Spectroscopy

Physics Laboratory 1

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Abstract In this experiment we studied optical spectroscopy using a Czerny-Turner spectrometer equipped with a CCD camera. The spectrometer was first calibrated with the well-known emission spectrum of a helium discharge lamp in two steps: the dependence of the central wavelength on the dial position and the mapping between dial position and pixel coordinate on the CCD. A linear fit to the helium lines yielded a slope of $m = (0.783 \pm 0.002)$ nm per dial unit and showed that the spectrum shifts by about 25 pixels per dial unit across the CCD. Using this calibration, we determine the wavelengths of the visible Balmer lines of hydrogen. For the Hα and Hβ lines we obtained $\lambda_\alpha = (655.52 \pm 2.89)\,\text{nm}$ and $\lambda_\beta = (490.36 \pm 2.63)\,\text{nm}$, in agreement with the literature values within $1\,\%$. From these wavelengths we extracted the Rydberg frequency, $R_H = (3.28 \pm 0.02) \times 10^{15}\,\text{Hz}$, and deduced the Balmer series limit $\lambda_{\text{lim}} = (365.97 \pm 2.54)\,\text{nm}$ as well as the ionisation energy of hydrogen, $E_I = (13.55 \pm 0.09)\,\text{eV}$. All results were consistent with the accepted values to better than $1\,\%$, demonstrating that precise atomic constants can be obtained even with a relatively simple student-lab spectrometer.

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Introduction

Scope of this experiment In this experiment we study optical spectroscopy using a Czerny-Turner spectrometer as described in the student manual [2] and in Ref. [1]. The main goals are to become familiar with the working principle of a grating spectrometer with a CCD camera, to calibrate the relation between wavelength, dial position and pixel position using the well-known emission spectrum of helium, and to use this calibration to measure the Balmer series of hydrogen. From the measured wavelengths of the Balmer lines we finally determine the Rydberg frequency and the ionisation energy of the hydrogen atom and compare our results with literature values.

Spectroscopy and discrete spectra Spectroscopy is a fundamental tool to investigate the interaction between light and matter. The observation that atoms and molecules emit and absorb light only at discrete wavelengths was historically crucial for the development of quantum mechanics. In particular, the Balmer series of hydrogen (the visible part of the hydrogen emission spectrum corresponding to electronic transitions to the second energy level) provides direct evidence for quantised energy levels in atoms. Measuring these spectral lines and relating them to the Rydberg formula allows one to extract the Rydberg constant and thus the binding energy of the electron in the ground state of hydrogen.

Helium spectrum as a calibration source Helium has a rich but well-tabulated emission spectrum with several isolated and bright lines in the visible range. This makes a helium discharge lamp an ideal calibration source for the spectrometer: the known wavelengths can be assigned to the spectral lines recorded by the CCD, which allows us to determine the linear dependence of the central wavelength on the dial position as well as the mapping between dial position and pixel coordinate on the camera chip. A schematic representation of the helium spectrum in first diffraction order is shown in Fig. 1 and was used as a reference when searching for the corresponding lines in our measurements.

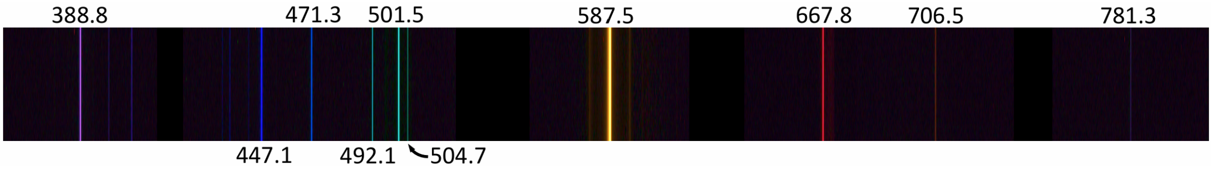


Figure 1: Known He-spectrum of first order. [2]

Experiment

In this experiment a Czerny-Turner spectrometer, with a spectral resolution about 0.1 nm [1], including a CCD camera, and the ThorCam software were used. An overview of the Czerny-Turner spectrometer can be seen in Fig. 2. To generate the helium and hydrogen spectra, He and H lamps were used. In this setup, the grating can act either as a simple mirror, producing the so-called *zero diffraction order*, or it can disperse the incoming light according to its wavelength, which produces the *first diffraction order*.

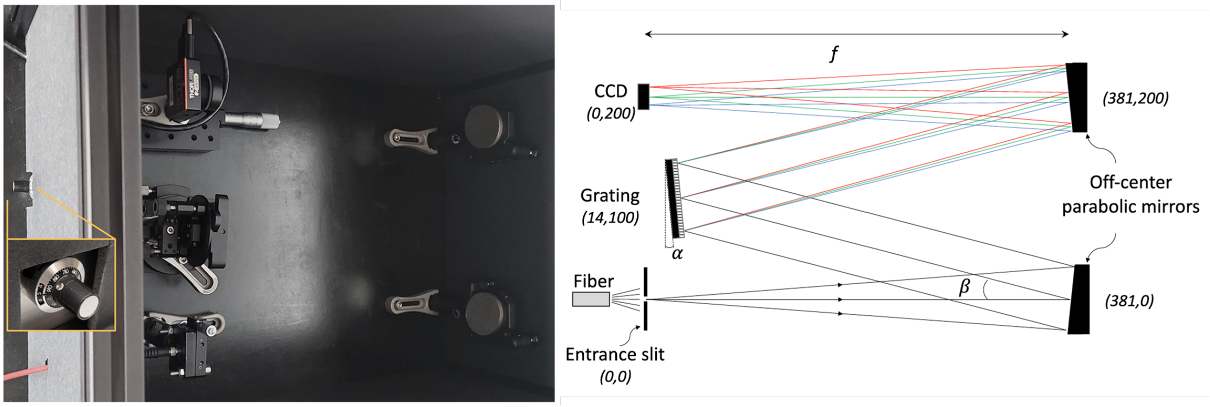


Figure 2: On the left a photograph and on the right a schematic of the spectrometer. [2]

For the calibration of the spectrometer, the He lamp was connected to the spectrometer, using a glass fiber. The grating was oriented so that it was parallel to the parabolic mirrors to find the zero diffraction order spectral line. After orienting the peak of the spectral line at the central pixel, the dial position k was determined and a .bmp file was recorded. By turning the grating-wheel clockwise, the first diffraction order spectral lines were found. The measurements were repeated for all visible spectral lines red, orange, green, blue and violet, as seen in Fig. 1. Afterwards, the He lamp was exchanged with the H lamp. For the next measurement, the lamp was turned off for 30 seconds, every 30 seconds, to prolong the service life of the lamp. By turning the grating anticlockwise, the spectral lines of the Balmer series were found and the measurements were performed as in the previous steps. During the first calibration step, each visible helium spectral line was positioned precisely at the central pixel of the CCD. This allowed us to determine the relation between the dial position k and the corresponding central wavelength. For the second calibration step, a bright helium line was moved stepwise across the CCD by adjusting the grating angle. For each position, both the pixel position and the dial position k were recorded in order to establish the linear relation between k and the pixel coordinate. All recorded data from both calibration steps were subsequently analysed using Python, where linear regressions were used to determine the calibration parameters needed for the wavelength reconstruction.

Results

The gathered data from the calibration process can be found in Tab.1 and Tab.2.

Table 1: Overview of all measured results from the calibration process, regarding the correspondence between the central wavelength λ_c and the dial position k.

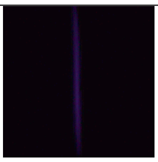
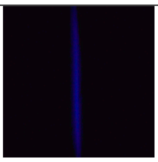
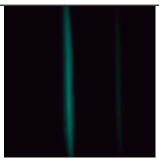
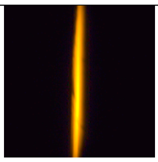
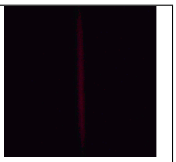
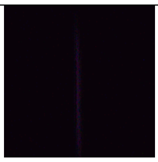
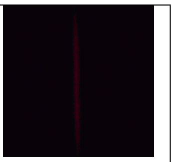
image					
λ_c / **nm**	388.8	447.1	501.5	587.5	667.8
$\boldsymbol{k}$	841 ± 1	914 ± 1	984 ± 1	1094 ± 1	1197 ± 1

Table 2: Overview of all measured results from the calibration process, regarding the correspondence between the pixels and the dial position k.

pixel	20	120	420	520	620	820	920	1020	1320	1420
$\boldsymbol{k}$	1120 ± 1	1116 ± 1	1108 ± 1	1100 ± 1	1099 ± 1	1089 ± 1	1086 ± 1	1080 ± 1	1070 ± 1	1066 ± 1

The data collected from the measurement of the Balmer series of hydrogen can be found in Tab. 3.

Table 3: Overview of all measured results from the measurement of the Balmer series of hydrogen

image				
$\boldsymbol{k}$	350 ± 1	–	970 ± 1	1181 ± 1

For one of the recorded hydrogen spectra no reliable dial position could be assigned. This spectrum is therefore indicated as "-" in Tab. 3 and was not used for the subsequent quantitative analysis.

Data Analysis

Calibration

For the helium lamp we first determined how the central wavelength displayed by the spectrometer depends on the dial position. Assuming a linear relation

$$\lambda_c(k) = mk + b,$$

a linear regression of the five measured helium lines (Tab 1) yields

$$m = (0.783 \pm 0.002)\,\text{nm per dial unit},$$
$$b = (-268.907 \pm 1.813)\,\text{nm}.$$

Thus, turning the dial by one unit shifts the central wavelength by approximately 0.78 nm. The effective zero point of the dial, defined by the condition $\lambda_c(k_0) = 0$, is

$$k_0 = -\frac{b}{m} = 343.540.$$

In a second calibration step we determined how the position of a bright helium line on the CCD shifts when the dial is rotated. Fitting

$$p(k) = m_2 k + b_2$$

to the corresponding data gives

$$m_2 = B = (-25.373 \pm 0.673)\,\text{pixels per dial unit},$$
$$b_2 = (2.846 \pm 0.074) \times 10^4\,\text{pixels}.$$

This means that the spectrum moves by about 25 pixels across the CCD per dial unit. The two calibration steps can be combined into the general wavelength relation

$$\lambda(p, k) = m_\lambda\,(k - k_0) + \frac{p - p_{\text{central}}}{B_\lambda},$$

where $m_\lambda = m$ and $B_\lambda = m_2$ are taken from the regression parameters. Here, p_{central} denotes the pixel position corresponding to the optical axis of the spectrometer, i.e. the pixel where a centred spectral line appears.
In the hydrogen measurements the spectral lines were centred on the CCD ($p \approx p_{\text{central}}$). Therefore the wavelength can be obtained directly from the simplified expression

$$\lambda(k) = mk + b.$$

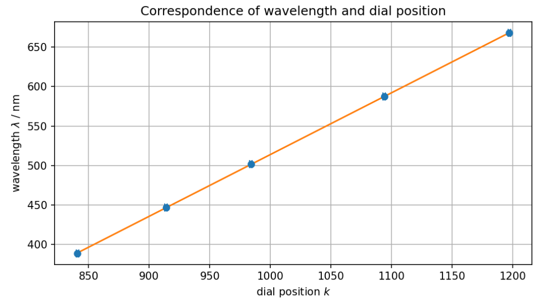


Figure 3: Linear calibration of wavelength vs. dial position.

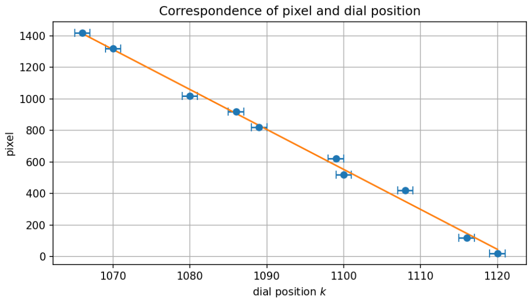


Figure 4: Linear calibration of pixel position vs. dial position.

For the hydrogen lamp we recorded several spectra of the Balmer series. From the images (see Tab. 3) we could reliably extract two dial positions: $k = 1181$ for the bright red line and $k = 970$ for the blue-green line. These lines were identified as the Hα ($n = 3$) and Hβ ($n = 4$) transitions,respectively.

Balmer series

For the hydrogen lamp we recorded several spectra of the Balmer series. From the images (see Tab. 3) we could reliably extract two dial positions: $k = 1181$ for the bright red line and $k = 970$ for the blue-green line. These lines were identified as the Hα ($n = 3$) and Hβ ($n = 4$) transitions, respectively.

Using the simplified calibration relation $\lambda(k) = mk + b$ (valid for centred spectral lines), we obtain the wavelengths

$$\lambda_\alpha = (655.52 \pm 2.89)\,\mathrm{nm} \qquad (\mathrm{H}\alpha,\ n = 3),$$
$$\lambda_\beta = (490.36 \pm 2.63)\,\mathrm{nm} \qquad (\mathrm{H}\beta,\ n = 4).$$

The corresponding literature values are $\lambda_\alpha^{\mathrm{lit}} = 656.3\,\mathrm{nm}$ and $\lambda_\beta^{\mathrm{lit}} = 486.1\,\mathrm{nm}$. Our measurements deviate by only 0.12 % (Hα) and 0.88 % (Hβ), which is well within the expected accuracy of the experimental setup.

From the measured wavelengths we compute the frequencies $\nu_i = c/\lambda_i$ and use the Rydberg formula

$$\nu_i = R_H \left(\frac{1}{4} - \frac{1}{n_i^2} \right)$$

to determine the Rydberg frequency from each line. This yields

$$R_{H,\alpha} = (3.29 \pm 0.02) \times 10^{15}\,\mathrm{Hz},$$
$$R_{H,\beta} = (3.26 \pm 0.02) \times 10^{15}\,\mathrm{Hz}.$$

Taking the mean of the two values and using their spread as an estimate of the uncertainty gives

$$R_H = (3.28 \pm 0.02) \times 10^{15}\,\mathrm{Hz}.$$

This agrees with the literature value $R_H^{\mathrm{lit}} = 3.29 \times 10^{15}\,\mathrm{Hz}$ within approximately 0.4 %. The series limit of the Balmer series follows from $\nu_{\mathrm{lim}} = R_H/4$, leading to

$$\lambda_{\mathrm{lim}} = \frac{c}{\nu_{\mathrm{lim}}} = (365.97 \pm 2.54)\,\mathrm{nm}.$$

This wavelength lies in the near ultraviolet, where the sensitivity of the lamp, optics, and CCD camera drops significantly; therefore the series limit cannot be observed directly in our spectra.

Finally, the ionisation energy of hydrogen is obtained from

$$E_I = hR_H = (13.55 \pm 0.09)\,\mathrm{eV}.$$

This result agrees very well with the literature value $E_I^{\mathrm{lit}} = 13.60\,\mathrm{eV}$ (relative deviation $\approx 0.4\,\%$).

Discussion

The two-step calibration of the spectrometer yielded consistent and reliable results. The first calibration, relating wavelength to dial position, showed an excellent linear behaviour over the entire scanned range, with a slope of $m = (0.783 \pm 0.002)\,\mathrm{nm\,per\,dial\,unit}$. The second calibration demonstrated that the spectrum shifts by approximately 25 pixels per dial unit on the CCD. Both regressions show small uncertainties, indicating that the mechanical control of the grating is sufficiently stable for the purpose of this experiment.

The measured hydrogen wavelengths agree very well with the literature values: the deviations are only $0.12\,\%$ for Hα and $0.88\,\%$ for Hβ. Such small deviations are remarkable given the relatively coarse dial scale and the limited number of calibration points. The residual discrepancies can be explained by (i) the mechanical play in the grating rotation mechanism, (ii) the finite linewidths of the lamp spectra, (iii) uncertainties in determining the exact dial position, and (iv) the assumption that the hydrogen lines are perfectly centred on the CCD, which neglects any possible pixel offset. In addition, one of the recorded Balmer spectra could not be assigned a reliable dial position and was therefore excluded from the analysis, which further reduces the number of available data points and slightly increases the statistical uncertainty of our results.

The extracted Rydberg frequency, $R_H = (3.28 \pm 0.02) \times 10^{15}\,\mathrm{Hz}$, agrees with the accepted value to within $0.4\,\%$. Using this value, the Balmer series limit was determined to be $\lambda_{\mathrm{lim}} = (365.97 \pm 2.54)\,\mathrm{nm}$, which lies in the near ultraviolet. The fact that no Balmer lines close to the series limit were observed is consistent with the decreasing sensitivity of the CCD and optics in this wavelength region.

Finally, the ionisation energy derived from the measured Rydberg frequency, $E_I = (13.55 \pm 0.09)\,\mathrm{eV}$, agrees very well with the literature value of $13.60\,\mathrm{eV}$. The relative deviation is again below $0.5\,\%$, confirming that the calibration procedure and evaluation method are robust despite the limited experimental resolution. Overall, the experiment demonstrates that even with a simple Czerny-Turner spectrometer and modest measurement precision, key atomic constants such as the Rydberg frequency and the ionisation energy of hydrogen can be extracted with surprisingly high accuracy.

Conclusion

In this experiment we calibrated a Czerny-Turner spectrometer using helium emission lines and applied this calibration to determine the wavelengths of the visible Balmer series of hydrogen. The two-step calibration showed a clear linear dependence of both the central wavelength and the CCD pixel position on the dial setting, enabling a consistent description of the spectrometer response.

Using the calibrated relation $\lambda(k) = mk + b$, the wavelengths of the Hα and Hβ lines were determined with deviations below $1\,\%$ from their respective literature values. From these wavelengths we extracted the Rydberg frequency, $R_H = (3.28 \pm 0.02) \times 10^{15}$ Hz, and obtained an ionisation energy of $E_I = (13.55 \pm 0.09)$ eV, both in excellent agreement with the accepted values.

Overall, the results demonstrate that even with a relatively simple spectrometer setup, fundamental atomic constants can be measured with high accuracy. The experiment thus successfully illustrates the power of optical spectroscopy in probing the structure of the hydrogen atom.

Appendix

AI Usage Declaration

This report was prepared with assistance from ChatGPT (OpenAI) for language polishing, formatting suggestions, and for helping to develop, debug, and correct the syntax of the Python code. The AI was not used to generate raw data, to select results, or to determine the final conclusions. All scientific content (methods, calculations, results, and interpretation) was critically reviewed and validated by the authors. The authors take full responsibility for the accuracy of the analysis and for any remaining errors. No confidential or personal data were provided to the AI system during the preparation of this report.

References

[1] Andreas Eggenberger, Tomasz Smolenski, and Martin Kroner. “A simple state-of-the-art spectrometer for student labs: Cost-efficient, instructive, and widely applicable”. In: *American Journal of Physics* 92.2 (Feb. 2024), pp. 146–153. ISSN: 0002-9505. DOI: `10.1119/5.0164044`. eprint: `https://pubs.aip.org/aapt/ajp/article-pdf/92/2/146/20107891/146_1_5.0164044.pdf`. URL: `https://doi.org/10.1119/5.0164044`.

[2] *Physikpraktikum für 3. Semester — Experiment 24 Grundlagen zur Spektroskopie*. Lab manual. Restricted access (ETH login required). ETH Zürich, Departement Physik, Nov. 10, 2025. URL: `https://ap.phys.ethz.ch/Anleitungen/Bilingual/24_Manual_PHYS.pdf`.

Python Code

```python
import numpy as np
import matplotlib.pyplot as plt
from math import atan2, sqrt
from dataclasses import dataclass

# ---------- 0) Messdaten aus der Tabelle (nm, k) ----------
# He: bekannte Wellenlngen und dazugehrige Dial-Positionen
hew = np.array([388.8, 447.1, 501.5, 587.5, 667.8], dtype=float)
herad = np.array([841,   914,   984,   1094,  1197], dtype=float)

# He: Pixelposition einer hellen Linie vs. Dial-Position (Kalibration 2)
hepix   = np.array([20, 120, 420, 520, 620, 820, 920, 1020, 1320, 1420],
                   dtype=float)
hepirad = np.array([1120, 1116, 1108, 1100, 1099,
                    1089, 1086, 1080, 1070, 1066],
                   dtype=float)

# ---------- 1) Lineare Regression fr die Kalibration ----------
# plot 1: lambda vs. k
(m, b), cov = np.polyfit(herad, hew, 1, cov=True)

# Standardfehler der Parameter
m_err = np.sqrt(cov[0, 0])
b_err = np.sqrt(cov[1, 1])

print(f"Kalibration 1: lambda(k) = m*k + b")
print(f"  m  = {m:.6f} pm {m_err:.6f} nm pro Dial-Einheit")
print(f"  b  = {b:.6f} pm {b_err:.6f} nm")

# plot 2: pixel vs. k
(m2, b2), cov2 = np.polyfit(hepirad, hepix, 1, cov=True)
m2_err = np.sqrt(cov2[0, 0])
b2_err = np.sqrt(cov2[1, 1])

print(f"\nKalibration 2: pixel(k) = m2*k + b2")
print(f"  m2 = B = {m2:.6f} pm {m2_err:.6f} pixel pro Dial-Einheit")
print(f"  b2 = {b2:.6f} pm {b2_err:.6f} pixel")

# ---------- 2) Plots (mit Fehlerbalken) ----------
# Plot 1: lambda vs. k
```

```python
plt.figure(figsize=(7.2, 4.2))
plt.errorbar(herad, hew, xerr=1, fmt='o', capsize=4, label="Messpunkte")

x_reg = np.linspace(min(herad), max(herad), 200)
y_reg = m * x_reg + b
plt.plot(x_reg, y_reg, '-', label=f"Regression: y = {m:.3f}x + {b:.1f}")

plt.xlabel("dial position $k$")
plt.ylabel(r"wavelength $\lambda$ / nm")
plt.title("Correspondence of wavelength and dial position")
plt.grid(True)
plt.tight_layout()
plt.legend()
plt.savefig("cor1.png", dpi=150)
plt.close()

# Plot 2: pixel vs. k
plt.figure(figsize=(7.2, 4.2))
plt.errorbar(hepirad, hepix, xerr=1, fmt='o', capsize=4, label="Messpunkte")

x_reg2 = np.linspace(min(hepirad), max(hepirad), 200)
y_reg2 = m2 * x_reg2 + b2
plt.plot(x_reg2, y_reg2, '-', label=f"Regression: y = {m2:.3f}x + {b2:.1f}")

plt.xlabel("dial position $k$")
plt.ylabel("pixel")
plt.title("Correspondence of pixel and dial position")
plt.grid(True)
plt.tight_layout()
plt.legend()
plt.savefig("cor2.png", dpi=150)
plt.close()

# ---------- 3) Kalibrationsparameter ableiten ----------
# effektiver Nullpunkt des Dials
k0 = -b / m
print(f"\nEffektiver Nullpunkt des Dials: k0 = {k0:.2f}")

# mittlerer Pixel der Kamera (angenommen), wurde bei uns fr H zentriert
p_central = 720.0

```

```python
def lambda_from_k_p(k, p, m, b, k0, B, p_central):
    """
    Wellenlnge in nm als Funktion von Dialposition k und Pixel p.
    Allgemeine Formel aus der doppelten Kalibration.
    """
    # zentrale Wellenlnge bei diesem k
    lam_center = m * (k - k0)
    # zustzliche Verschiebung durch Pixelposition
    delta_lam_pixel = (p - p_central) / B
    return lam_center + delta_lam_pixel + m * k0 + b  # identisch zu m*k + b + (p-pc)/B

# Fr unsere H-Messungen haben wir die Linie jeweils auf den Zentralpixel gesetzt,
# daher setzen wir im Folgenden p = p_central und benutzen lambda(k) = m*k + b.
def lambda_from_k(k, m, b):
    """vereinfachte Kalibration fr zentrierte Linien"""
    return m * k + b


# ---------- 4) Balmerdaten (nur Dial-Positionen) ----------
# Aus Tabelle 3: k-Werte der sichtbaren H-Linien.
# Wir verwenden nur 970 (H_beta) und 1181 (H_alpha); 350 liegt weit ausserhalb der
# Kalibration und ergibt eine unphysikalische Wellenlnge.
k_H = np.array([1181.0, 970.0])      # Dialpositionen
names_H = np.array(["H_alpha", "H_beta"])
n_H = np.array([3, 4], dtype=float)  # Quantenzahlen n

# angenommene Unsicherheit in k
sigma_k = 1.0

# Wellenlngen und Unsicherheiten bestimmen
lambda_H = lambda_from_k(k_H, m, b)  # in nm

# Fehlerfortpflanzung fr lambda = m*k + b
sigma_lambda_H = np.sqrt((k_H * m_err)**2 + b_err**2 + (m * sigma_k)**2)

print("\n--- Balmer-Linien (aus Dial-Positionen) ---")
for name, k_val, lam, lam_err in zip(names_H, k_H, lambda_H, sigma_lambda_H):
    print(f"{name:8s}: k = {k_val:.0f} pm {sigma_k:.0f}, "
```

```python
          f"lambda = {lam:.2f} pm {lam_err:.2f} nm")

# ---------- 5) Rydberg-Konstante aus den Balmerlinien ----------
c = 2.99792458e8       # Lichtgeschwindigkeit (m/s)
h_ev = 4.135667696e-15 # Planckkonstante in eV s

# Frequenzen und Fehler
lambda_H_m = lambda_H * 1e-9
sigma_lambda_H_m = sigma_lambda_H * 1e-9

nu_H = c / lambda_H_m
sigma_nu_H = c * sigma_lambda_H_m / (lambda_H_m**2)

# Faktor (1/4 - 1/n^2) fr Balmer-Serie
f_H = 0.25 - 1.0 / (n_H**2)

R_vals = nu_H / f_H
sigma_R_vals = sigma_nu_H / f_H

R_mean = np.mean(R_vals)
R_std  = np.std(R_vals, ddof=1)     # Streuung zwischen den Linien

print("\n--- Rydberg-Frequenz ---")
for name, lam, R, sR in zip(names_H, lambda_H, R_vals, sigma_R_vals):
    print(f"{name:8s}: lambda = {lam:.2f} nm  ->  "
          f"R_H = ({R:.3e} pm {sR:.3e}) Hz")

print(f"\nGemittelter Wert:")
print(f"R_H = ({R_mean:.3e} pm {R_std:.3e}) Hz")

# ---------- 6) Reihengrenze und Ionisationsenergie ----------
nu_lim = R_mean / 4.0
nu_lim_err = R_std / 4.0

lambda_lim_m = c / nu_lim
lambda_lim_err_m = c * nu_lim_err / (nu_lim**2)

lambda_lim_nm = lambda_lim_m * 1e9
lambda_lim_err_nm = lambda_lim_err_m * 1e9

E_I = h_ev * R_mean
```

```python
E_I_err = h_ev * R_std

print("\n--- Balmer-Reihengrenze ---")
print(f"lambda_limit = ({lambda_lim_nm:.2f} pm {lambda_lim_err_nm:.2f}) nm")

print("\n--- Ionisationsenergie von Wasserstoff ---")
print(f"E_I = ({E_I:.3f} pm {E_I_err:.3f}) eV")
```