WAVELENGTH DEPENDENT RAMAN SPECTROSCOPY ON CHEMICAL WARFARE AGENT SIMULANTS

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Student Conference 2026

Motivation

Motivation

1914-1918

- WWI
  chlorine
  phosgene
  mustard gas
  casualities: ~ 100,000

1939-1945

- WWII
  Zyklon B
  casualities: ~ 1,1 m

1980s

- Iran-Iraq war
  mustard gas
  casualities: ~ 100,000

1988

- Halabja
  mustard
  gas
  sarin
  tabun
  VX
  casualities: ~ 5,000

1995

- Tokyo subway
  sarin
  casualities: ~ 12

2013

- Syrian Civil war
  sarin
  mustard gas
  chlorine
  casualities: ~ 2,000

A Brief History of Chemical War, Science History Institute, Accessed: 2026-02-16, https://www.sciencehistory.org/stories/magazine/a-brief-history-of-chemical-war
History of chemical warfare, Wikipedia, Accessed: 2026-02-16, https://en.wikipedia.org/wiki/History_of_chemical_warfare

Motivation

! Sensitive and reliable detection possibilities are necessary

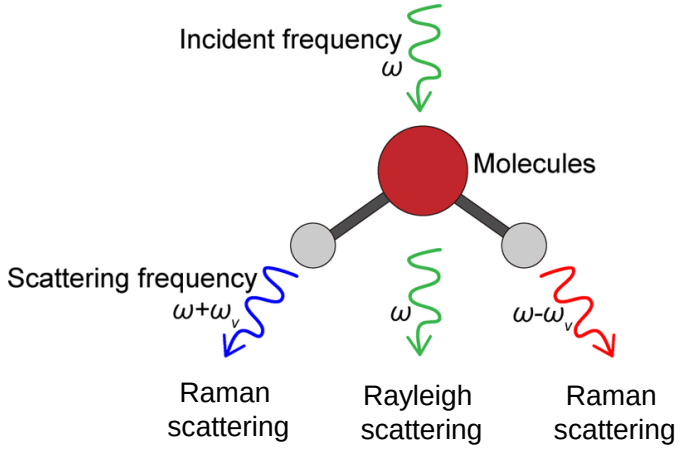
Methods:

- Colorimetric assay
- Ion mobility spectrometry

→ Raman spectroscopy as a standoff detection method

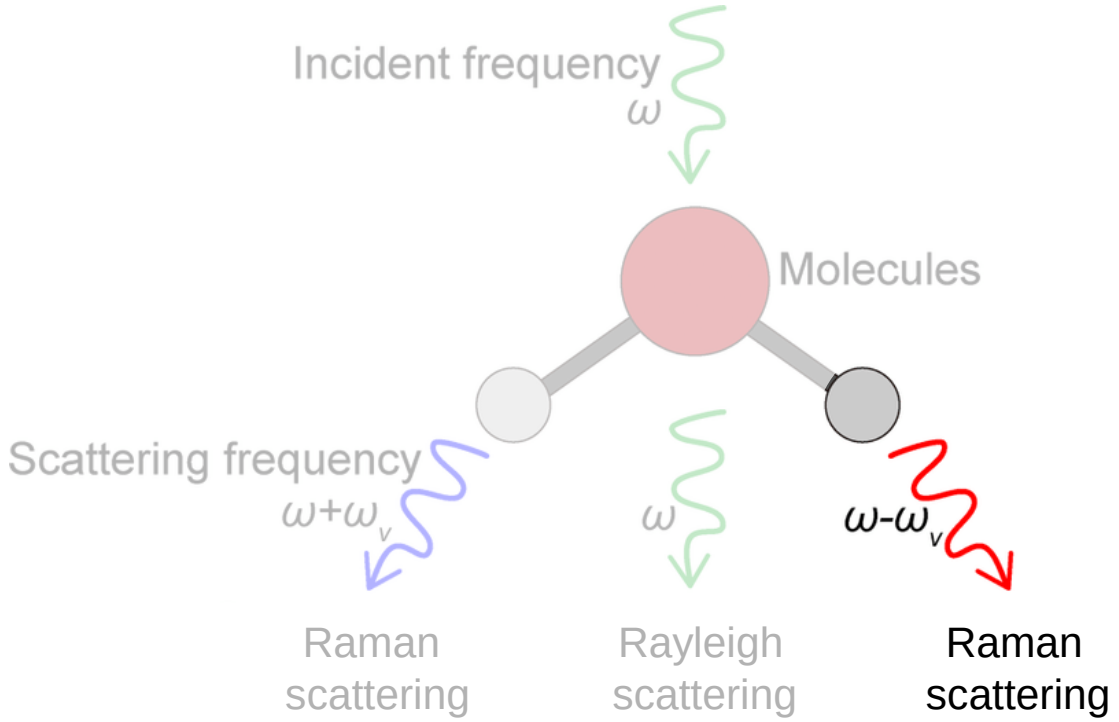
Challenges:

- sensitivity
- specificity
- detection distance



L. Lin, X. Bi, and et. al . Surface-enhanced Raman scattering nanotags for bioimaging. Journal of Applied Physics, 2021, DOI: 10.1063/5.0047578

Raman Effect

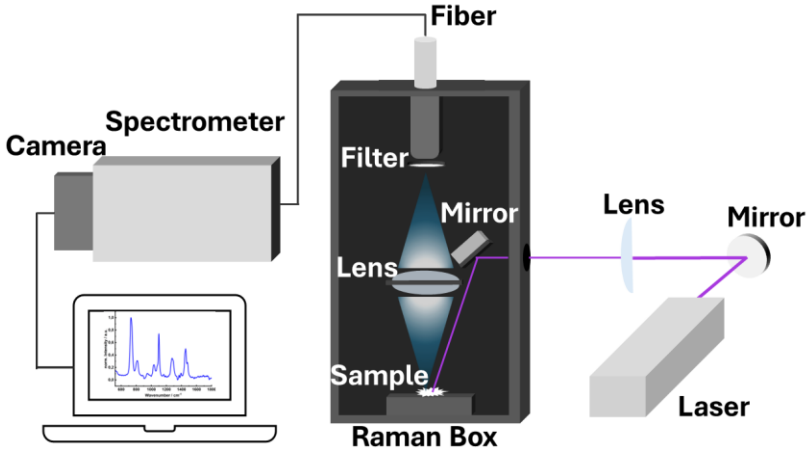


$$\text{Raman intensity} \propto \frac{1}{\lambda^4}$$

L. Lin, X. Bi, and et. al . Surface-enhanced Raman scattering nanotags for bioimaging. Journal of Applied Physics, 2021, DOI: 10.1063/5.0047578

Experimental

Setups



785 nm excitation

- portable Raman spectrometer MIRA XTR (Metrohm)
- contact detection
- FWHM: 17 cm^{-1}

355 nm excitation

- newly developed Raman setup
- 9 cm detection distance
- FWHM: 11 cm^{-1}

266 nm excitation

- inhouse built Raman setup
- 75 cm detection distance
- FWHM: 33 cm^{-1}

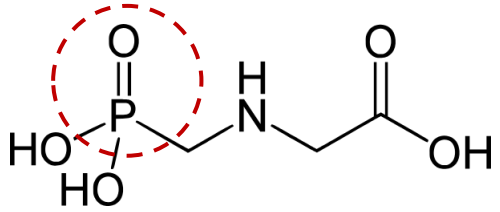
FWHM: Full Width at Half Maximum

CWA-Simulants

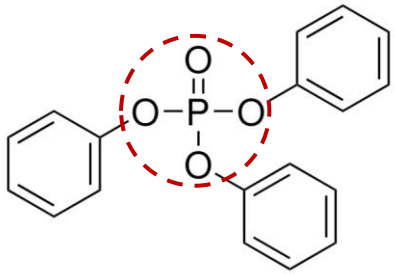
CWA simulants as alternative for research → less toxic
have some similar physical and chemical properties (e.g. vapor pressure and relevant functional groups)

Powders

Glyphosate (GPH)

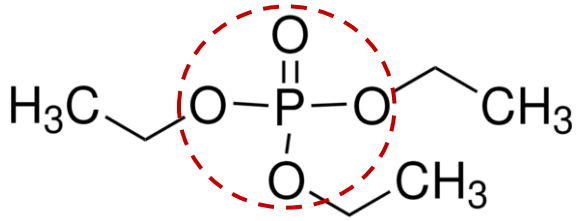


Triphenyl phosphate (TPP)

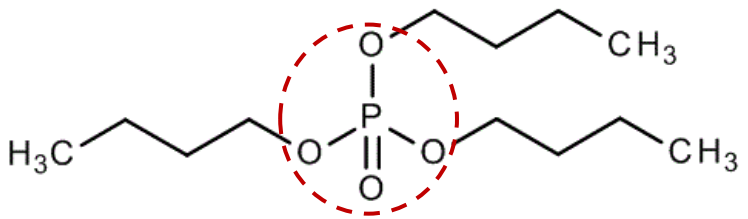


Liquids

Triethyl phosphate (TEP)



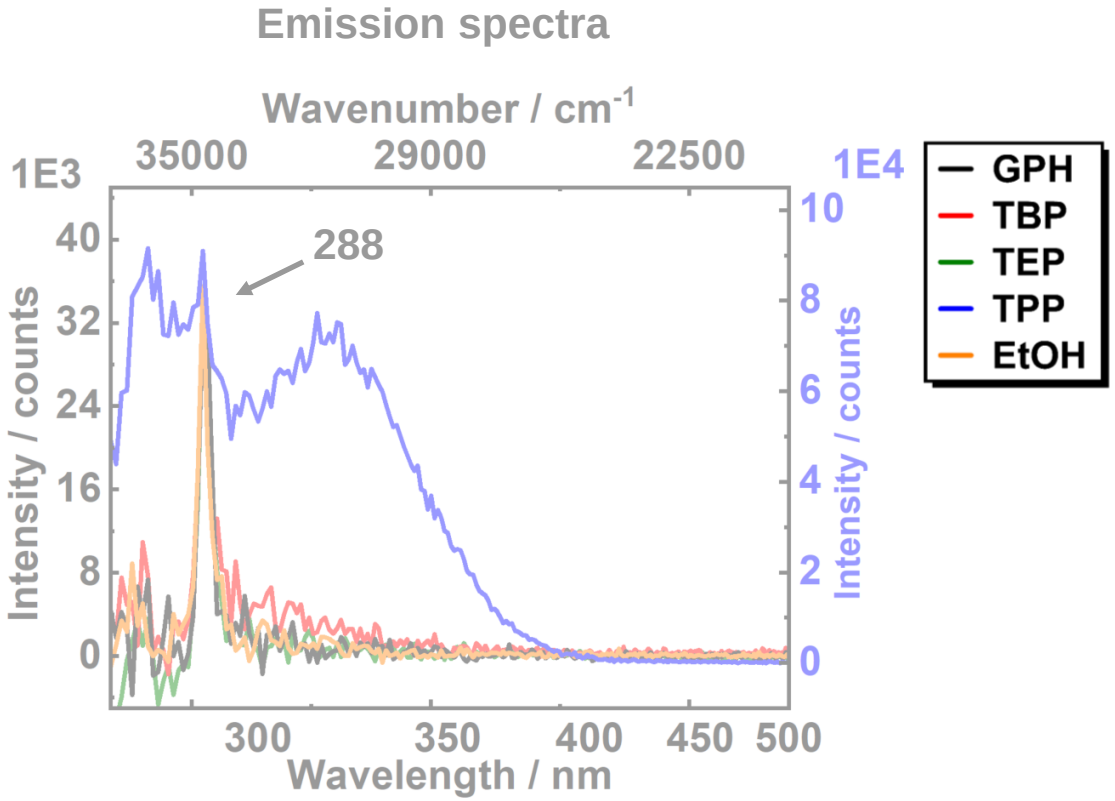
Tributyl phosphate (TBP)



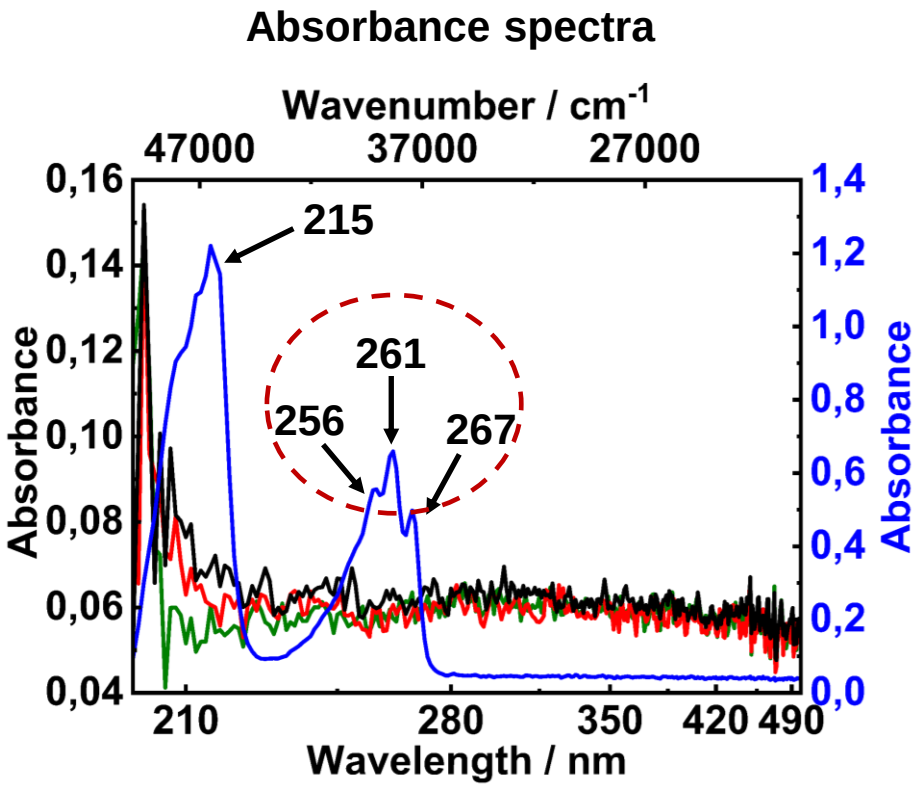
Triethylphosphate, Merck, Accessed: 2026-02-23, https://www.sigmaaldrich.com/DE/de/product/aldrich/538728
Tributylphosphate, Merck, Accessed: 2026-02-23, https://www.merckmillipore.com/DE/de/product/Tributyl-phosphate,MDA_CHEM-818604
Triphenylphsphate, Merck, Accessed: 2026-02-23, https://www.sigmaaldrich.com/DE/de/product/aldrich/241288
Glyphosate, Wikipedia, Accessed: 2026-02-23, https://de.wikipedia.org/wiki/Glyphosat

Results

UV-VIS measurements of solutions



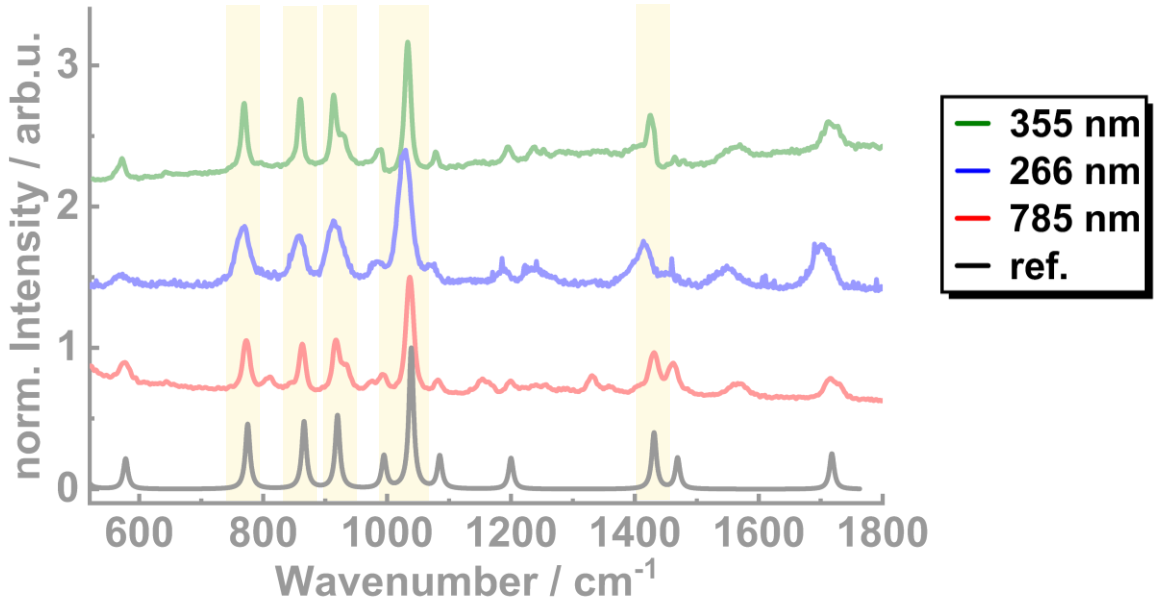
- excitation wavelength of 266 nm
- emission of ethanol or quartz at 288 nm in all spectra visible
- strong fluorescence of TPP



- multiple absorbance peaks of TPP

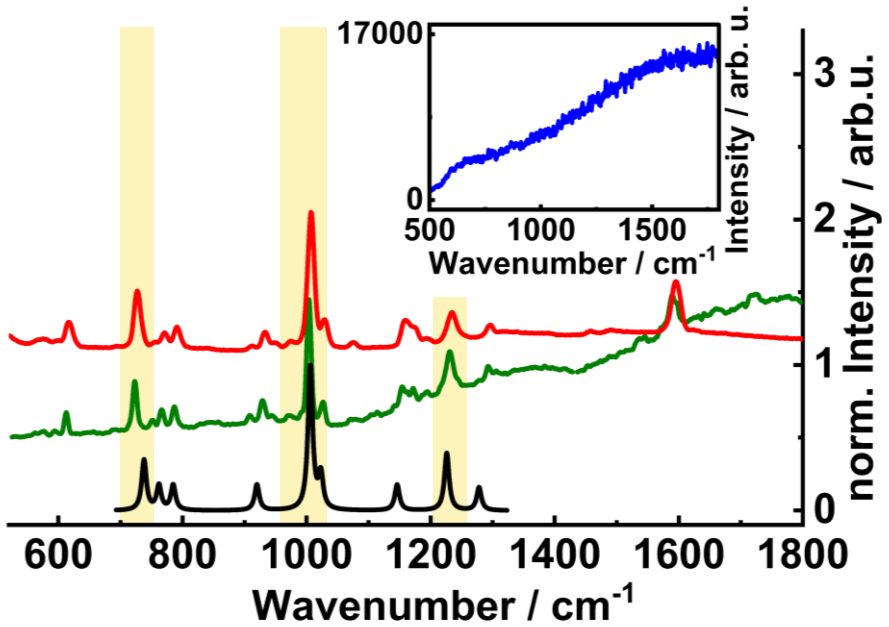
Raman measurements

Glyphosate



- very similar Raman spectra of all setups
- all band positions comparable with literature band positions[1]

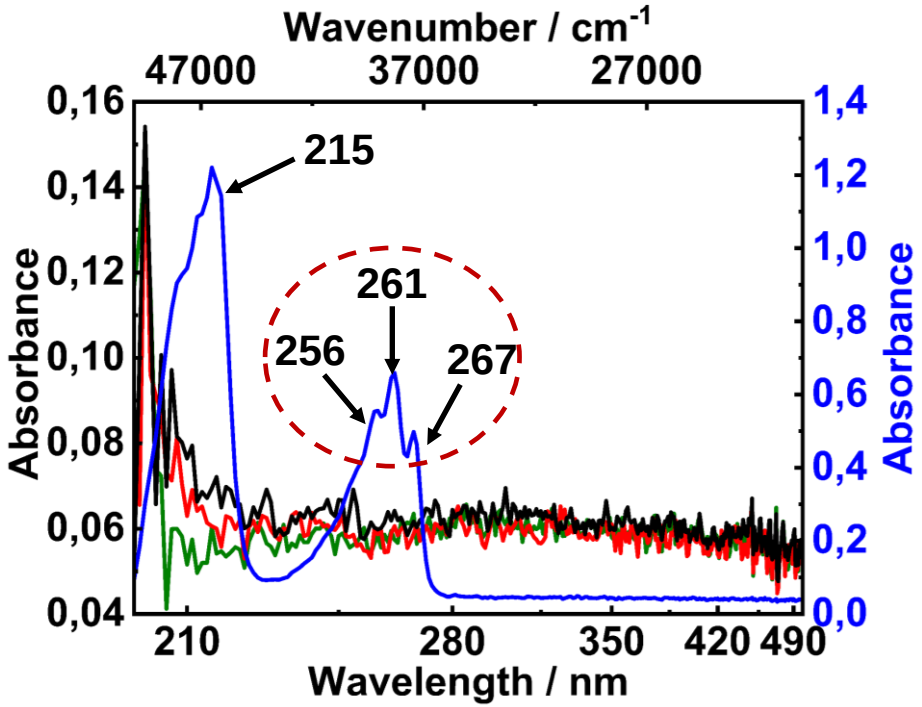
Triphenyl phosphate

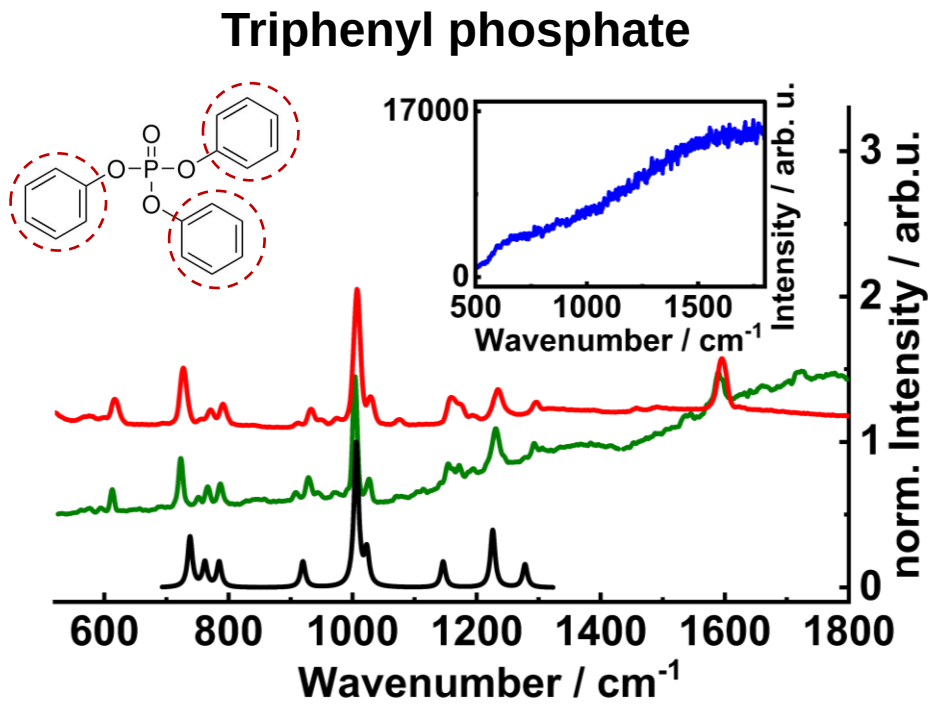


- strong fluorescence of TPP at 266 nm exc. excitation wavelength → no Raman peaks observable
- some of fluorescence at 355 nm also visible, but less intense
- band positions comparable to the literature[2]

[1] L. Mikac, I. Rigó, and et al. Comparison of glyphosate detection by surface-enhanced raman spectroscopy using gold and silver nanoparticles at different laser excitations. MDPI Molecules, (18), 2022, doi:10.3390/molecules27185767
[2] L. Cantu and E. Gallo. Explosives and warfare agents remote raman detection on realistic background samples. Eur. Phys. J. Plus, 137(207), 2022, doi:https://doi.org/10.1140/epjp/s13360-022-02416-0.

Raman measurements





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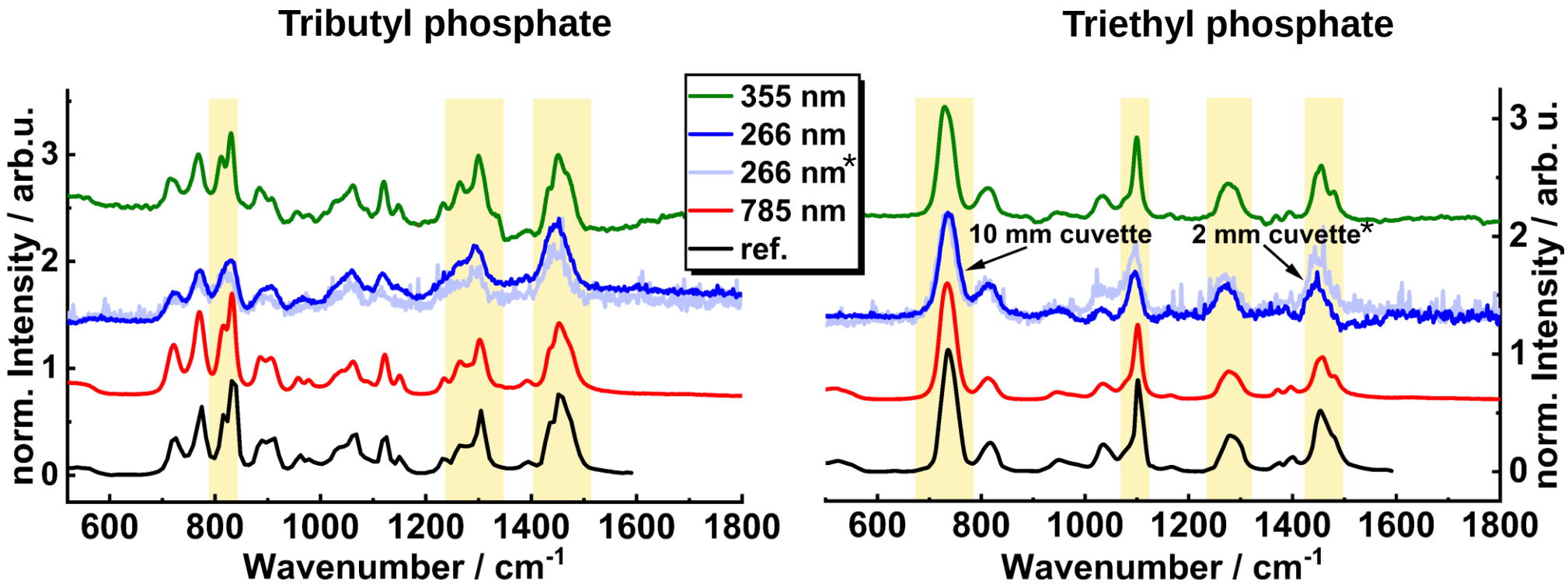
Raman measurements



- very similar Raman spectra of all setups
- all band positions comparable with literature band positions[3,4]
- lower SNR in cuvette with low amount of sample (2 mm cuvette)

SNR: signal-to-noise ratio

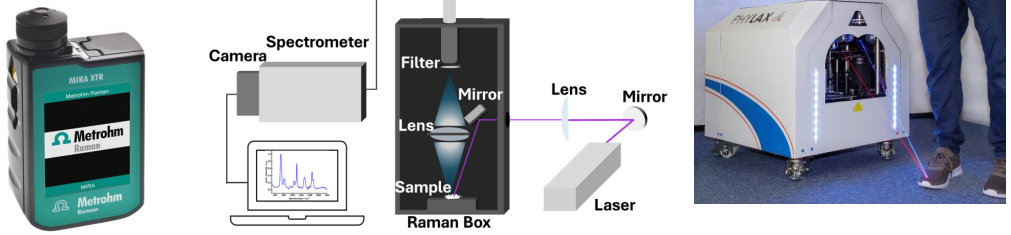
[3] N. I. of Advanced Industrial Science and Technology, Accessed: 2026-01-12, 1999. https://sdbs.db.aist.go.jp/CompoundView.aspx?sdbsno=2164
[4] N. I. of Advanced Industrial Science and Technology, Accessed: 2026-01-12, 1999. https://sdbs.db.aist.go.jp/CompoundLanding.aspx?sdbsno=2905

Conclusion and Outlook

Conclusion

- direct and quantitative comparison of the spectra is difficult

→ differences in optical design, spectrometer resolution and detection distance among the setups

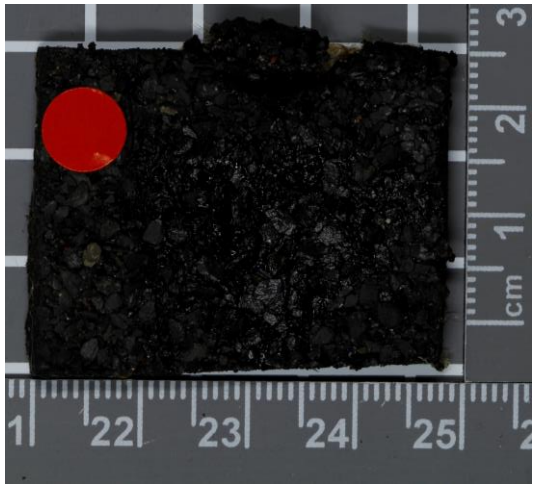


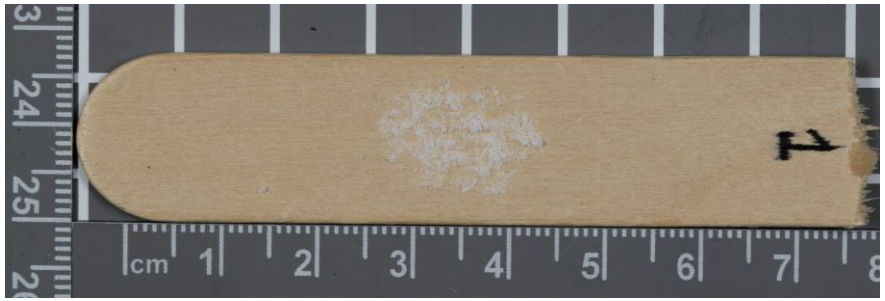
- BUT: initial impression could be obtained ✓
  - Raman bands correlate well with literature values, except TPP at 266 nm excitation
  - Raman peaks detectable in smaller amounts

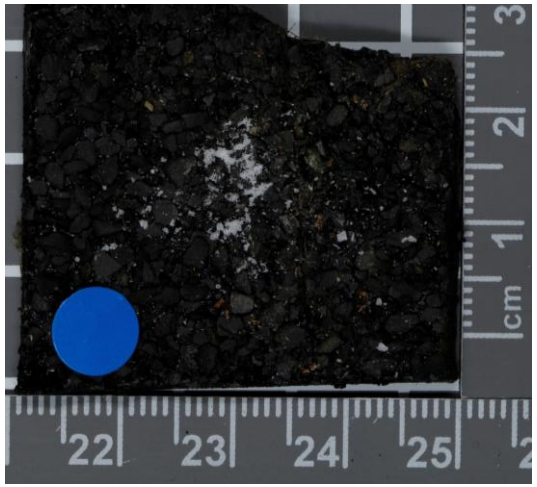
Outlook

more studies are still ongoing, with the focus on:

- determination of detection limit → various concentrations of the sample
- simulation of realistic scenarios → samples on various materials/substrates







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THANK YOU FOR YOUR ATTENTION!