Optical Spectroscopy

Protocol for the PC 2 lab course by
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date of experiment:	28.01.2026
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submission date:	January 29, 2026

Abstract: In this experiment,

Contents

1 Theory

Fig. 1: Scheme of the .[1]

[1]

$$R = \frac{\lambda}{\Delta\lambda} = k \cdot N \tag{1}$$

$$\alpha = ... + \Delta\alpha \tag{2}$$

2 Procedure

The DIY spectrometer was already built prior to the start of the experiment as shown in Figure 1 and was set up so that the zeroth diffraction order was centered on the exit slit. First, the reference spectrum of the lamp was recorded with the Python script `Spektrometersoftware.py`, using a step count of 6000 and a stepping speed of 1000 steps per second. Then the bandpass filter was inserted between the entrance slit and the concave mirror and the spectrum of the filtered light was recorded. For calibration, the transmission spectrum was compared to theoretical transmission data using the Python script `calibration.py` and the parameters scale, f and $\Delta\alpha$ were adjusted according to Equation 2 to fit the measured spectrum to the theoretical spectrum. For all subsequent measurements, the calibration parameters scale = 1.0, $f = 0.925$ and $\Delta\alpha = 0.59$ were used.
Next, a cuvette was filled with distilled water and placed between exit slit and concave mirror. The spectrum was recorded and used as a reference for the potassium permanganate and chlorophyll solutions. After replacing the water cuvette with a cuvette filled with concentrated and then diluted potassium permanganate solution, their spectrum were recorded separately. In the next part, a single drop of chlorophyll solution was added to the water cuvette and the spectrum was recorded. Then, another drop was added and the spectrum recorded again. This was repeated until a total of five drops were added to the cuvette. In the last part of the experiment, both slits were closed first, then the entrance slit was opened by half a turn and the exit slit by 6 turns. Then the background spectra of pure nitric acid and the solution of holmium oxide in nitric acid were recorded separately. This was repeated with the exit slit opened by 3 turns and one and a half turn, respectively.

3 Results and Analysis

3.1 Lamp and filter spectra

3.2 Potassium permanganate spectra

3.3 Chlorophyll spectra

3.4 Holmium oxide spectra

The absorption spectra of Holmium oxide in nitric acid for different exit slit widths are generated from the measured transmission spectra analog to the spectra of $KMnO_4$ und Chlorophyll and are plotted together in Figure 2.

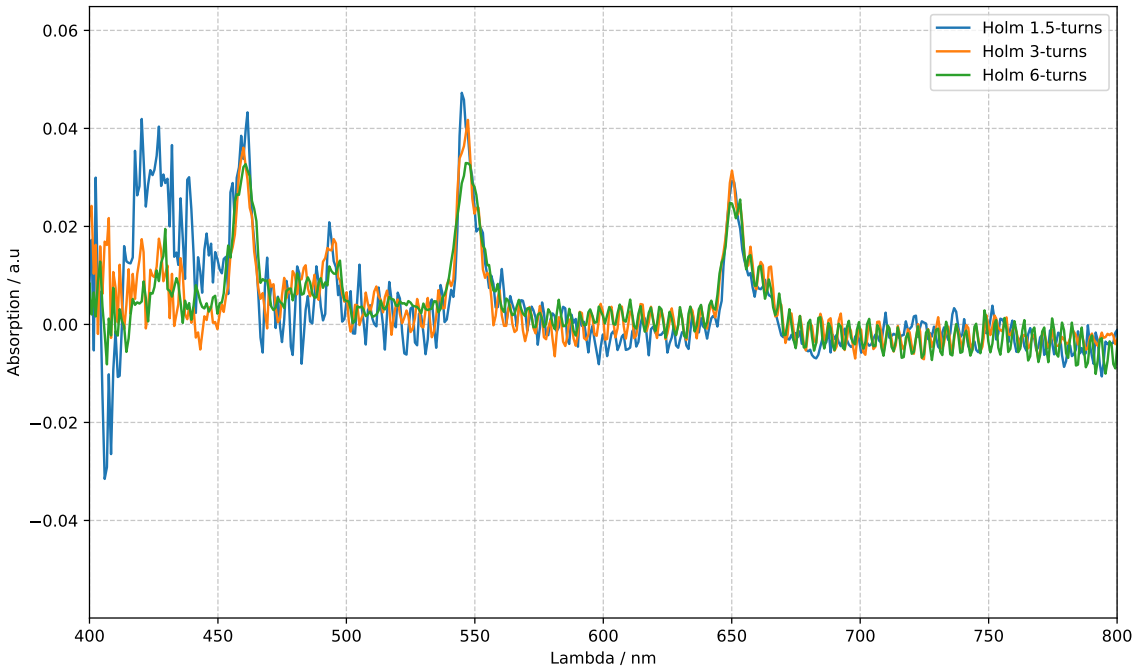

Fig. 2: Absorption spectrum of Holmium oxide in nitric acid for different exit slit widths between 400 and 800 nm.

All three spectra show three distinct absorption peaks around 460 nm, 545 nm and 650 nm. With decreasing slit width, the absorption peaks become narrower and more pronounced. The absorption spectrum of Holmium oxide with an exit slit of 1.5 turns shows additional oscillations, which can be attributed to noise due to the lower light intensity reaching the detector at this slit width.
To analyze the absorption peaks further, a four-fold Lorentzian model is fitted to each of the three spectra. The fitted curves are shown together with the measured spectra in Figure 3, Figure 4 and Figure 5.

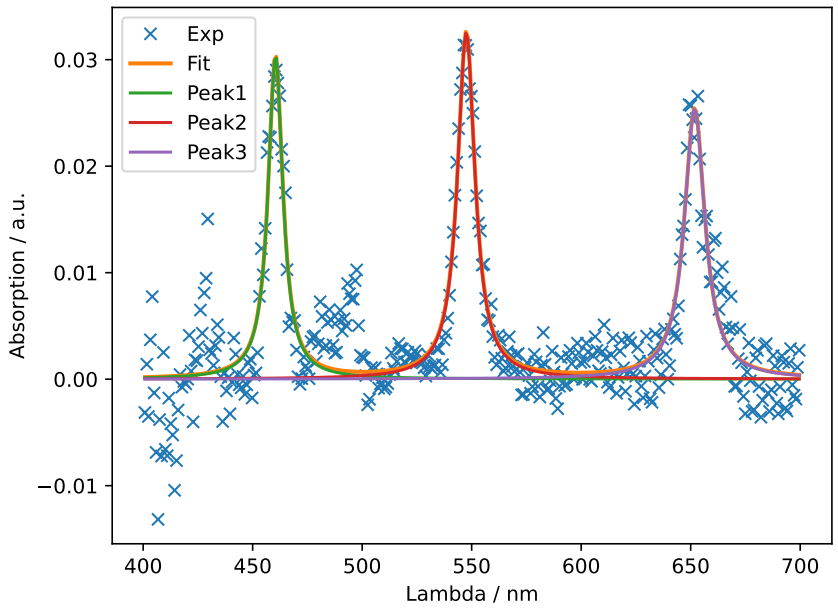

Fig. 3: Absorption signals of Holmium oxide in nitric acid with a four-fold Lorentzian model fit for 6 turns between 400 and 700 nm.

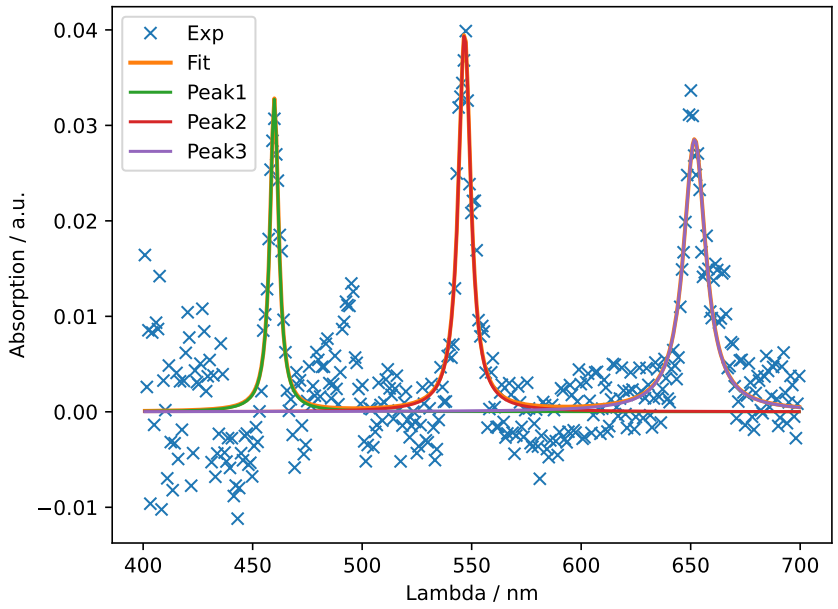

Fig. 4: Absorption signals of Holmium oxide in nitric acid with a four-fold Lorentzian model fit for 3 turns between 400 and 700 nm.

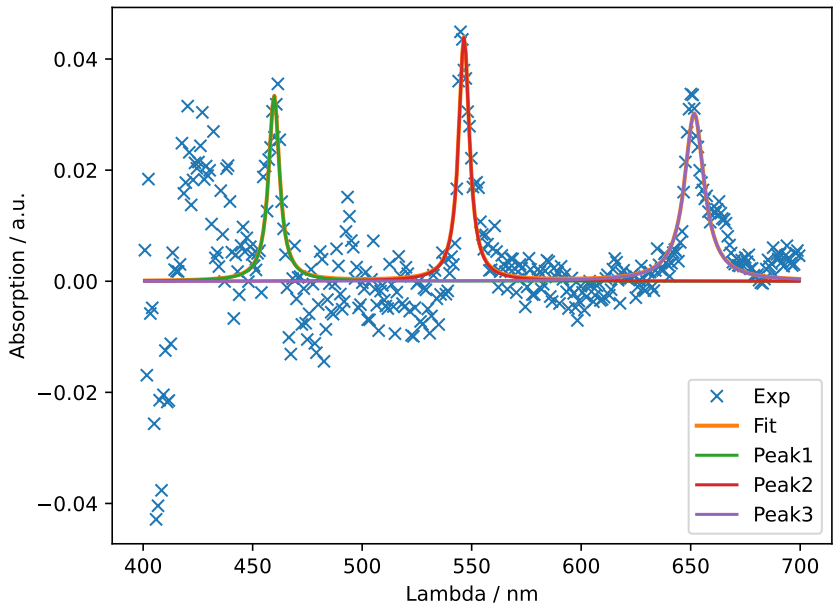

Fig. 5: Absorption signals of Holmium oxide in nitric acid with a four-fold Lorentzian model fit for 1.5 turns between 400 and 700 nm.

The extracted fit parameters, namely the position, half width at half maximum (HWHM, gam) and the peak amplitude of the three main absorption peaks for 6 turns in Figure 3 are summarized in Table 1.

Tab. 1: Fit parameters of the Lorentzian model for the absorption spectrum of Holmium oxide in nitric acid with an exit slit width of 6 turns.

pos / nm	gam / nm	amp / a.u.
460.45	8.12	0.39
547.54	9.67	0.49
651.81	11.40	0.46

The corresponding fit parameters for the fits in Figure 4 and Figure 5 are summarized in Table 2 and Table 3.

Tab. 2: Fit parameters of the Lorentzian model for the absorption spectrum of Holmium oxide in nitric acid with an exit slit width of 3 turns.

pos / nm	gam / nm	amp / a.u.
460.45	4.79	0.25
547.54	6.82	0.43
651.81	12.27	0.55

Tab. 3: Fit parameters of the Lorentzian model for the absorption spectrum of Holmium oxide in nitric acid with an exit slit width of 1.5 turns.

pos / nm	gam / nm	amp / a.u.
460.45	5.95	0.31
547.54	5.92	0.41
651.81	10.88	0.52

What can be observed from the fit parameters is that with decreasing slit width, the HWHM of the two absorption peaks at 460.5 nm and 547.5 nm decreases, indicating a higher resolution of the spectrometer at smaller slit widths. However, the peak amplitudes do not show a clear trend with changing slit width. Only the peak amplitude of the absorption peak at 547.5 nm decreases with decreasing slit width, matching the expectation that less light reaches the detector at smaller slit widths. The peak amplitude of the absorption peak at 460.5 nm first decreases from 6 turns to 3 turns, but then increases again for 1.5 turns and for the peak at 651.8 nm, the peak amplitude first increases from 6 turns to 3 turns and then decreases again for 1.5 turns. A possible explanation for this is the manual adjustments of the slit widths, which can lead to slight misalignments of the spectrometer and thus affect the measured intensities.
The line width is characterized by the full width at half maximum (FWHM) of the fitted Lorentzian peaks, which is 2 times the HWHM, expressed in the fit parameter 'gamma' and can be calculated for every absorption peak and slit width from Table 1, Table 2 and Table 3 using the equation:

$$\mathrm{FWHM} = 2 \cdot \mathrm{gam} \tag{3}$$

The calculated FWHM values for the three main absorption peaks at different slit widths are listed with the corresponding peak amplitudes in Table 4.

Tab. 4: Line widths (FWHM) and peak amplitudes of the Lorentzian model fits for different slit widths.

	6-turns		3-turns		1.5-turns	
pos / nm	FWHM/nm	amp/a.u.	FWHM/nm	amp/a.u.	FWHM/nm	amp/a.u.
460.45	16.24	0.39	9.58	0.25	11.90	0.39
547.54	19.34	0.49	13.64	0.43	11.84	0.49
651.81	22.80	0.46	24.54	0.55	21.76	0.52

The resolution of the spectra for the different slit widths is calculated by inserting the full width at half maximum (FWHM) with the extracted position of the absorption peak into Equation 1.

$$R = \frac{\lambda}{\Delta\lambda} = \frac{\mathrm{pos}}{\mathrm{FWHM}} \tag{4}$$

The calculation for the resolution of the spectrometer at a slit width of 6 turns yields:

$$R_{6-\mathrm{turns}} = \frac{1}{3} \cdot \left(\frac{460.45\ \mathrm{nm}}{16.24\ \mathrm{nm}} + \frac{547.54\ \mathrm{nm}}{19.34\ \mathrm{nm}} + \frac{651.81\ \mathrm{nm}}{22.80\ \mathrm{nm}} \right) = 26.6$$

By calculating the resolution for the slit widths of 3 turns and 1.5 turns in the same way with the mean value of the resolution for each peak from Equation 4, the resolution $R_{3-\text{turns}} = 38.3$ and $R_{1.5-\text{turns}} = 38.3$ are determined. The calculation matches the expectation that the resolution of the spectrometer increases with decreasing slit width, as less light reaches the detector and thus a more precise measurement of the absorption peaks is possible. But this trend is not observed for the reduction of the slit widths from 3 turns to 1.5 turns, indicating that a further decrease in slit width to 0.5 turns as described in the script[1] could have led to an even higher spectrometer resolution.

4 Conclusion

In this experiment,

5 References

[1] H. Dilger, *2025-pc2-script-en*, **2025**.