Wavelength dependent Raman spectroscopy on chemical warfare agent simulants

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Introduction

- multiple occasions of chemical warfare agent (CWA) use throughout history [1] ➞ valid detection possibilities are needed
- direct investigation of CWAs is very challenging ➞ CWA-simulants as a safer approach
- identification of CWAs using Raman spectroscopy
- Raman cross section is highly wavelength dependent

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

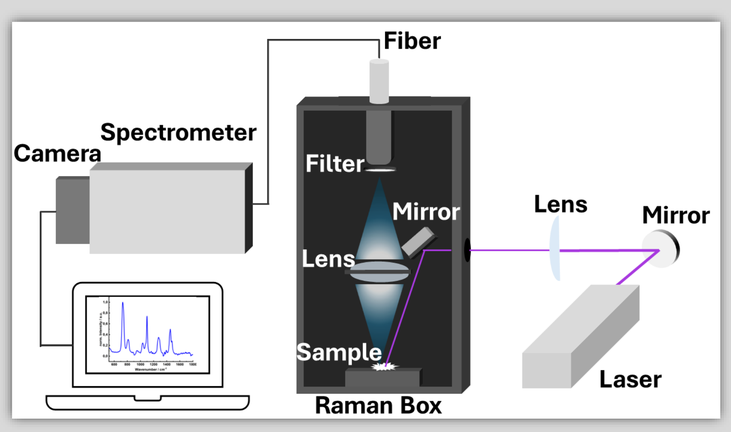
Aim of this Work

- Feasibility of Raman spectroscopy studies on CWA-simulants: Glyphosate (GPH), Triphenyl phosphate (TPP), Triethyl phosphate (TEP) and Tributyl phosphate (TBP) with different excitation wavelengths ➞ 266, 355 and 785 nm

Experimental setups

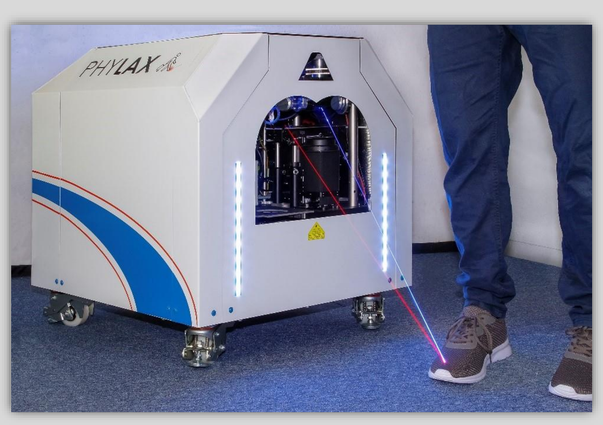
785 nm excitation

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



355 nm excitation

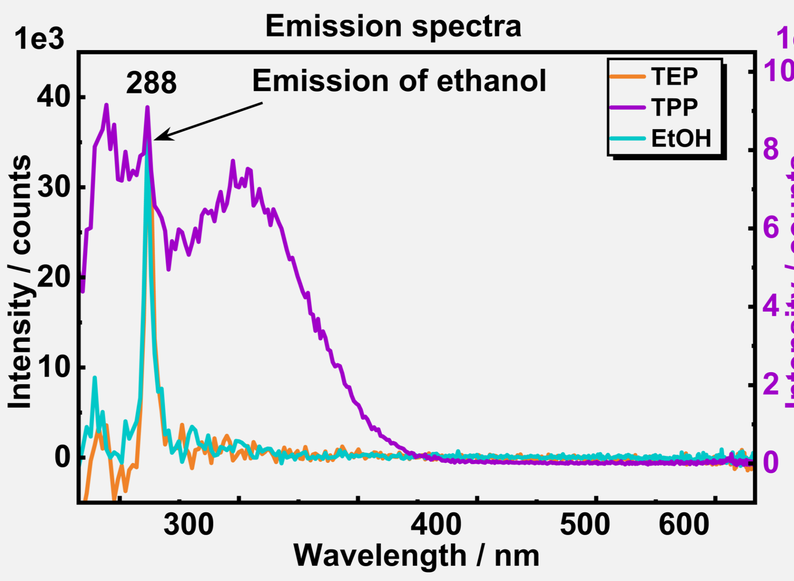
- newly developed Raman setup
- 9 cm detection distance
- FWHM: 11 cm^{-1}

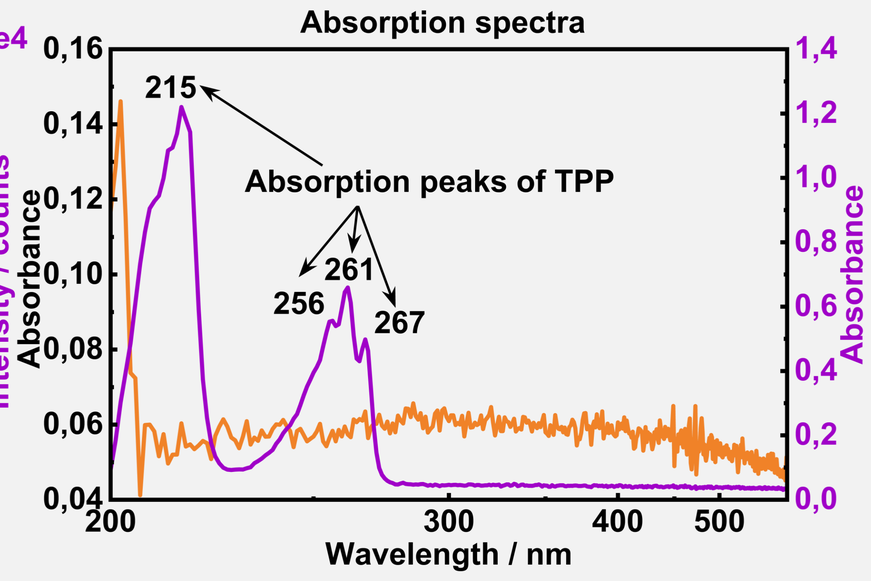


266 nm excitation

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

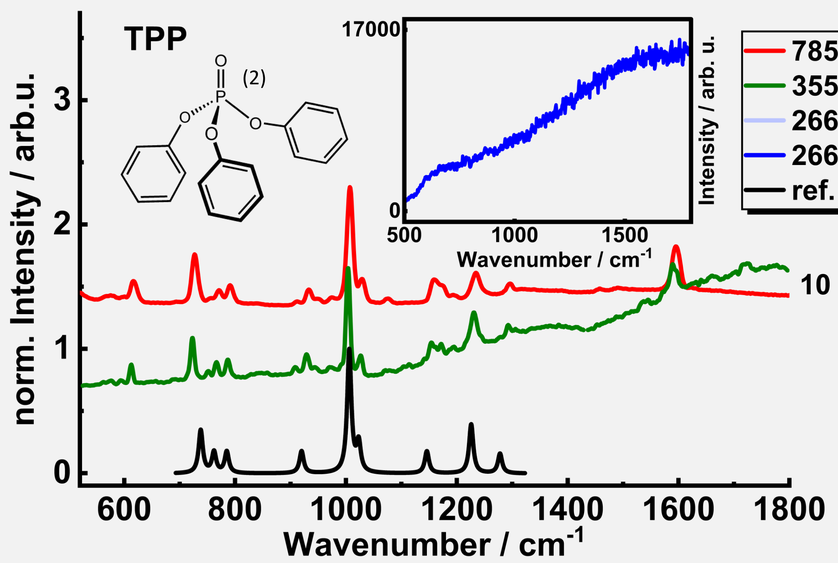
Results and Discussion

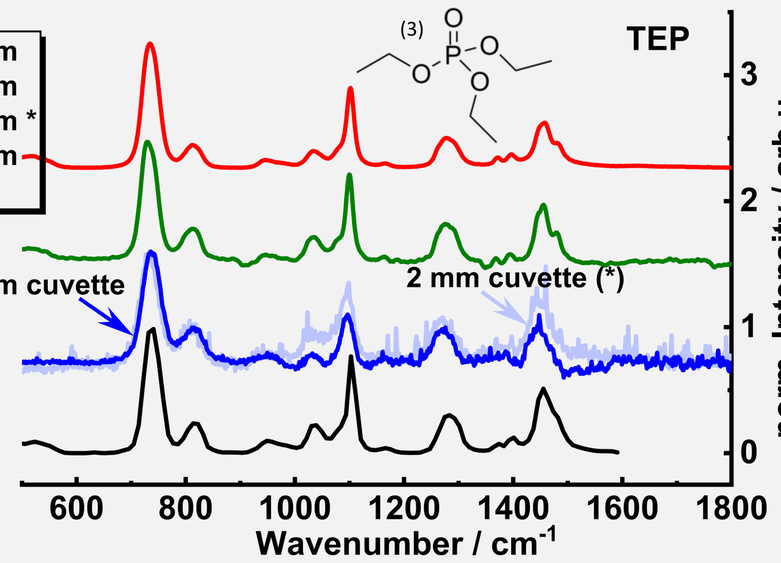




Fluorescence measurements

- ethanol solutions of CWA simulants show possible emission of ethanol at 288 nm
- broad fluorescence of TPP
- absorbance peaks of TPP at 215, 256, 261 and 267 nm detected





Raman measurements

- very similar spectra of all of the setups
- strong fluorescence of TPP at 266 nm excitation wavelength ➞ chemical structure of TPP is the cause
- measurement of TEP in different path length cuvettes ➞ lower SNR in thinner cuvettes
- lower spectral resolution of 266 nm setup ➞ slightly broader peaks
- all Raman bands comparable with literature band positions [4,5]

Conclusion

- characteristic Raman bands visible in almost all spectra
- 266 nm excitation is less suitable for TPP
- Raman peaks also visible for low amounts of sample

Outlook

- measurements at different concentrations ➞ determine the detection limit
- tests on various background materials to simulate realistic scenarios

References

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Acknowledgments

The work has been carried out at the Institute of Technical Physics in Hardthausen, German Aerospace Center (Deutsches Zentrum für Luft- und Raumfahrt) and supervised by Prof. Dr. Christian Hübner, Institute of Physics, Universität zu Lübeck, Lübeck.
Sincere gratitude is expressed to the Department of Atmospheric Propagation and Effect for providing the opportunity to complete the internship at their institution. Additional thanks to Björn Prietzel for his assistance with the chemicals.