# Fine structure, one-electron and two-electron spectra

(Item No.: P2510600)

## **Curricular Relevance**



#### Keywords:

Diffraction spectrometer, spin, angular moment, spin-orbital angular moment interaction, multiplicity, energy level, excitation energy, selection rules, doublets, parahelium, orthohelium, exchange energy, singlet series, triplet series, forbidden transitions

## Overview

## **Short description**

#### Principle

A level energy calculation with the Schrödinger equation predicts a level energy degeneracy for all electron states inside an atom belonging to the same shell having main quantum number n, and same orbit with orbital angular momentum quantum number l. This ignores the effects of magnetic spin-orbit interactions and relativistic effects which shift the energy of levels in atoms causing the fine structure thus lifting this level degeneracy.

By observation of the wavelength of light from transitions between atomic levels this energy shift can be determined. To determine the wavelength, a spectrometer-goniometer is used. It consists of a dispersive element, which deflects light through an angle depending on the wavelength, and a goniometer to determine the angle of deflection of the light beam. As dispersive elements a grating and a flint prism are used.





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### **Materials**

Position No.	Material	Order No.	Quantity
1	PHYWE Spectrometer-Goniometer with vernier SG1 PRO	35635-03	1
2	Diffraction grating, 600 lines/mm	08546-00	1
3	Prism, 60 degrees, height = 36.4 mm, flint	08237-00	1
4	Spectral lamp He, pico 9 base	08120-03	1
5	Spectral lamp Na, pico 9 base	08120-07	1
6	Spectral lamp Hg 100, pico 9 base	08120-14	1
7	Spectral lamp Cd, pico 9 base	08120-01	1
8	Spectral lamp Zn, pico 9 base	08120-11	1
9	Magnifier with handle, 4x, d=50 mm	87004-03	1
10	Power supply for spectral lamps	13662-97	1
11	Lamp holder pico 9 for spectral lamps	08119-00	1
12	Tripod base PHYWE	02002-55	1

#### Tasks

One-electron spectra:

- 1. Set up the spectrometer as a grating spectrometer and determine the grating constant using literature values for the visible spectral lines from a helium lamp.
- 2. With the determined grating constant measure the wavelengths of the observable sodium spectral lines belonging to the split  $3^2 P$  level, determine the energy difference between the  $3^2 P_{1/2}$  and  $3^2 P_{3/2}$  level

Two-electron spectra:

- 1. Set up the spectrometer as a prism spectrometer and determine the dispersion function of the flint prism using literature values for the visible spectral lines from a helium lamp.
- 2. Determine the wavelengths of spectral lines of zinc, cadmium, and mercury. Observe the increase of triplet-singulet transitions with increasing atomic number.

#### **General remarks:**

Darken the room in order to see fainter lines of the spectral lamps and to percieve lines on the red or blue end of the visible spectrum. It is advisable to have a separate lamp for reading the angle scales that can be easily switched off when observing the spectral lines through the ocular telescope.

Align the grating or the prism on the spectrometer table according to the operating instructions of the spectrometer-goniometer 35635-03. Align the slit vertical and the reticule parallel to the slit image. For the grating be sure to check that the vertical position of the slit image is equal on both sides of the undeflected beam as else deviations from verticality of the slit produce angle errors. Also for the prism the slit image vertical position should be constant throughout the whole spectrum. Be aware that because of the dispersion of the lenses the slit image has to be focused for every spectral line.

To avoid lateral play of the focussing mechanics after exerting lateral force to slit or eyepiece, turning the focussing knob back and forth brings the movable part to its reproducable neutral position.



## Fine structure of single electron spectra - grating spectrometer

### Set up and procedure

#### *a)* Determination of the grating constant

Insert the helium (He 10) lamp into the lamp holder, connect this to the power supply and turn on.

Note the reticule angle position on the outer scale where the undiffracted light ("zero" order) appears, use this as reference for the angle you measure to both sides of the zero order. Identify the spectral lines of Table 3 and measure first order deflection angles to both sides, - data taken from U.S. National Institute of Standards and Technology (NIST), NIST Atomic Spectroscopy Database (ASD), refer to

#### http://physics.nist.gov/PhysRefData/ASD/lines\_form.html

Be aware that relative line intensities vary with the specific conditions in the glow discharge of the lamp, that is pressure, temperature, and position inside the lamp. For ease of line identification a spread sheet calculating the expected angle from the wavelength assuming a grating constant of 600 l/mm can be helpful.

b) Determination of sodium spectral line wavelengths

Turn off the power supply and let cool down the lamp, then exchange the He lamp with the sodium (Na 10) lamp. Use paper or cloth to touch the lamps.

Measure the angle of the first order diffracted light for the visible double lines for both sides, and if possible, also for the second order of diffraction. Depending on the quality of the specific grating in use, second order light may not be equally intense on both sides, if the transmission function of the grating is not precisely a rectangular one.

#### Data and results

For the angle  $\alpha$  of n-th order of diffraction for the light of wavelength  $\lambda$  on a grating with line spacing d or grating constant 1/d it is  $n \lambda = d \sin \alpha$ , which can be used to calculate 1/d for given  $\lambda$  and n.

With a result for 1/d on the other hand unknown wavelengths can be determined.

For sodium the level splitting of the  $3^2 P$  level is to be determined by the wavelength differences in each doublet.





purple	396.47	1s4p, $^{1}P_{1}$	1s2s, ${}^{\scriptscriptstyle 1}S_0$	7.0 x 10 <sup>6</sup>	23.7421	20.6158
blue	402.62	1s5d, ${}^3_{ m o}D$	1s2p, ${}^3P$	1.2 x 10 <sup>7</sup>	24.0427	20.9641
blue	412.08	1s5s, ${}^3S_1$	1s2p, ${}^3P$	2.5 x 10 <sup>6</sup>	23.9720	20.9641
blue	414.49	1s6d, ${}^1D_2$	1s2p, $^1P_1$	4.9 x 10 <sup>6</sup>	24.2092	21.2180
blue	438.92	1s5d, $^1D_2$	1s2p, $^1P_1$	9.0 x 10 <sup>6</sup>	24.0428	21.2180
blue	447.15	1s4d, ${}^3_{ m o}D$	1s2p, ${}^3P$	2.5 x 10 <sup>7</sup>	23.7361	20.9641
cyan	471.31	1s4s, ${}^3S_1$	1s2p, ${}^3P$	9.5 x 10 <sup>6</sup>	23.5940	20.9641
green	492.19	1s4d, ${}^{1}D_{2}$	1s2p, $^1P_1$	1.2 x 10 <sup>7</sup>	23.7363	21.2180
green	501.71	1s3p, $^1P_1$	1s2s, ${}^1S_0$	1.3 x 10 <sup>7</sup>	23.0870	20.6158
green	504.91	1s4s, $^1S_0$	1s2p, $^1P_1$	6.8 x 10 <sup>6</sup>	23.6736	21.2180
yellow	587.73	1s3d, ${}^3D$	1s2p, $^{3}P$	7.1 x 10 <sup>7</sup>	23.0737	20.9641
red	668.00	1s3d, ${}^{1}D_{2}$	1s2p, $^1P_1$	6.4 x 10 <sup>7</sup>	23.0741	21.2180
red	706.72	1s3s, ${}^3S_1$	1s2p, ${}^3P$	2.8 x 10 <sup>7</sup>	22.7185	20.9641
red	728.34	1s3s, $^1S_0$	1s2p, $^1P_1$	$1.8 \times 10^{7}$	22.9203	21.2180

Table 1: Transitions that are observable with the prism - helium (He) – NIST data for level energies and wavelengthes  $\lambda$ 



Table 2: Transitions that are observable with the prism - sodium (Na) – NIST data for level energies and wavelengths  $\lambda$ 

Note that a 600 l/mm grating has a better spectral resolution than most prisms. But only a fraction of the light gets diffracted – the other part of the light is in zero order and some light gets absorbed and reflected. Also the diffracted fraction is distributed to two sides and several orders of diffraction. So some spectral lines that can be evaluated with the prism may not be visible with the grating.

Table 3 shows a measurement example for the helium spectrum. Note that here the deflection angle is assumed positive in both directions to get positive grating constants for the left and right side, so the 360° circle mark and the 353° zero order position have to be taken into account differently left and right.



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measured angle left		ngle left	right				calculated grating of	const.
8	18	15.30	337	39	15.35	438.92	601.2	603.1
8	37	15.62	337	20	15.67	447.15	602.0	603.9
9	27	16.45	336	27	16.55	471.31	600.8	604.4
10	14	17.23	335	41	17.32	492.19	601.9	604.8
10	34	17.57	335	21	17.65	501.71	601.6	604.3
10	40	17.67	335	15	17.75	504.91	601.1	603.8
13	41	20.68	332	14	20.77	587.73	601.0	603.3
16	44	23.73	329	15	23.75	668	602.5	602.9
							average:	602.7

Table 3: Measurement example for He, angle calculated with zero order position at  $$353.00^\circ$$ 

The NIST wavelengths are used to calculate the grating constant. With the grating constant of Table 3 the sodium lines evaluate as Table 4:

<b>measured</b> 1st order	l angl	e left	right			calculated	l wavelen	gth	
10	25	17.42	335	30	17.50	496.7	499.0	497.8	497.9
10	26	17.43	335	29	17.52	497.1	499.4	498.3	498.3
11	2	18.03	334	53	18.12	513.7	516.0	514.8	514.9
11	3	18.05	334	52	18.13	514.1	516.4	515.3	515.3
13	0	20.00	332	57	20.05	567.5	568.9	568.2	568.3
13	1	20.02	332	56	20.07	568.0	569.3	568.7	568.8
13	48	20.80	332	11	20.82	589.2	589.7	589.5	589.0
13	50	20.83	332	10	20.83	590.1	590.1	590.1	589.6
14	45	21.75	331	12	21.80	614.9	616.2	615.5	615.4
14	46	21.77	331	11	21.82	615.3	616.7	616.0	616.1
2nd order									
			316	8	36.87		497.8		497.9
			316	6	36.90		498.1		498.3
			314	40	38.33		514.6		514.9
			314	39	38.35		514.8		515.3
36	20	43.33	309	50	43.17	569.3	567.6	568.5	568.3
36	22	43.37	309	47	43.22	569.7	568.1	568.9	568.8
38	21	45.35	307	52	45.13	590.2	588.0	589.1	589.0
38	25	45.42	307	49	45.18	590.9	588.5	589.7	589.6
			305	12	47.80		614.6		615.4
			305	9	47.85		615.1		616.1

Table 4: Measured angles with the sodium lamp, calculated wavelengths with gratingconstant from Table 3 and NIST data for comparison

## **Evaluation**

In atoms with more than one electron the $n-l$ degeneracy is already lifted because the electrons see a screend potential of the atomic nucleus because of the other electrons. The resulting devation of the central potential from the $1/r$ -law lifts the level energies of orbits with higher $l$ .	<b>λ [nm]</b> 497.8	<b>▲E</b> [meV]
For single electrons outside completely filled orbits it can be assumed that there is a magnetic interaction	498.3	2.3
energy between the spin magnetic moment and the orbital magnetic moment. For orbits with zero angular	515.3	2.1
momentum ( $S$ -orbits) the orbital magnetic moment is zero. For $P$ -orbits the e.g. $z$ -component of spin	568.2	2.1
and orbit magnetic moments can be in the same direction, so there is a positive interaction energy	568.7	17
increasing the level energy – the magnetic fields of both moments add and the outer field is larger, so the	589.5	1.7
energy stored in magnetic field integrated over the whole space is larger. Else the spin and orbit magnetic	590.1	2.4
moments can be opposed, so the magnetic field weakened and the level energy lowered. Thus the energy of the ${}^{2}P_{\rm c}$ is level, for all arbitrary magnetic field weakened and the level for all arbitrary magnetic field.	615.5	
of the $13/2$ level should be expected to be higher than of the $11/2$ level. For all orbits with an orbital	616.0	1.5
magnetic moment this situation is the same and because radiative transitions are allowed from both	497.8	
upper and lower sub-level, the spectrum appears as doublet system.	498.1	1.9
Since the electron spin magnetic moment is fixed, the size of the spin orbit interaction depends on the	514.6	
magnetic moment of the orbit. For a magnetic need the speed of the charge is essential, that is	514.8	0.9
the average kinetic energy is higher to the corresponding magnetic moments can be stronger though the	568.5	
angular momentum is smaller. Even more so in atoms with several electrons where the inner electrons	568.9	1.7
screen the electric field of the atomic nucleus – they deform the central potential such that the potential is	589.1	<u> </u>
lower at the outside.	589.7	2.1
This causes in sodium the splitting of the $^2D$ -levels to be far smaller than of the $^2P$ -levels.	615 1	1.6
The technique to calculate this is perturbation theory taking into account the screening of the electric	015.1 Av [me]/]	· 18
central potential by the filled inner electron shells. There are many different possible formalisms here so	Table 5: N	. 1.0 Aeasured
for the calculation refer to literature, starting e.g. with Wikipedia,	enerav d	ifference
https://en.wikipedia.org/wiki/Spin%E2%80%93orbit_interaction	between	the Na
https://en.wikipedia.org/wiki/Fine_structure	$3^2P_{1/2}$ ar	nd $3^2P_{3/2}$
From the measured wavelength $\lambda$ data of Table 4 the wavelength splitting can be calculated to an energy		/el
splitting assuming only the $3$ " $P_{1/2}$ and $3$ " $P_{3/2}$ levels differ in energy of the levels involved with the		

transition. For calculation of energies E the wavelength in air is to be corrected for air refractive index of n = 1.00028 as is done by NIST in their data, so with speed of light c and Planck constant h the energy is  $E = h \cdot c/(n \cdot \lambda)$  and to be divided by electron charge e for results in eV. Table 5 shows the result. The result of 1.8 meV is to be compared with NIST value of 2.13202 meV for the splitting of Na  $3\ ^2P_{1/2}$  and  $3\ ^2P_{3/2}$  level. The large deviation here is due to the angle precision of 0°1' corresponding to an energy of 0.6 meV at 589 nm in second order and 1.6 meV at 589 nm in first order.

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## Fine structure of two electron spectra - prism spectrometer

### Set up and procedure

a) Determination of the dispersion function

Insert the helium (He 10) lamp into the lamp holder, connect this to the power supply and turn on.

Align the gonio-spectrometer according to the operating instructions and record the reticule angle where the slit image appears without prism.

Mount and align the diffraction prism according to the operating instructions.

Measure the minimum angle of deviation for visible He spectral lines reading the reticule angle position on the outer scale and calculating the angle difference with the reticule angle without prism. The table angle data read on the inner scale are far less precise and needn't be used for evaluation because at the angle of least deflection also the change of deflection angle with change of table angle is smallest. But they can help to check if there are errors like unintentional change of prism position or badly fixed table and the like. The table angle change should be half the ocular angle change.

Use a spread sheet to plot the angle of least deflection over the wavelength and to identify the He spectral lines, refer to Table 1. You can assume a smooth dispersion curve to identify the lines. Use this plot as calibration curve for wavelength measurement of the spectral lines of the other lamps.

Calculate the refractive index of the prism for each wavelength with the spread sheet and plot the dispersion curve fro the prism in use.

b) Determination of two-electron spectral line wavelengths

Turn off the power supply and let cool down the lamp, then exchange the He lamp with the zinc (Zn 10), cadmium (Cd 10) and mercury (Hg 100) lamp. For each lamp record the angle of least deflection for the visible lines. Determine the wavelength from the angle using the calibration curve.

Compare the results with the theoretical values.



#### **Data and results**

If a prism with inner angle  $\alpha_{prism}$  at its corner deflects a light beam of wavelength  $\lambda$  at the angle of least deflection through the angle  $\beta_{\lambda}$ , then the refractive index of the prism  $n_{\lambda}$  for this light is according to Snell's Law

$$n_\lambda = rac{\sin((lpha_{prism}+eta_\lambda)/2)}{\sin(lpha_{prism}/2)}$$

A measurement example is shown in Table 6. For the helium spectral line and transition data refer to the data of Table 1 and Fig. 2.



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A spline may be used for interpolation of the wavelength over angle data as it can be assumed that the function is a smooth convex one.

Fig. 5: Wavelength over angle of minimum deviation  $eta_\lambda$  and inserted spline, data of Table 6

Then this diagram can be used to read off the wavelenght from the measured angle data for the visible spectral lines of the other spectral lamps.

Tables 7 through 9 and Fig. 7 through 9 show the expected data for zinc, cadmium and mercury.



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blue	462.98	3d $^{10}$ 4s5d, $^1D_2$	3d $^{10}$ 4s4p, $^1P_1$	1.4 x 10 <sup>6</sup>	8.4729	5.7957
blue	468.01	3d $^{10}$ 4s5s, $^3S_1$	3d $^{10}$ 4s4p, $^{3}P_{0}$	$1.4 \times 10^{7}$	6.6545	4.0061
blue	472.22	3d $^{10}$ 4s5s, $^{3}S_{1}$	3d $^{10}$ 4s4p, $^{3}P_{1}$	$1.9 \times 10^{7}$	6.6545	4.0297
blue	481.05	3d $^{10}$ 4s5s, $^3S_1$	3d $^{10}$ 4s4p, $^{3}P_{2}$	$1.9 \times 10^{7}$	6.6545	4.0779
green	507.0	3d $^{ t 10}$ 4s9p, $^{ t 3}P_{0,1,2}$	3d $^{10}$ 4s5s, $^3S_1$	5 x 10 <sup>5</sup>	9.0998	6.6545
green	518.20	3d $^{10}$ 4s6s, $^{1}S_{0}$	3d $^{10}$ 4s4p, $^1P_1$	1 x 10 <sup>7</sup>	8.1876	5.7957
green	530.9	3d $^{ t 10}$ 4s8p, $^{ t 3}P_{ extrm{0,1,2}}$	3d $^{10}$ 4s5s, $^3S_1$	1 x 10 <sup>6</sup>	8.9890	6.6545
red	636.23	3d $^{10}$ 4s4d, $^1D_2$	3d $^{10}$ 4s4p, $^1P_1$	4.7 x 10 <sup>7</sup>	7.7439	5.7957
Fig. 7: Zn transitions - NIST data						

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blue	441.30	$_{4d^{10}5c6c} {}^{1}S_{0}$	$4d^{10}550 + {}^{3}P_{1}$	$2 \times 10^{5}$	6.6096	3.8009
blue	466.24	4d $^{10}$ 5s6d, $^{1}D_{2}$	4d $^{10}$ 5s5p, $^{1}P_{1}$	$5.5 \times 10^{6}$	8.0757	5.4172
blue	467.81	4d $^{10}$ 5s6s, $^3S_1^{-1}$	4d $^{10}$ 5s5p, $^{3}P_{0}^{1}$	1.3 x 10 <sup>7</sup>	6.3832	3.7337
blue	479.99	4d $^{10}$ 5s6s, $^{3}S_{1}$	4d $^{10}$ 5s5p, $^{3}P_{1}$	4.1 x 10 <sup>7</sup>	6.3832	3.8009
green	508.58	4d $^{10}$ 5s6s, $^3S_1^{-}$	4d $^{10}$ 5s5p, $^{3}P_{2}^{-}$	5.6 x 10 <sup>7</sup>	6.3832	3.9460
green	515.47	4d $^{10}$ 5s7s, $^1S_0$	4d $^{10}$ 5s5p, $^1P_1$	3 x 10 <sup>5</sup>	7.8218	5.4172
red	632.52	4d $^{10}$ 5s5d, $^{3}D_{2}$	4d $^{10}$ 5s5p, $^1P_1$	6 x 10 <sup>6</sup>	7.3768	5.4172
red	633.00	4d $^{10}$ 5s5d, $^{3}D_{1}$	4d $^{10}$ 5s5p, $^1P_1$	2 x 10 <sup>6</sup>	7.3753	5.4172
red	643.85	4d $^{10}$ 5s5d, $^1D_2^-$	4d $^{10}$ 5s5p, $^1P_1$	5.9 x 10 <sup>7</sup>	7.3423	5.4172

Table 8: Cd transitions - NIST data



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colour	v [um]	upper (1)	lower (2)	A[s]	$L_1 [ev]$	$L_2 [ev]$
purple	365.3	5d $^{10}$ 6s6d, $^{3}D_{1}$ ,3	5d $^{10}$ 6s6p, $^{3}P_{2}$	1.3 x 10 <sup>8</sup>	8.8500	5.4606
blue	404.66	5d $^{10}$ 6s7p, $^3S_1$	5d $^{10}$ 6s6p, $^{3}P_{0}$	2.1 x 10 <sup>7</sup>	7.7305	4.6674
blue	407.78	5d $^{10}$ 6s7s, $^1S_0$	5d $^{10}$ 6s6p, $^{3}P_{1}$	4.0 x 10 <sup>6</sup>	7.9261	4.8865
blue	410.81	5d $^{10}$ 6s8s, $^1S_0$	5d $^{10}$ 6s6p, $^1P_1$	3.0 x 10 <sup>6</sup>	9.7209	6.7037
blue	433.92	5d $^{10}$ 6s7d, $^{3}D_{2}$	5d $^{10}$ 6s6p, $^1P_1$	2.9 x 10 <sup>6</sup>	9.5601	6.7037
blue	434.75	5d $^{10}$ 6s7d, $^1D_2$	5d $^{10}$ 6s6p, $^1P_1$	8.4 x 10 <sup>6</sup>	9.5547	6.7037
blue	435.83	5d $^{10}$ 6s7p, $^3S_1$	5d $^{10}$ 6s6p, $^{3}P_{1}$	5.6 x 10 <sup>7</sup>	7.7305	4.8865
cyan	491.61	5d $^{10}$ 6s8s, $^1S_0$	5d $^{10}$ 6s6p, $^1P_1$	5.8 x 10 <sup>6</sup>	9.2250	6.7037
green	546.08	5d $^{10}$ 6s7p, $^3S_1$	5d $^{10}$ 6s6p, $^{3}P_{2}$	4.9 x 10 <sup>7</sup>	7.7305	5.4606
yellow	576.96	5d $^{10}$ 6s6d, $^{3}D_{2}$	5d $^{10}$ 6s6p, $^1P_1$	2.4 x 10 <sup>7</sup>	8.8520	6.7037
yellow	578.97	5d $^{10}$ 6s6d, $^{3}D_{1}$	5d $^{10}$ 6s6p, $^1P_1$	2.4 x 10 <sup>7</sup>	8.8445	6.7037
red	623.44	5d $^{10}$ 6s9p, $^1P_1$	5d $^{10}$ 6s7s, $^1S_0$	5.3 x 10 <sup>5</sup>	9.9143	7.9261
red	690.75	5d $^{10}$ 6s8p, $^{3}P_{2}$	5d $^{10}$ 6s7p, $^3S_1$	2.8 x 10 <sup>6</sup>	9.5249	7.7305
		Table 9: H	a transitions -NIST	Г data		

Table 10 and 11 show a comparison of the wavelength determined by reading off the wavelength from the interpolated data measured with the prism assuming the He wavelength known (Fig. 5) with the reference data from NIST.

Zn		_			Cd		_		
deg.	min	$\beta_{\lambda}$	λ, Fig. 5	λ, NIST	deg.	min	$\beta_{\lambda}$	λ, Fig. 5	λ, NIST
		[°]	[nm]	[nm]			[°]	[nm]	[nm]
288	25	64.52	414	411.3	289	14	63.70	429	430.7
289	9	63.78	427	429.3	289	42	63.23	439	441.3
289	11	63.75	428	429.8	290	40	62.27	466	466.2
290	32	62.40	462	463.0	290	42	62.23	467	467.8
290	43	62.22	468	468.0	291	7	61.82	480	480.0
290	52	62.07	474	472.2	291	55	61.02	512	508.6
291	9	61.78	481	481.1	292	3	60.88	518	515.5
291	54	61.03	511	507.0	293	42	59.23	612	609.9
292	7	60.82	520	518.2	293	43	59.22	613	611.1
292	24	60.53	534	530.9	294	0	58.93	636	632.5
294	2	58.90	640	636.2	294	0	58.93	636	633.0
					294	7	58.82	646	643.8

Table 10: Measurement data for zinc (Zn) and cadmium (Cd)



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Hg		0		
deg.	min.	$\beta_{\lambda}$	λ, Fig. 5	λ, NIST
		[°]	[nm]	[nm]
287	48	65.13	406	404.7
287	58	64.97	408	407.8
288	9	64.78	410	410.8
289	21	63.58	432	433.9
289	24	63.53	433	434.7
289	28	63.47	434	435.8
291	27	61.48	492	491.6
292	43	60.22	550	546.1
293	14	59.70	580	577.0
293	15	59.68	581	579.0
293	52	59.07	626	623.4
294	40	58.27	684	690.8
Tab	ole 11	: Measu	irement data	for mercury
			(Hg)	

#### **Evaluation**

While for helium eight lines were observable and identifyable with the grating, with the prism it was 14 lines. With the grating for sodium the averaged absolute value of deviation of first order measured wavelength from literature values was 0.16 nm. Compared to that this value is for the prism for Zn, Cd and Hg with 2 nm more than ten times larger.

For zinc with atomic number 30 no transitions between singulett and tripplett states are observable.

For cadmium with atomic number 48 transitions at 441 nm and 633 nm are just observable, which are transitions between singulett and tripplett states.

For mercury with atomic number 80 the yellow doublett at 578 nm is one of the most prominent lines and other transitions between singulett and tripplett states are well observable, too.

This means that for light elements with low atomic number different selection rules apply for transitions than for heavy elements.

For light elements the selection rule for spin quantum number S is  $\Delta S=0$ . LS or Russel-Sounders coupling applies: The two spins  $s_i$  couple to form a total spin S and the two orbital moments  $l_i$  couple to form a total orbital angular moment L,  $L = \sum_i l_i$ ,  $S = \sum_i s_i$ , J = L + S.

For heavy atoms for the outermost electrons the interaction between the individual spin  $s_i$  and orbit  $l_i$  is stronger than between different spins so first each  $s_i + l_i = j_i$  couple and  $J = \sum_i j_i = \sum_i (l_i + s_i)$ . This is referred to as jj-coupling. Here the selection rule  $\Delta S = 0$  is lifted.

Refer to:

https://en.wikipedia.org/wiki/Angular momentum coupling https://en.wikipedia.org/wiki/Spin%E2%80%93orbit interaction

## Appendix

## Atomic level data (source: NIST)

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	He levels	Na levels
config	. term E [eV]	config. term E [eV]
-	singulett	doublett
1s <sup>2</sup>	$S_0 = 0.0000$	$_{2p^{6}3s}$ $_{2}^{2}S_{1/2}$ 0.0000
1s2s	$^{1}S_{0}$ 20.6158	$_{ m 2p^63p}$ $^2P_{1/2}$ 2.1023
1s2p	$^{1}P_{1}$ 21.2180	2p $^{6}$ 3p $^{2}P_{3/2}$ 2.1044
1s3s	$^{1}S_{0}$ 22.9203	2p $^{6}$ 4s $^{2}S_{1/2}$ 3.1914
1s3d	$^{1}D_{2}$ 23.0741	2p $^{6}$ 3d $^{2}D_{5/2,3/2}$ 3.6170
1s3p	$^{1}P_{1}$ 23.0870	2p $^{6}$ 4p $^{2}P_{1/2}$ 3.7526
1s4s	$^{1}S_{0}$ 23.6736	$_{ m 2p^{6}4p}$ $^{2}P_{ m 3/2}$ 3.7533
1s4p	$^{1}P_{1}$ 23.7421	2p $^{6}$ 5s $^{2}S_{1/2}$ 4.1164
1s4d	$^{1}D_{2}$ 23.7363	$_{ m 2p^64d}$ $^2D_{5/2,3/2}$ 4.2835
1s4f	$^{1}F_{3}$ 23.7370	$_{ m 2p^64f}$ $^2F_{7/2,5/2}$ 4.2882
1s5s	$^{1}S_{0}$ 24.0112	$_{ m 2p^65p}$ $^2P_{ m 1/2}$ 4.3445
1s5d	$^{1}D_{2}$ 24.0428	$_{ m 2p^65p}$ $^2P_{ m 3/2}$ 4.3448
1s5f	$^{1}F_{3}$ 24.0432	$_{ m 2p^6_{6s}}$ $^2S_{ m 1/2}$ 4.5096
1s5p	$^{1}P_{1}$ 24.0458	2p $^{6}$ 5d $^{2}D_{5/2,3/2}$ 4.5920
1s6s	$^{1}S_{0}$ 24.1690	2p <sup>6</sup> 5f ${}^2F_{7/2,5/2}$ 4.5946
1s6d	$^{1}D_{2}$ 24.2092	2p $^{6}$ 6p $^{2}P_{1/2}$ 4.6242
	triplett	2p $^{6}$ 6p $^{2}P_{3/2}$ 4.6243
1s2s	$^3S_1$ 19.8196	2p $^{6}$ 7s $^{2}S_{1/2}$ 4.7129
1s2p	${}^3P_{0,1,2}$ 20.9641	$_{ m 2p^6_{6d}}{}^2D_{5/2,3/2}$ 4.7594
1s3s	${}^3S_1$ 22.7185	2p <sup>6</sup> 6f ${}^2F_{7/2,5/2}$ 4.7610
1s3p	${}^{3}P_{0,1,2}$ 23.0071	$_{ m 2p^{6}7p}$ $^{2}P_{ m 1/2}$ 4.7784
1s3d	${}^{3}D_{1,2,3}$ 23.0737	$_{ m 2p^67p}$ $^2P_{ m 3/2}$ 4.7785
1s4s	$^3S_1$ 23.5940	2p $^{6}$ 8s $^{2}S_{1/2}$ 4.8315
1s4p	${}^{3}P_{0,1,2}$ 23.7079	
1s4d	${}^{3}D_{1,2,3}$ 23.7361	
1s4f	${}^3F_{2.3.4}$ 23.7370	
1s5s	$^3S_1$ 23.9720	
1s5p	${}^{3}P_{0,1,2}$ 24.0282	
1s5f	${}^3F_{2.3.4}$ 24.0432	
1s5d	${}^{3}D_{123}^{-,0,-}$ 24.0427	
	1,4,0	

Zn levels	Zn levels
config. term E [eV]	config. term E [eV]
$\begin{array}{c} singulett\\ 3d^{10}4s2 & S_0 & 0.0000\\ 3d^{10}4s4p & ^1P_1 & 5.7957\\ 3d^{10}4s5s & ^1S_0 & 6.9170\\ 3d^{10}4s5p & ^1P_1 & 7.7999\\ 3d^{10}4s5p & ^1P_1 & 7.7999\\ 3d^{10}4s6s & ^1S_0 & 8.1876\\ 3d^{10}4s5d & ^1D_2 & 8.4729\\ 3d^{10}4s6p & ^1P_1 & 8.5062\\ 3d^{10}4s6p & ^1P_1 & 8.5062\\ 3d^{10}4s4f & ^1F_3 & 8.5344\\ 3d^{10}4s7p & ^1S_0 & 8.6794\\ 3d^{10}4s6d & ^1D_2 & 8.8091\\ 3d^{10}4s7p & ^1P_1 & 8.8300\\ 3d^{10}4s5f & ^1S_0 & 8.9214\\ 3d^{10}4s6s & ^1S_0 & 8.9214\\ 3d^{10}4s8p & ^1P_1 & 9.0045\\ 3d^{10}4s8p & ^1P_1 & 9.0045\\ 3d^{10}4s8p & ^1P_1 & 9.0999\\ 3d^{10}4s9p & ^1P_1 & 9.1090\\ \end{array}$	$\begin{array}{c} triplett\\ 3d^{10}454p & {}^{3}P_{0} & 4.0061\\ 3d^{10}454p & {}^{3}P_{1} & 4.0297\\ 3d^{10}455p & {}^{3}P_{2} & 4.0779\\ 3d^{10}455p & {}^{3}P_{1} & 6.6545\\ 3d^{10}455p & {}^{3}P_{1} & 7.5971\\ 3d^{10}455p & {}^{3}P_{1} & 7.5971\\ 3d^{10}455p & {}^{3}P_{2} & 7.6041\\ 3d^{10}456p & {}^{3}P_{1} & 7.7823\\ 3d^{10}454d & {}^{3}D_{1} & 7.7823\\ 3d^{10}454d & {}^{3}D_{2} & 7.7827\\ 3d^{10}454d & {}^{3}D_{2} & 7.7834\\ 3d^{10}456p & {}^{3}P_{1} & 8.4409\\ 3d^{10}456p & {}^{3}P_{1} & 8.4409\\ 3d^{10}456p & {}^{3}P_{1} & 8.4409\\ 3d^{10}456p & {}^{3}P_{1} & 8.4435\\ 3d^{10}456p & {}^{3}P_{1} & 8.4435\\ 3d^{10}456p & {}^{3}P_{1} & 8.4435\\ 3d^{10}456p & {}^{3}P_{1,2,3} & 8.5030\\ 3d^{10}456f & {}^{3}F_{2,3,4} & 8.5433\\ 3d^{10}456f & {}^{3}F_{2,3,4} & 8.8445\\ 3d^{10}455g & {}^{3}G_{3,4,5} & 8.8492\\ 3d^{10}456g & {}^{3}F_{2,3,4} & 9.0125\\ 3d^{10}456f & {}^{3}F_{2,3,4} & 9.0125\\ 3d^{10}456f & {}^{3}F_{2,3,4} & 9.0149\\ 3d^{10}456g & {}^{3}G_{3,4,5} & 9.0149\\ 3d^{10}456g & {}^$
	- 3 - 7 7



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Cd levels		Cd levels		
config.	term E [eV]	config.	term	E [eV]
4d <sup>10</sup> 5s2	${}^{1}S_{0}$ 0.0000	4d <sup>10</sup> 5s5p	$^{3}P_{0}$	3.7337
4d <sup>10</sup> 5s5p	${}^{1}P_{1}$ 5.4172	4d <sup>10</sup> 5s5p	${}^{3}P_{1}$	3.8009
4d <sup>10</sup> 5s6s	$^{1}S_{0}$ 6.6096	4d <sup>10</sup> 5s5p	${}^{3}P_{2}$	3.9460
4d <sup>10</sup> 5s5d	$^{1}D_{2}$ 7.3423	4d <sup>10</sup> 5s6s	${}^3S_1$	6.3832
4d <sup>10</sup> 5s6p	$^{1}P_{1}$ 7.4276	4d <sup>10</sup> 5s6p	$^{3}P_{0}$	7.2396
4d <sup>10</sup> 5s7s	$^{1}S_{0}$ 7.8218	4d <sup>10</sup> 5s6p	${}^{3}P_{1}$	7.2483
4d <sup>10</sup> 5s6d	${}^{1}D_{2}$ 8.0757	4d <sup>10</sup> 5s6p	${}^{3}P_{2}$	7.2699
4d <sup>10</sup> 5s7p	${}^{1}P_{1}$ 8.1211	4d <sup>10</sup> 5s5d	$^{\circ}D_1$	7.3753
4d <sup>10</sup> 5s8s	${}^{1}S_{0}$ 8.2952	4d <sup>10</sup> 5s5d	$^{3}D_{2}$	7.3768
4d <sup>10</sup> 5s7d	$^{1}D_{2}$ 8.4109	4d <sup>10</sup> 5s5d	$^{3}D_{3}$	7.3790
4d <sup>10</sup> 5s8p	$^{1}P_{1}$ 8.4383	4d <sup>10</sup> 5s7s	${}^{3}S_{1}$	7.7569
4d <sup>10</sup> 5s9s	$^{1}S_{0}$ 8.5300	4d <sup>10</sup> 5s7p	$^{\circ}P_0$	8.0585
4d <sup>10</sup> 5s8d	$^{1}D_{2}$ 8.5917	4d <sup>10</sup> 5s7p	$^{\circ}P_1$	8.0621
4d <sup>10</sup> 5s9p	$P_1 8.6094$	4d <sup>10</sup> 5s7p	$^{\circ}P_2$	8.0706
4d <sup>10</sup> 5s10s	$^{-5}0$ 8.6634	4d <sup>10</sup> 5s6d	$^{\circ}D_{1}$	8.1028
4d <sup>10</sup> 5s9d	$^{-}D_{2}$ 8.6999	4d <sup>10</sup> 5s6d	$^{\circ}D_{2}$	8.1035
4d <sup>10</sup> 5s10p	$^{-}P_{1}$ 8.7120	4d <sup>10</sup> 5s6d	$^{-}D_{3}$	8.1045
4d <sup>10</sup> 5s11s	${}^{50}$ 8.7411	4d <sup>10</sup> 5s4f	${}^{\circ}F_{2,3,4}$	8.1320
4d <sup>10</sup> 5s10d	$D_2 8.7/01$	4d <sup>10</sup> 5s8s	$\frac{3}{3}$	8.2675
4d <sup>10</sup> 5s10f	$-F_3$ 8.8566	4d <sup>10</sup> 5s8p	$^{2}P_{0}$	8.4098
		4d <sup>10</sup> 5s8p	3 D	8.4113
		4d <sup>10</sup> 5s8p	$r_2$	8.4155
		4d <sup>10</sup> 5s7d	$^{\circ}D_{1,2,3}$	8.4302
		4d <sup>10</sup> 5s5f	<sup>°</sup> F <sub>2,3,4</sub>	8.4425
		4d <sup>10</sup> 5s9s	3D	8.5155
		4d <sup>10</sup> 5s9p	$^{\circ}P_{0,1,2}$	8.5959
		4d <sup>10</sup> 5s8d	$^{\circ}D_{1,2,3}$	8.6049
		4d <sup>10</sup> 5s6f	${}^{-F_{2,3,4}}_{3C}$	8.6115
		4d <sup>10</sup> 5s10s	3D	ö.0549
		4d <sup>10</sup> 5s10p	$3 r_{0,1,2}$	ö./U39
		4d <sup>10</sup> 5s7f	${}^{r_{2,3,4}}_{3c}$	ö./133
		4d <sup>10</sup> 5s11s	$\mathcal{D}_1$	ö./411

Hg levels					
config. term E [eV]					
singulett					
5d <sup>10</sup> 6s2 $\frac{1}{50}$	0.0000				
5d <sup>10</sup> 6s6p $^{1}P_{1}$	6.7037				
$5d^{10}6s7s$ $^{1}S_{0}$	7.9261				
$5d^{10}6s7p$	8.8394				
$5d^{10}6s6d$ $^{1}D_{2}$	8.8442				
5d $^{10}$ 6s8s $^1_1S_0$	9.2250				
$5d^{10}6s8p$ $^{1}P_{1}$	9.5298				
$5d^{10}6s7d^{-1}D_2$	9.5547				
$5d^{10}6s5f_{1}^{1}F_{3}$	9.5767				
5d $^{10}$ 6s9s $^1S_0$	9.7209				
triplett					
$5d^{10}6s6p^{-3}P_0$	4.6674				
$5d^{10}6s6p$ $^{3}P_{1}$	4.8865				
$5d^{10}6s6p$ $^{3}P_{2}$	5.4606				
$5d^{10}6s7p^{-3}S_1$	7.7305				
$5d^{10}6s7p^{-3}P_0$	8.6190				
$5d^{10}6s7p^{-3}P_1$	8.6370				
$5d^{10}6s7p^{-3}P_2$	8.8286				
$5d^{10}6s6d^{3}D_{1}$	8.8445				
$5d^{10}6s6d^{3}D_{2}$	8.8520				
$5d^{10}6s6d^{3}D_{3}$	8.8563				
5d $^{10}$ 6s8s $^3S_1$	9.1700				
$5d^{10}6s8p^{3}P_{0}$	9.4782				
5d <sup>10</sup> 6s8p $^{3}P_{1}$	9.4807				
$5d^{10}6s8p$ $^{3}P_{2}$	9.5249				
$5d^{10}6s7d^{3}D_{1}$	9.5573				
$5d^{10}6s7d^{-3}D_2$	9.5601				
$5d^{10}6s7d^{3}D_{3}$	9.5628				
5d <sup>10</sup> 6s5f ${}^{3}F_{2}$	9.5762				
5d <sup>10</sup> 6s5f ${}^{3}F_{3}$	9.5764				
3F	0 5000				

5d $^{10}$ 6s5f  $^{3}F_{4}$  9.5823