

Optical Spectroscopy

Protocol for the PC 2 lab course by
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Abstract: In this experiment, a DIY spectrometer with a rotatable grating was used to measure the absorption spectra of different samples, including potassium permanganate, chlorophyll and holmium oxide in nitric acid. The spectrometer was calibrated using a bandpass filter to establish a precise relationship between motor steps and wavelength. Potassium permanganate spectra were analyzed, identifying an absorption maximum at 525 nm consistent with its characteristic LMCT-induced purple color. Chlorophyll concentration series were evaluated, confirming the Beer-Lambert's law while identifying detector saturation and stray light as primary sources of spectral deviation. For holmium oxide in nitric acid, three absorption peaks of $f \rightarrow f$ transitions between $4f$ orbitals of holmium were measured and analyzed with a four-fold Lorentzian model fit. With decreasing slit width, the resolution of the spectrometer increased from $R_{6\text{-turns}} = 26.6$ to $R_{3\text{-turns}} = R_{1.5\text{-turns}} = 38.3$, as indicated by the decreasing FWHM of the absorption peaks at 460.5 nm and 547.5 nm and the decreasing amplitude of the peak at 547.5 nm.

Contents

1	Theory	1
1.1	Optical Spectroscopy	1
1.2	Wave interference at gratings	1
1.3	The spectrometer	2
1.4	Grating Equation for a Rotatable Grating	3
2	Procedure	3
3	Results and Analysis	4
3.1	Lamp and filter spectra	4
3.2	Potassium permanganate spectra	6
3.3	Chlorophyll spectra	8
3.4	Holmium oxide spectra	9
4	Conclusion	14
5	References	15

1 Theory

1.1 Optical Spectroscopy

Optical spectroscopy studies the interactions between matter and light of the visible and ultraviolet spectrum. This is done by analyzing the characteristic absorption and transmission spectra of different materials, which enables a qualitative and quantitative measurement of that material.

1.2 Wave interference at gratings

Optical gratings are often used in optical spectroscopy because they, like the classical double slit experiment, create characteristic interference patterns. But because of the higher number of slits, the gratings allow for a more complex pattern, which in turn results in better measurements. The interference patterns are created when light in the form of a linear wavefront passes through the grating. Each slit acts according to Huygens principle as the starting point of a new spherical wave that interferes with the other spherical waves.^[1] If the path width between those waves is an integer multiple, the waves interfere constructively, which leads to bright spots. If the path width is a half-integer multiple they interfere destructively, which leads to dark spots. An illustration of a grating is shown in Figure 1.

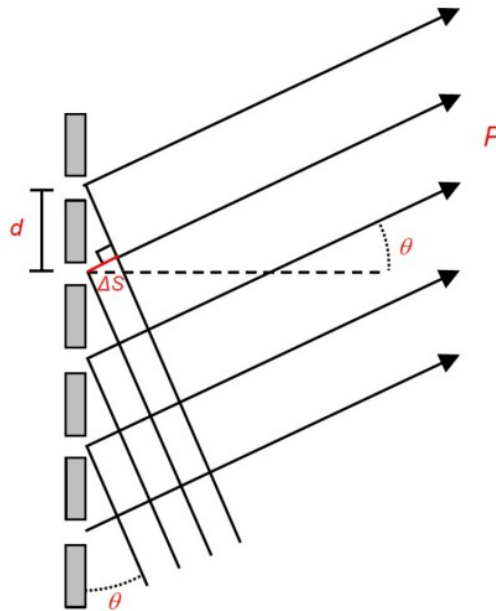


Fig. 1: A grating with the distance d between the slits, the deviation angle θ of the light and the path width ΔS .^[1]

The deviation angle of the constructive interference can be calculated by using Equation 1.

$$\sin \theta_k = \frac{k \cdot \lambda}{d} \quad (1)$$

Where k is the order of diffraction, λ is the wavelength and d is the distance between the slits.^[1]

1.3 The spectrometer

Figure 2 shows the setup of the DIY spectrometer used in the experiment.

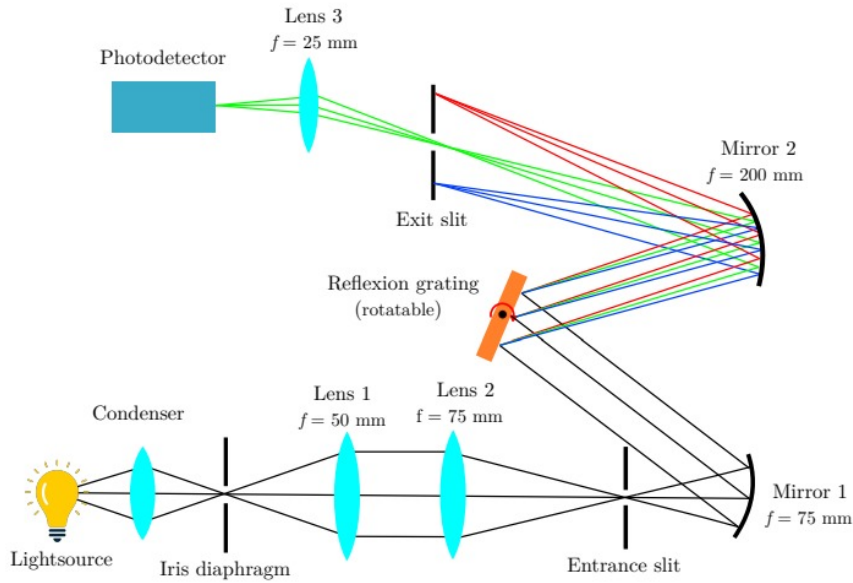


Fig. 2: Scheme of the different components, that make up the spectrometer used in the experiment.^[1]

The figure shows, that the light from a LED passes through a condenser and iris diaphragm, which collimate the light and regulate the intensity of the light used in the measurements. Afterwards it passes through two lenses, where the first lens refracts it back into parallel beams and the second focuses it again. The focused light then passes the entrance slit, as well as the sample, which is positioned directly behind the slit. After that it gets reflected by a mirror onto the rotating reflexion grating, where it gets reflected to another mirror. After that it passes through the exit slit and another lens to be focused onto the detector. The resolution of the spectrometer can be calculated using Equation 2.

$$R = \frac{\lambda}{\Delta\lambda} = k \cdot N \quad (2)$$

$\Delta\lambda$ is the smallest difference in wavelength that can be resolved at a wavelength λ and N is the total number of illuminated slits on the grating.

1.4 Grating Equation for a Rotatable Grating

The reflexion grating used in the experiment has to be rotated in order to measure the sample at the different wavelengths. This is achieved by using a stepper motor, where each step rotates the grating by 1.8° . Each step also consists of 16 micro steps z and have to factor in the gearbox of the motor which has a ratio of $\frac{1}{20}$.^[1] Using those factors, it is possible to calculate the degree of rotation α , as is shown in Equation 3.

$$\alpha = \frac{1.8 \cdot \pi}{16 \cdot 20 \cdot 180} \cdot z \quad (3)$$

To account for possible measurement errors the auxiliary values f and $\Delta\alpha$ are introduced into the equation, which leads to Equation 4.

$$\alpha = \frac{1.8 \cdot \pi}{16 \cdot 20 \cdot 180} \cdot z \cdot f + \Delta\alpha \quad (4)$$

Where f is a scaling factor and $\Delta\alpha$ accounts for the fact that the original angle of the grating is not known.^[1]

The rotation angle can now be used to calculate the outgoing wavelength of the light for every possible angle. This is shown in Equation 5.

$$k \cdot \lambda = \sin(\theta + \alpha) + \sin(\alpha) \quad (5)$$

2 Procedure

The DIY spectrometer was already built prior to the start of the experiment as shown in Figure 2 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 4 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

To evaluate the measuring setup, the spectrum of the used lightsource with and without the bandpass filter is plotted in Figure 3.

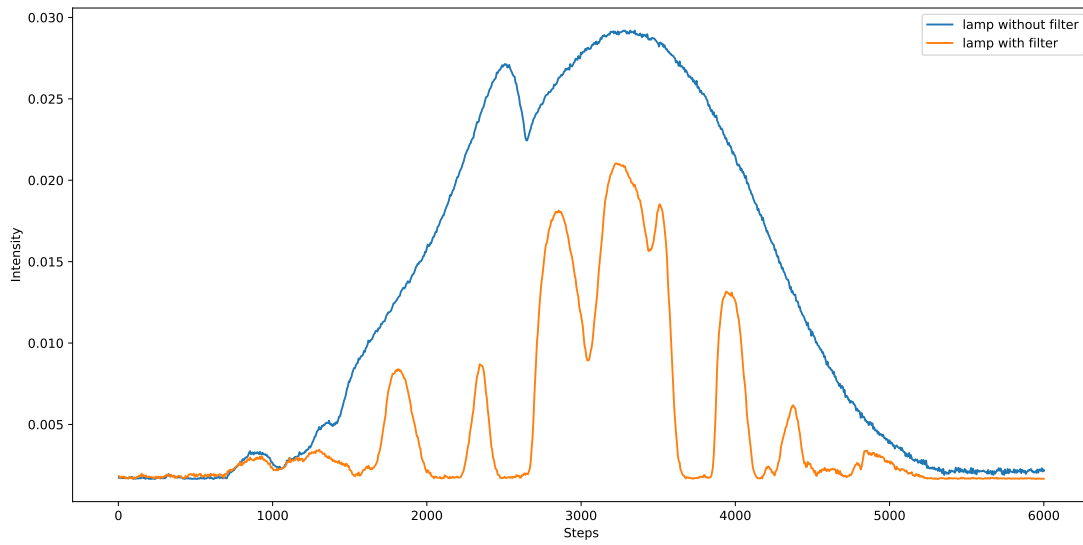


Fig. 3: The intensities of the measuring setup plotted over the number of steps with and without the bandpass filter.

Using Equation 4 the number of steps is converted into the wavelength λ . Then the transmission spectrum of the bandpass filter is calculated by dividing the intensity of the unfiltered light by the intensity of the filtered light of the lamp.

$$T_{\lambda} = \frac{I_{\text{lamp},\lambda}}{I_{\text{filter},\lambda}} \quad (6)$$

To adjust the paramers scale, f and $\Delta\alpha$, the transmission of said bandpassfilter was plotted over the wavelength together with the transmission spectrum for a theoretical, ideal bandpassfilter. The values were adjusted as in chapter 2 described. As a result of the adjustment the two spectra are plotted in Figure 4.

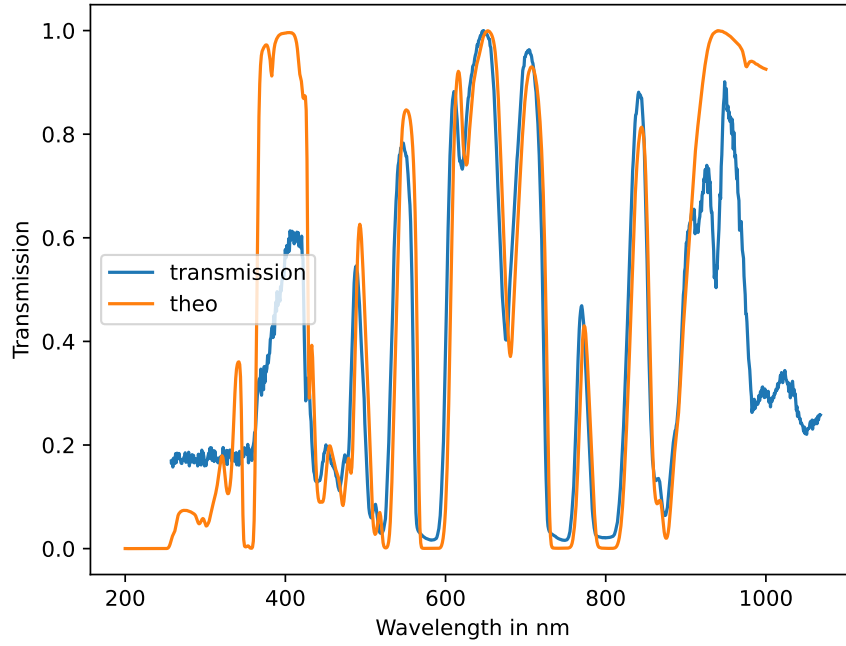


Fig. 4: The overlaid transmittance spectra of the measured and commercial bandpassfilter.

To interpret the taken spectra, the transmission spectra are also converted into absorption spectra using Equation 7, which is derived from the Beer-Lambert's law.

$$A_{\lambda} = -\log_{10}(T_{\lambda}) = \epsilon_{\lambda} \cdot c \cdot d \quad (7)$$

ϵ_{λ} is the extinction coefficient at the wavelength λ , c the concentration and d the thickness of the cuvette.

The absorption spectrum of the used bandpass filter is plotted in Figure 5. This conversion is essential to establish a linear relationship between the measured signal and the concentration of the sample, according to the Beer-Lambert's law. Furthermore, the filter's characteristic absorption bands allow for a precise verification of the spectrometer's wavelength accuracy across the relevant spectral range.

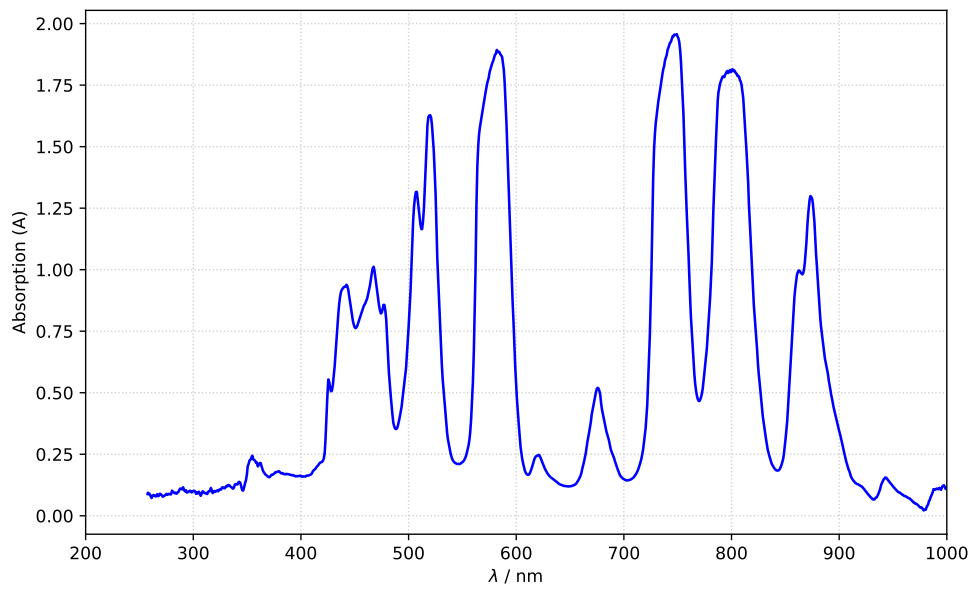


Fig. 5: The absorption spectrum of the bandpassfilter.

3.2 Potassium permanganate spectra

The transmittance of the potassium permanganate solution was determined by calculating the difference between the intensity of the sample and the intensity of a water-filled reference cuvette. This result is depicted in Figure 6. By applying this referencing procedure, the specific absorption of the solvent and the cuvette material is effectively eliminated from the spectra. Consequently, the resulting transmittance values represent the isolated optical properties of the permanganate ions, providing a reliable basis for the subsequent conversion into absorption units.

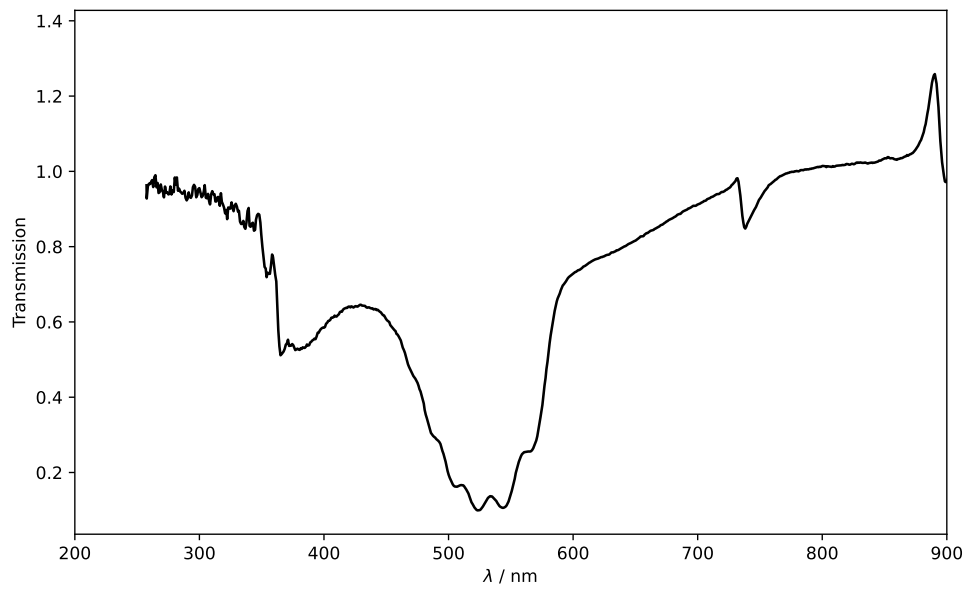


Fig. 6: Transmission spectrum of an aqueous potassium permanganate solution.

In the transmission spectrum, a clear minimum is observed at approximately 525 nm. It should be noted that the characteristic purple color of the permanganate solution does not correspond to the absorbed wavelength, but rather to its complementary color. This phenomenon occurs, because the absorption of the green component from the incident white light leaves the remaining spectral colors to be perceived by the observer. The corresponding absorption spectrum of permanganate is presented in Figure 7.

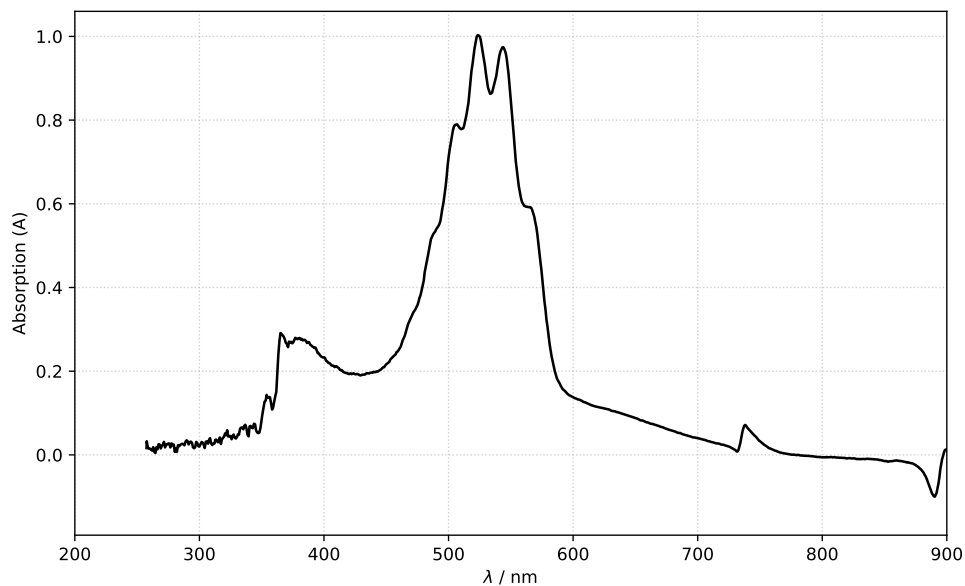


Fig. 7: Absorption spectrum of an aqueous potassium permanganate solution.

As observed in Figure 7 the maximum is around 525 nm, corresponding to the transmission minimum. This wavelength corresponds to green light, which implies a purple color of the sample, which is according to its real color. Said color is caused by the ligand to metal charge transfer (LMCT) from the oxygen ligands to the manganese cations. The observed absorption maxima and the characteristic structure of the MnO_4^- ions are in excellent agreement with literature values reported by Den Boef et al.^[2] Specifically, the peak at approximately 525 nm aligns with the established spectral data for aqueous potassium permanganate solutions, confirming the accuracy of the performed measurement.

3.3 Chlorophyll spectra

Since chlorophyll spectra of different concentrations were measured, these can now be compared. The absorptions of the different concentrations are plotted together in Figure 8, as this allows for the most effective analysis and comparison of the spectral features. By overlaying the absorption curves, the linear increase in peak intensity relative to the concentration becomes evident, consistent with the Beer-Lambert's law. This simultaneous representation also confirms that the positions of the characteristic absorption maxima remain constant, indicating that no significant chemical alterations or aggregation effects occurred within the studied concentration range. In Figure 8 the numbers in the legend of the graph corresponds to the drops added.

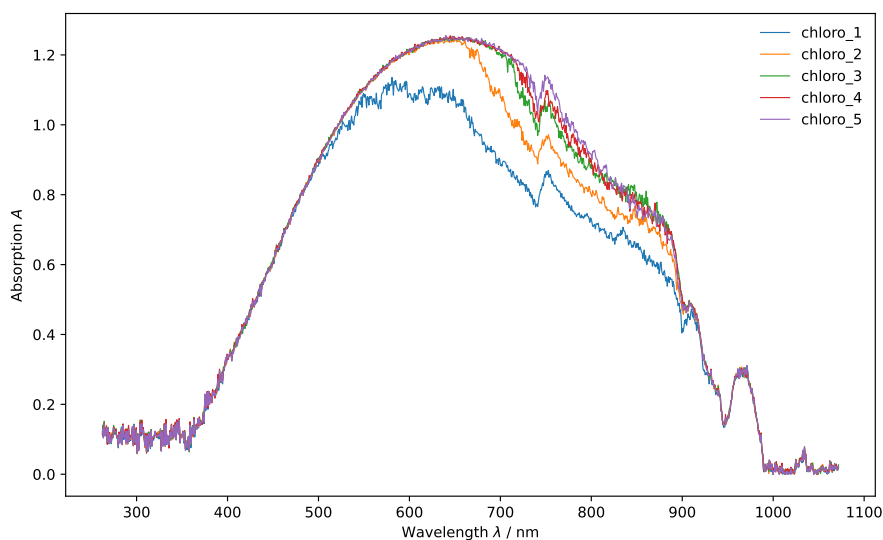


Fig. 8: The absorption spectra of the five measured chlorophyll solutions.

The absorption increases proportionally with the concentration of chlorophyll. However, in the spectra of samples 3, 4, and 5, no distinct differences are recognizable due to detector saturation.

Above a certain concentration, the number of molecules in the solution is too high, causing nearly all incident light to be absorbed. The lowest concentration provides the most accurate spectrum, exhibiting a maximum around 660 nm. This corresponds to the absorption of red light, which, along with the absorption in the blue region, results in the characteristic green color of the chlorophyll sample caused by $\pi \rightarrow \pi^*$ transitions.

However, the measured spectrum differs significantly from the ideal literature spectrum, reported by Lichtenthaler.^[3] While the literature suggests a prominent "absorption gap" between 500 nm and 600 nm, this feature is not observed in the experimental data. This discrepancy can be attributed to the limited resolution of the self-assembled spectrometer and potential stray light effects. Furthermore, the use of a broad-band light source and the simple setup may lead to an overlap of spectral orders, effectively "filling" the expected gap in the green spectral range. Additionally, the presence of various chlorophyll derivatives (a and b) in the sample could contribute to a broader absorption profile than seen in purified literature standards.

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 9.

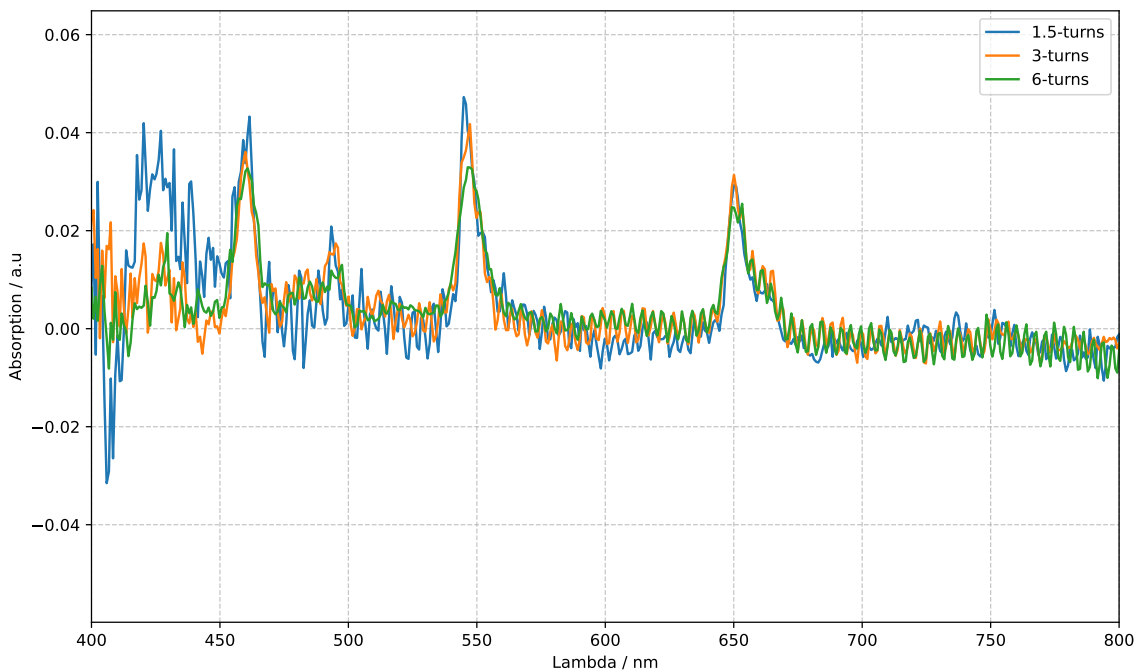


Fig. 9: Absorption spectrum of holmium oxide in nitric acid for different exit slit widths between 400 and 800 nm.

All three spectra show three distinct absorption peaks at around 460 nm, 545 nm and 650 nm, which can be assigned to $f \rightarrow f$ transitions between $4f$ orbitals of holmium. 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 10, Figure 11 and Figure 12.

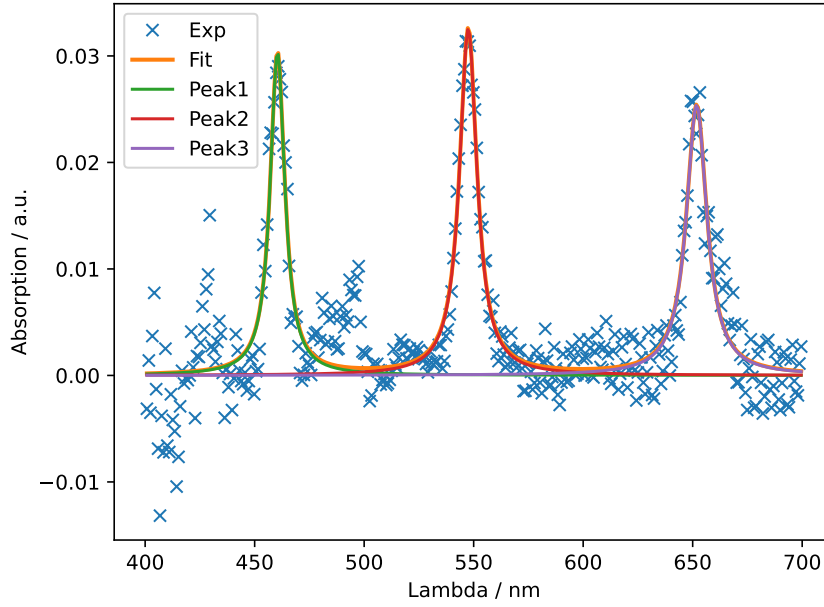


Fig. 10: Absorption signals of holmium oxide in nitric acid with a four-fold Lorentzian model fit for 6 turns between 400 and 700 nm.

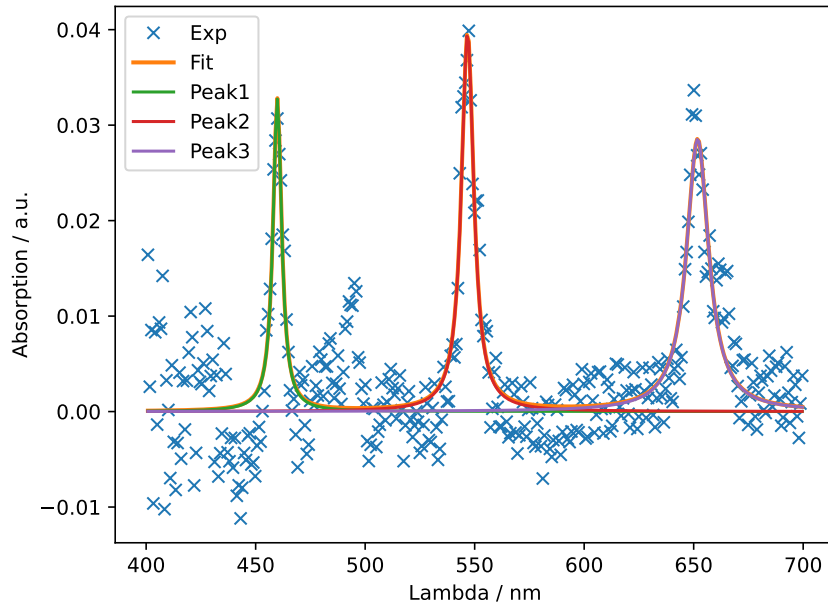


Fig. 11: Absorption signals of holmium oxide in nitric acid with a four-fold Lorentzian model fit for 3 turns between 400 and 700 nm.

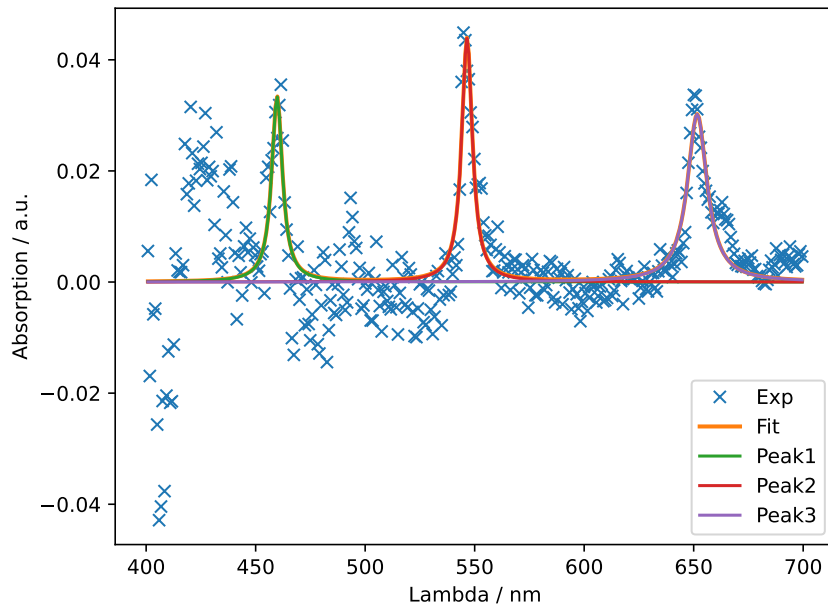


Fig. 12: Absorption signals of holmium oxide in nitric acid with a four-fold Lorentzian model fit for 1.5 turns between 400 and 700 nm.

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 10 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 11 and Figure 12 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:

$$\text{FWHM} = 2 \cdot \text{gam} \quad (8)$$

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.

pos/nm	6-turns		3-turns		1.5-turns	
	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

$$R = \frac{\lambda}{\Delta\lambda} = \frac{\text{pos}}{\text{FWHM}} \quad (9)$$

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

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

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 9, 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, a DIY spectrometer with a rotatable grating was used to measure the absorption spectra of different samples, including potassium permanganate, chlorophyll and holmium oxide in nitric acid. The spectrometer was calibrated by comparing the measured bandpass filter transmission to a theoretical model, allowing for a precise conversion of motor steps into wavelength units as shown in the resulting absorption profiles.

The potassium permanganate spectra reveal a characteristic absorption maximum at 525 nm, where the observed purple color originates from the absorption of the green spectral component via a ligand-to-metal charge transfer (LMCT) from the oxygen ligands to the manganese cations.

The concentration series of chlorophyll demonstrates a proportional increase in absorbance according to the Beer-Lambert's law, though detector saturation and stray light effects cause the experimental spectra to deviate from the ideal literature gap between 500 nm and 600 nm.

The absorption spectra of holmium oxide in nitric acid were measured at different exit slit widths and analyzed using a four-fold Lorentzian model fit. The results showed three absorption peaks of $f \rightarrow f$ transitions between $4f$ orbitals of holmium. With decreasing slit width, the resolution of the spectrometer increased from $R_{6\text{-turns}} = 26.6$ to $R_{3\text{-turns}} = R_{1.5\text{-turns}} = 38.3$, as indicated by the decreasing FWHM of the absorption peaks at 460.5 nm and 547.5 nm and the decreasing amplitude of the peak at 547.5 nm. However, the peak amplitudes of the other two absorption peaks and the FWHM of the peak at 651.8 nm did not show a clear trend with changing slit width, which could be attributed to manual adjustments of the slit widths leading to slight misalignments of the spectrometer and thus affecting the measured intensities. Overall, the experiment demonstrated the capabilities of the DIY spectrometer and showed the characteristic wavelengths of different electronic transitions in potassium permanganate, chlorophyll and holmium oxide.

5 References

- [1] H. Dilger, *2025-pc2-script-en*, **2025**.
- [2] G. Den Boef, H. J. van der Beek, T. Braaf, *Recueil des Travaux Chimiques des Pays-Bas* **1958**, 77, 1064–1070.
- [3] H. K. Lichtenthaler in *Methods in Enzymology*, Vol. 148, Elsevier, **1987**, pp. 350–382.