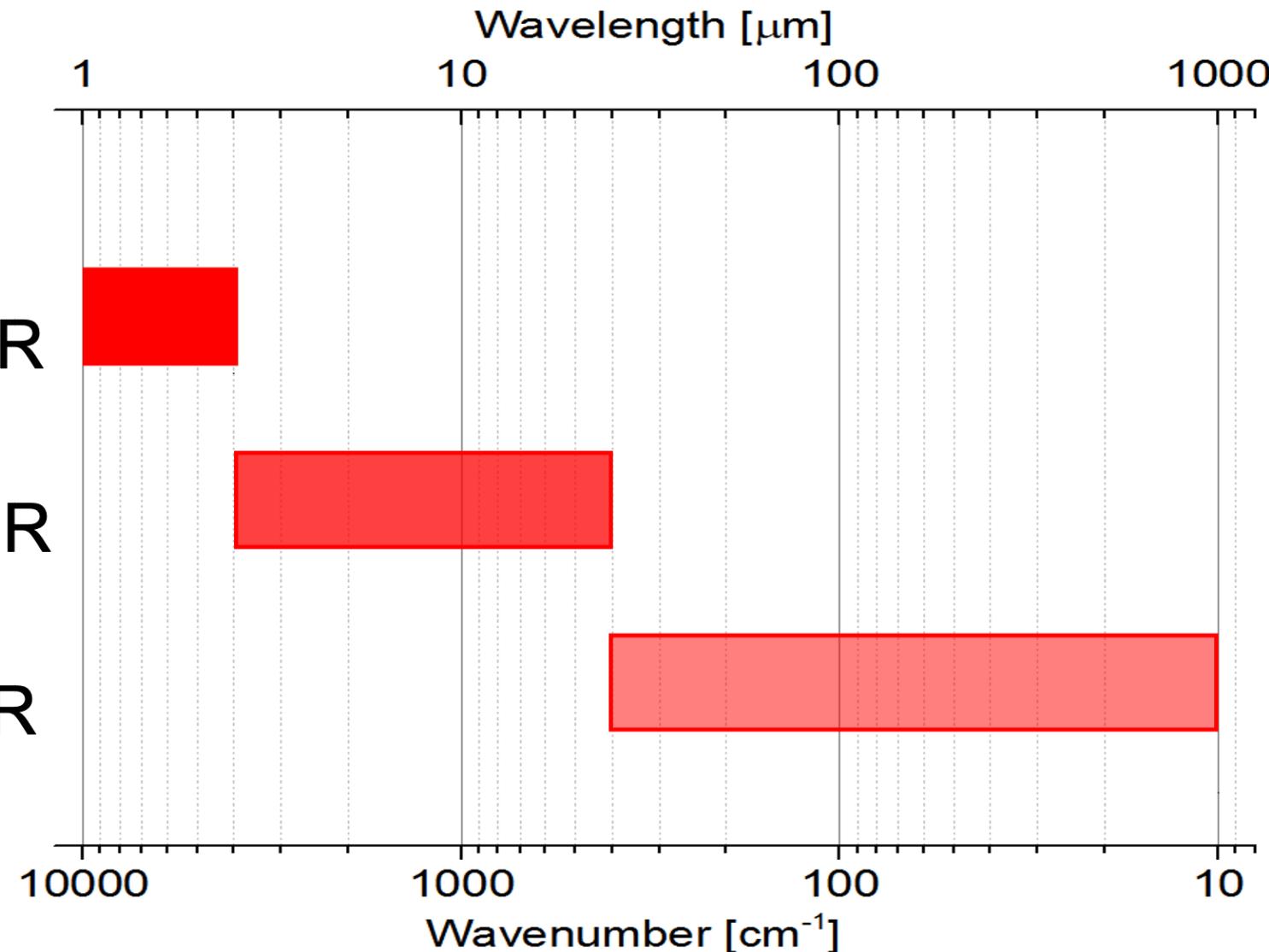
Principles of IR spectroscopy

- most organic molecules absorb light in the infrared region of the electromagnetic spectrum
- absorption at certain wavenumbers corresponds specifically to the bonds present
- every compound has unique spectral signature: absorbance of the infrared light versus the wavenumber

Method - Infrared spectroscopy

- various types of samples
- extensive database of spectra
- easily transferable
- specificity and selectivity
- adjusting the sampling method
- volatile samples (repeatability)
- complex chemical fingerprint - many variables
- required data processing

Spectral Ranges



Sampling Techniques

Transmission

Reflection

ATR

Diffuse Reflection (DRIFT)

Transmission

- method of choice, should be used whenever possible
- spectra of the highest quality and adhere to the Beer-Lambert law

Attenuated Total Reflection

- widely used FTIR sampling technique
- small depth of penetration (path length), virtually “surface” analysis
- relatively easy cleaning
- lower sensitivity than transmission
- response is wavelength dependent
- selection of crystal is required (refractive index and spectral range)

Liquid Samples

Classic Cell

window material
variable path
length
time consuming
cleaning

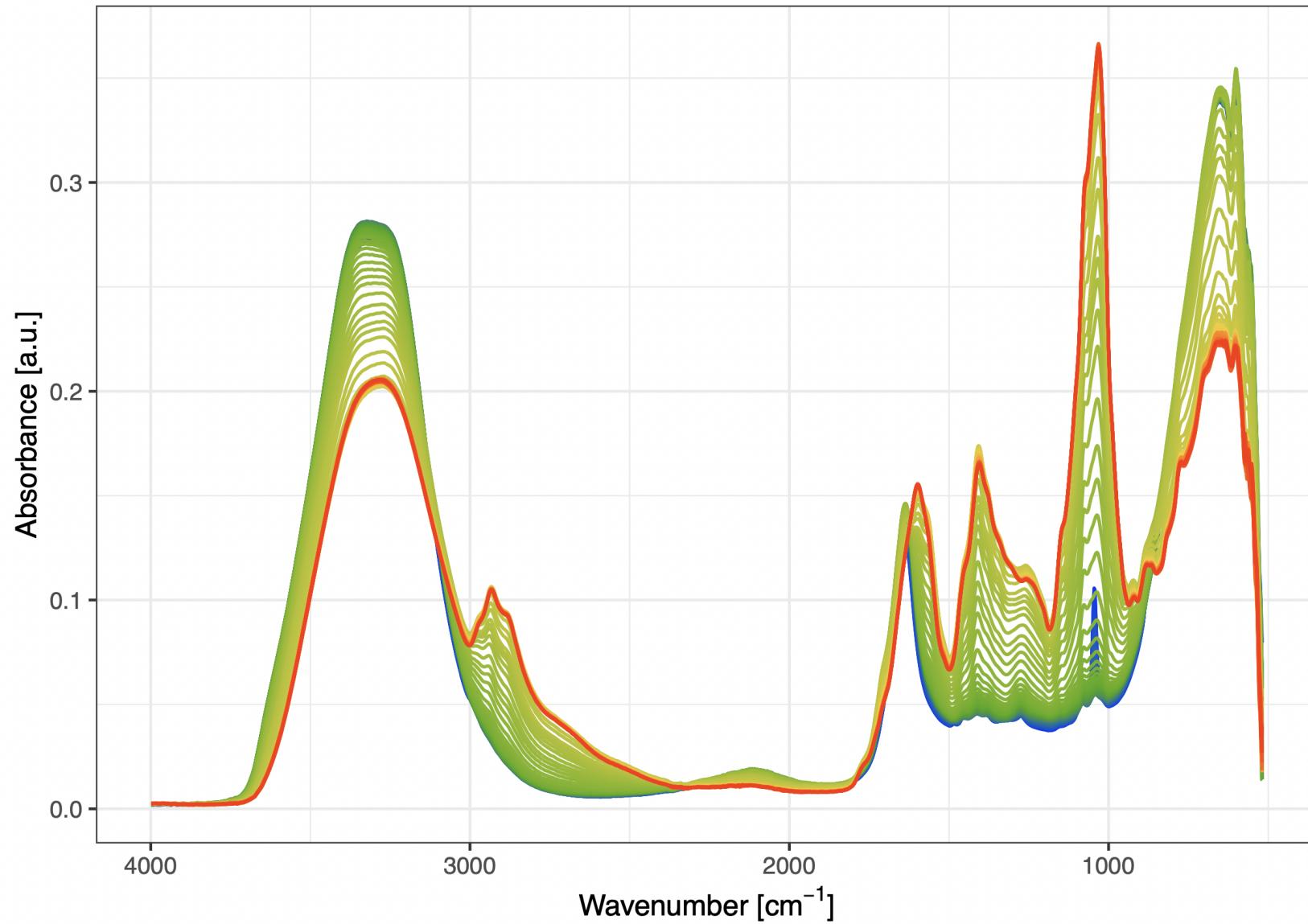
Sealed Cell

window material
constant path
length
extreme difficult
cleaning

ATR

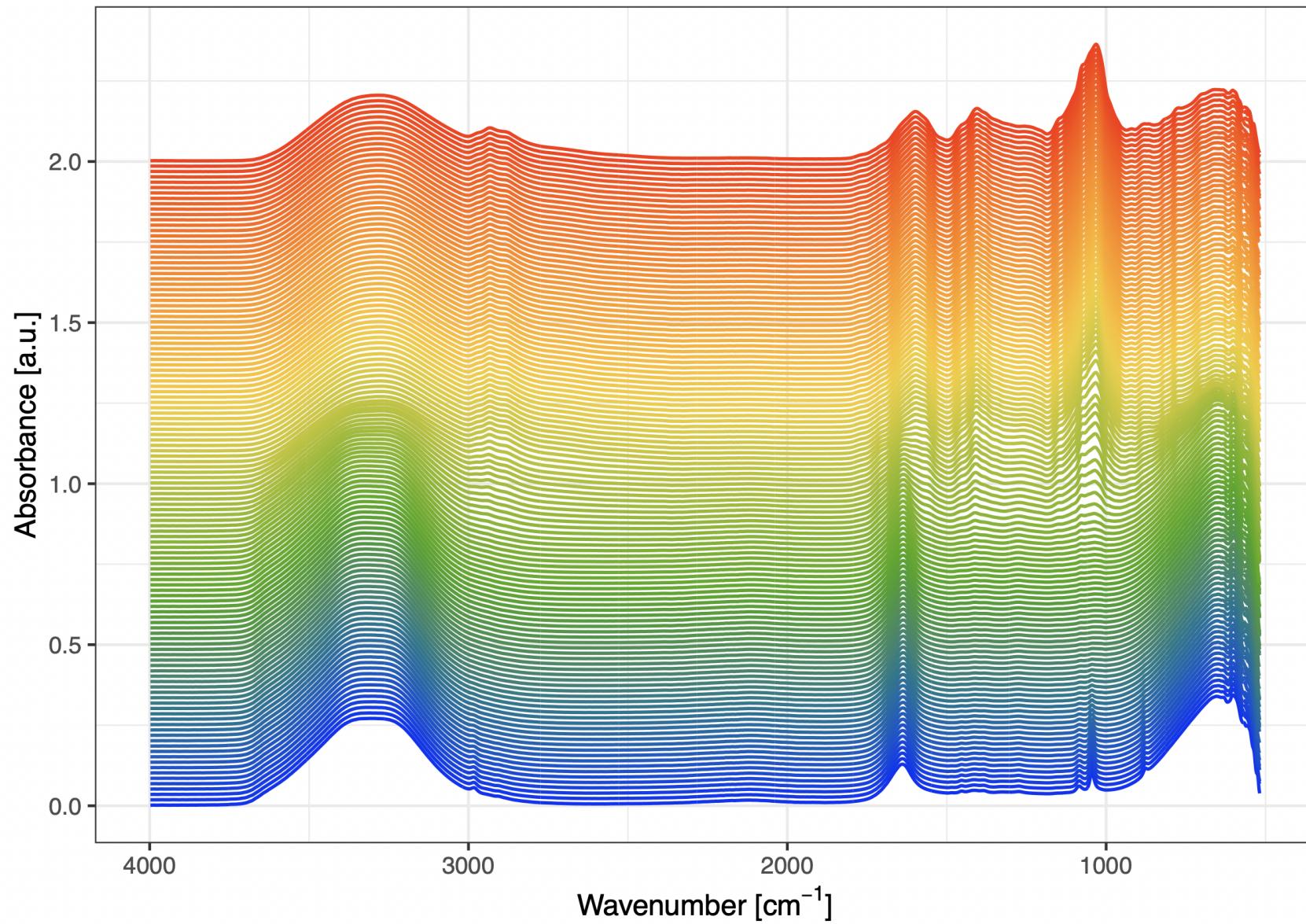
crystal material
small depth of
penetration
relatively easy
cleaning

Time Trial



2022.05.12, Nairobi

Time Trial - Spectra with the shift



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Examples of research

ATR-FTIR gasoline

ATR-FTIR Diesel

FTIR Bio-Diesel

Common oil parameters by FTIR

Parameter	Wavenumber [cm ⁻¹]
oxidation	1710
nitration	1630
sulfation	1150
Diesel fuel	810
gasoline	750
water	3420
glycol	1080, 1040, 880
soot	2000

Conclusions

- infrared spectroscopy: safe and label-free method for chemical evaluation
- repeatability and stability is required
- adequate experiment design
- careful spectral data processing especially for quantitative analysis

THANK YOU FOR YOUR ATTENTION