



Universidad de Valladolid

# MEASURING TRANSITION PROBABILITIES OF RARE-EARTHS: EXPERIMENTAL REQUIREMENTS AND CHALLENGES

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# OUTLINE

***1. Who are we?***

***2. Transition probabilities*** (what are they, why are they important, how do I measure them?)

***3. Experimental requirements and challenges***

***4. Is there any equilibrium?***

# Atomic Spectroscopy Laboratory (Faculty of Sciences)



**Dr Teruca Belmonte**



**Pratyush R Sen Sarma**

**(poster P5)**



**Prof Santiago Mar**



**Nuño Lorenzana**



**University of  
Valladolid (Spain)**



# Our laboratory – past...

1 H																2 He	
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	* 71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	* 103 Lr	* 104 Rf	* 105 Db	* 106 Sg	* 107 Bh	* 108 Hs	* 109 Mt	* 110 Ds	* 111 Rg	* 112 Cn	* 113 Nh	* 114 Fl	* 115 Mc	* 116 Lv	* 117 Ts	* 118 Og
		* 57 La	* 58 Ce	* 59 Pr	* 60 Nd	* 61 Pm	* 62 Sm	* 63 Eu	* 64 Gd	* 65 Tb	* 66 Dy	* 67 Ho	* 68 Er	* 69 Tm	* 70 Yb		
		* 89 Ac	* 90 Th	* 91 Pa	* 92 U	* 93 Np	* 94 Pu	* 95 Am	* 96 Cm	* 97 Bk	* 98 Cf	* 99 Es	* 100 Fm	* 101 Md	* 102 No		

Transition probabilities

Stark widths and shifts





**Dr Henrik Hartman**

**University of Malmö  
(Sweden)**



**Dr Gillian Nave**

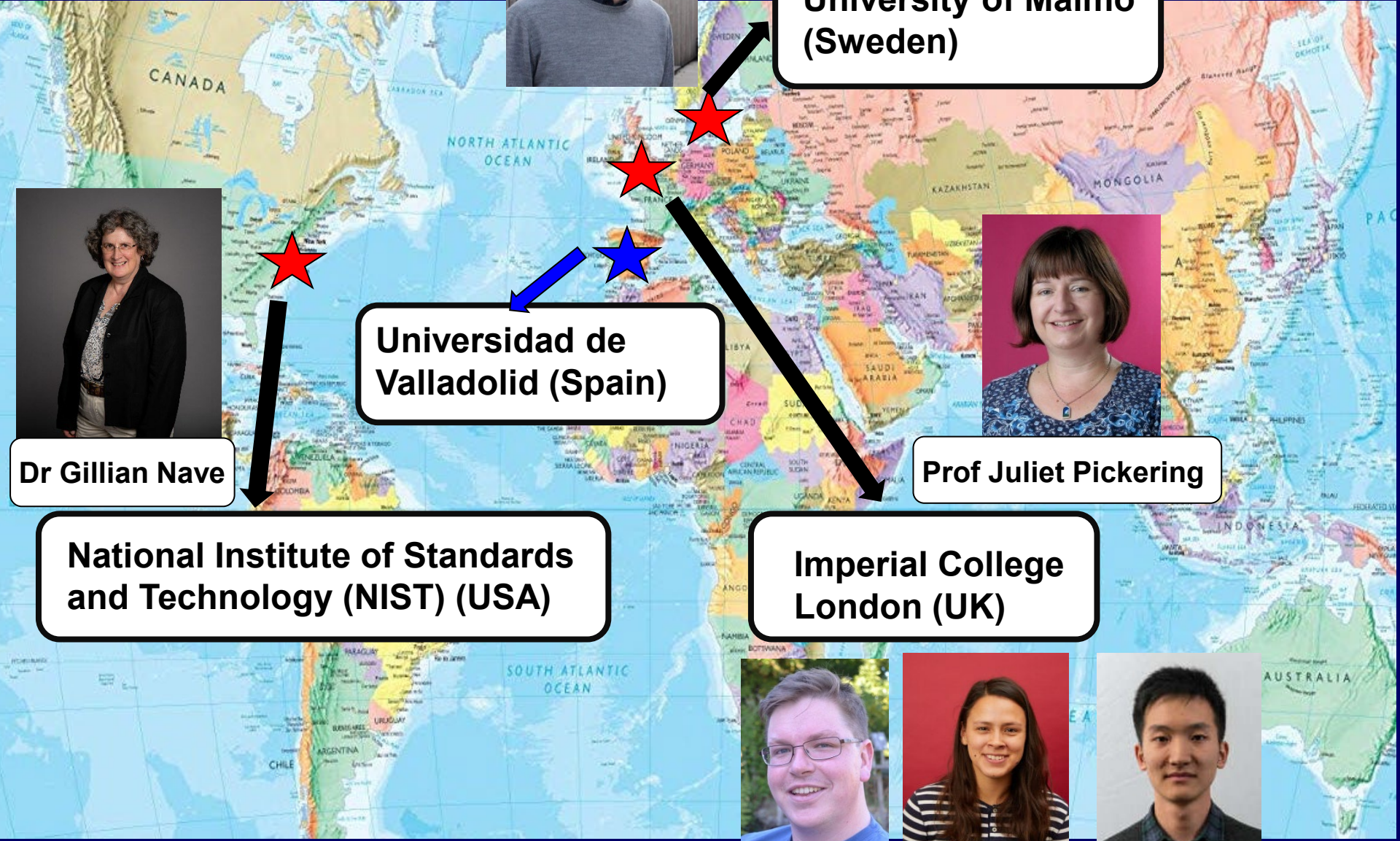
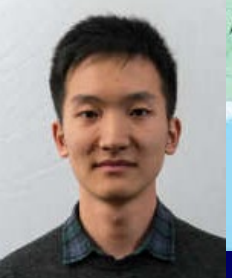
**Universidad de  
Valladolid (Spain)**



**Prof Juliet Pickering**

**National Institute of Standards  
and Technology (NIST) (USA)**

**Imperial College  
London (UK)**



# and present: the rare-earths

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Transition probabilities

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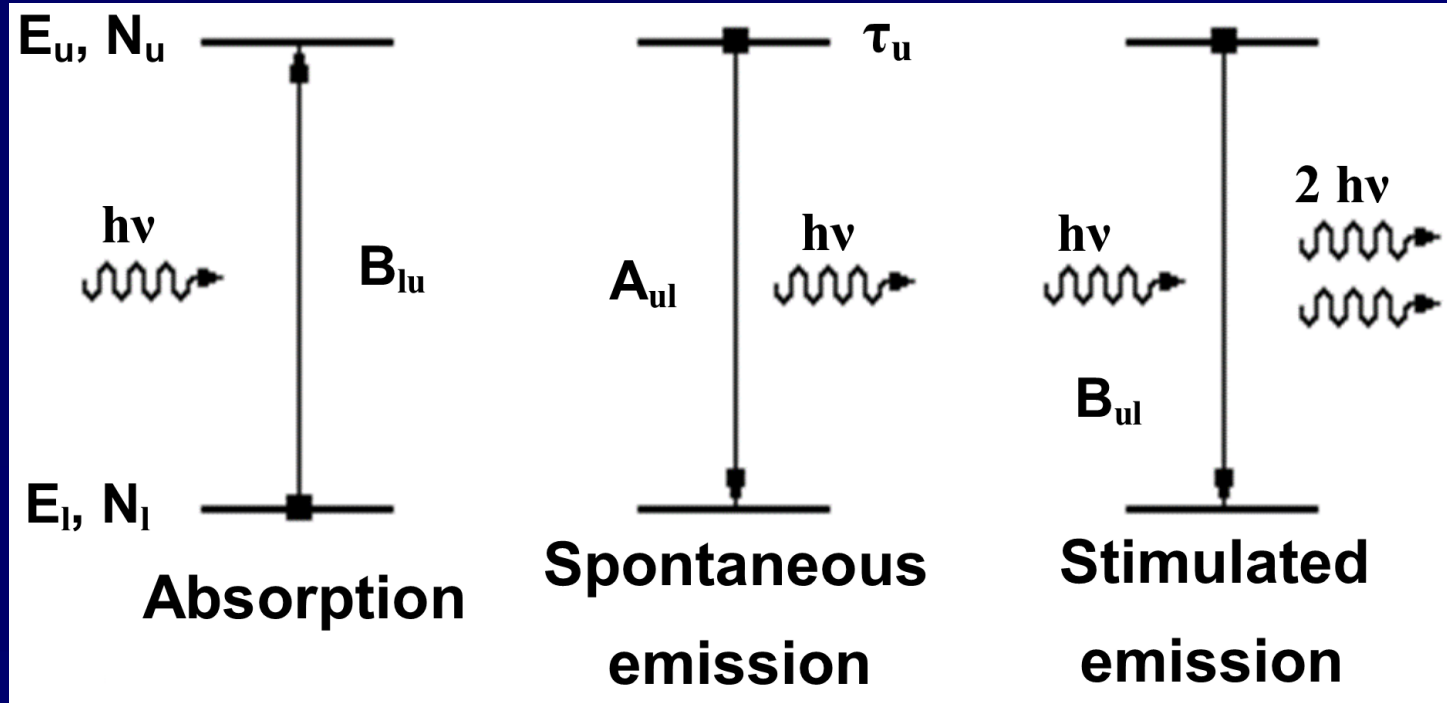
***3. Experimental requirements and challenges***

***4. Is there any equilibrium?***



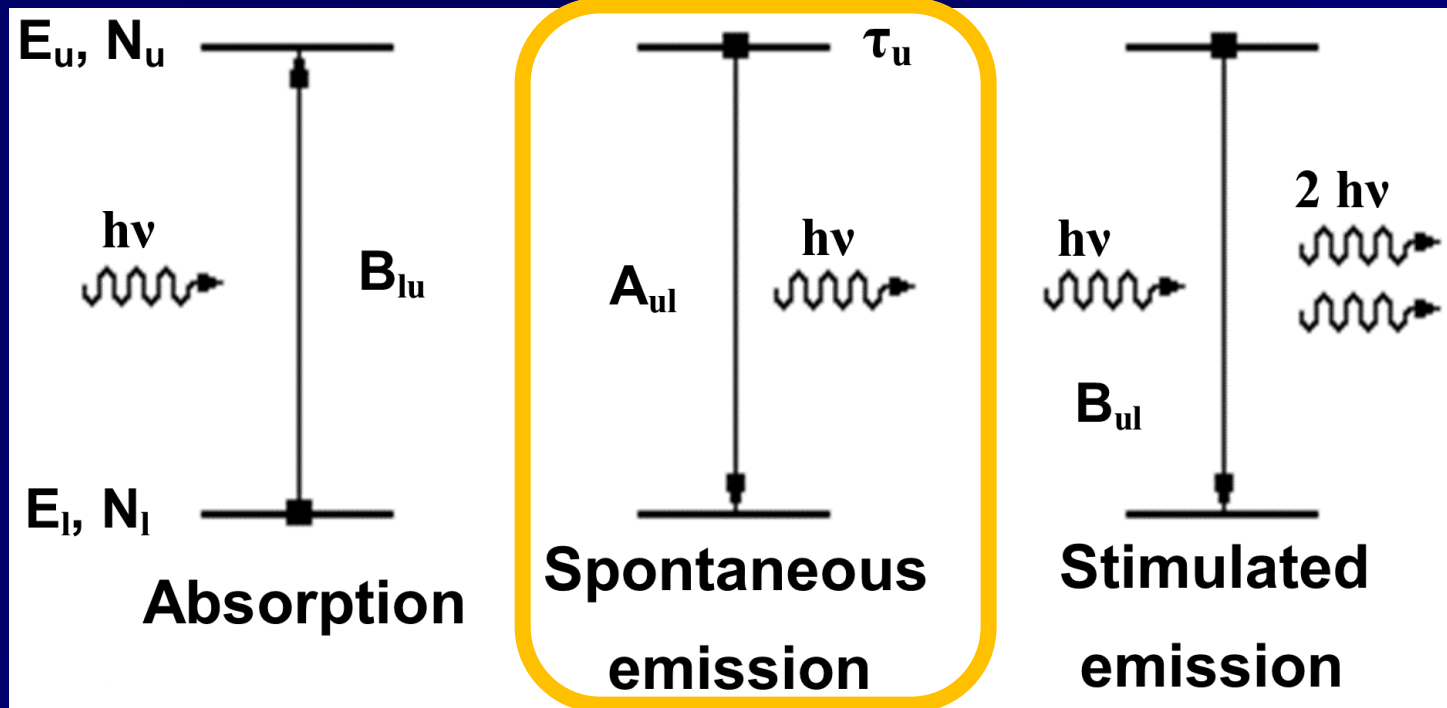
# What are Transition probabilities?

## Einstein coefficients



# What are Transition probabilities?

## Einstein coefficients



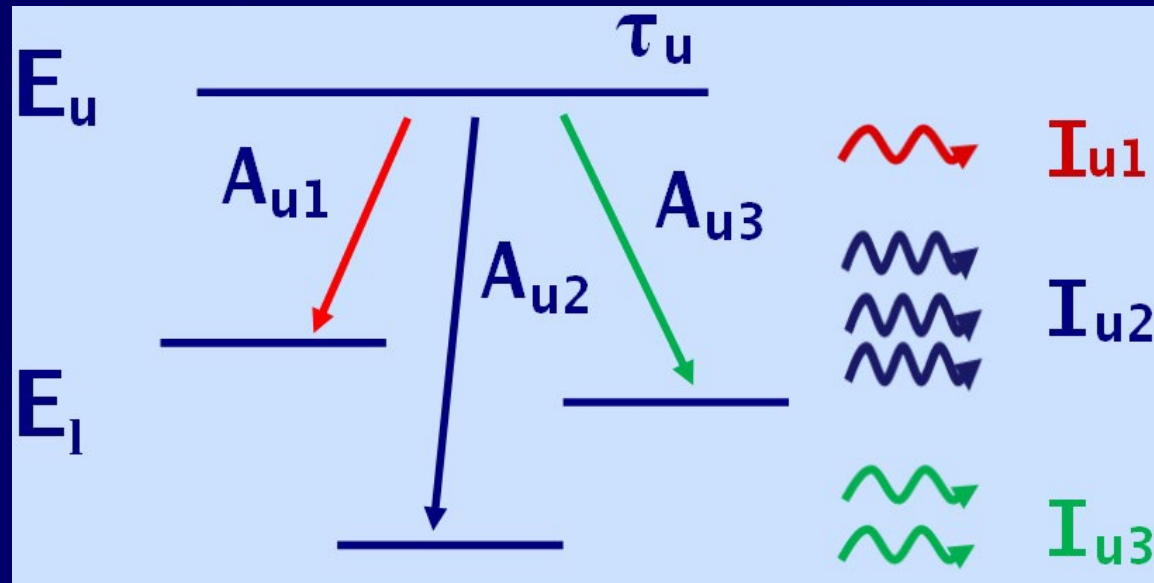
Lifetime (s)

$$\tau_u = \frac{1}{A_{ul}}$$

transition probability ( $s^{-1}$ )

# What are Transition probabilities?

Einstein  
coefficients



Lifetime (s)  $\leftarrow \tau_u = \frac{1}{\sum_i A_{ui}}$   $\rightarrow$  transition probability ( $s^{-1}$ )



## EMISSION OF RADIATION

Einstein A-values

Transition probabilities

Einstein coefficients for  
spontaneous emission

## ABSORPTION OF RADIATION

Oscillator strengths

f- values

$\log (g_l f_l)$

$$f_{lu} = \frac{mh}{\pi e^2} \nu_{lu} B_{lu}$$

## EMISSION OF RADIATION

Einstein A-values

Transition probabilities

Einstein coefficients for spontaneous emission

$$\log(g_l f) = \log\left(A_{ul} g_u \lambda^2 \times 1.499 \times 10^{-14}\right)$$

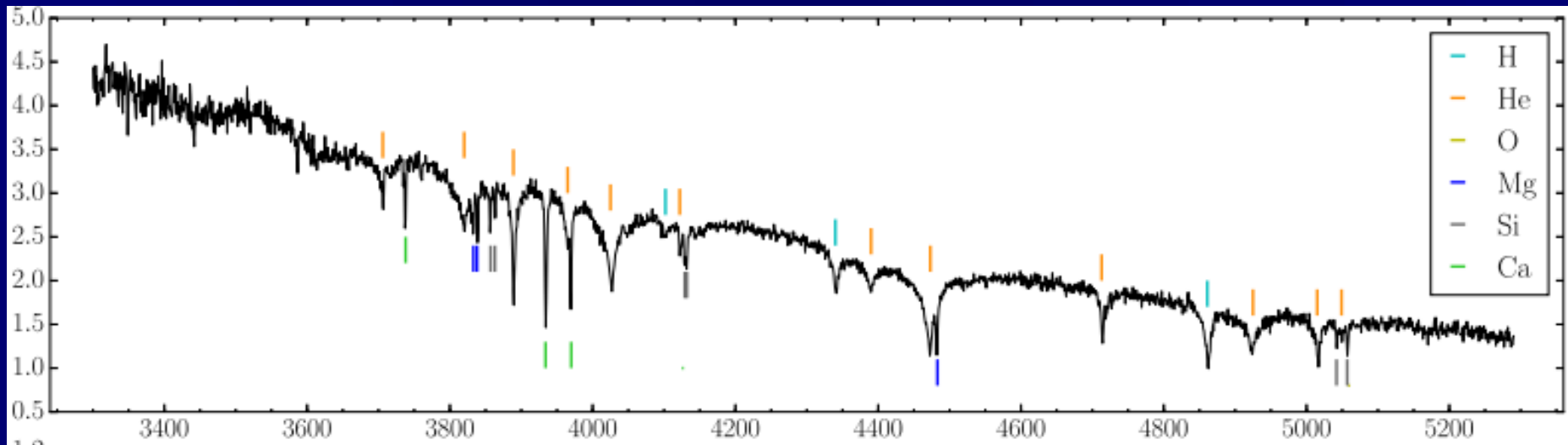
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Oscillator strengths

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*Izquierdo et al. GD 424 – a helium-atmosphere white dwarf with a large amount of trace hydrogen in the process of digesting a rocky planetesimal, MNRAS 501, 4276–4288 (2021)*

- Line POSITIONS → COMPOSITION (need of Wavelengths)
- Line INTENSITIES → ABUNDANCE (need of Transition probabilities)

$$\log \left( \frac{EW}{\lambda} \right) = \log(\text{Abundance}) + \log(\lambda g f) + C + \text{other parameters}$$



# How can we measure transition probabilities?

$$I_{ul} \propto A_{ul} N_u$$

$I_{ul}$  = intensity of the spectral line (area under the profile)

$A_{ul}$  = transition probability (Einstein coefficient for spontaneous emission)

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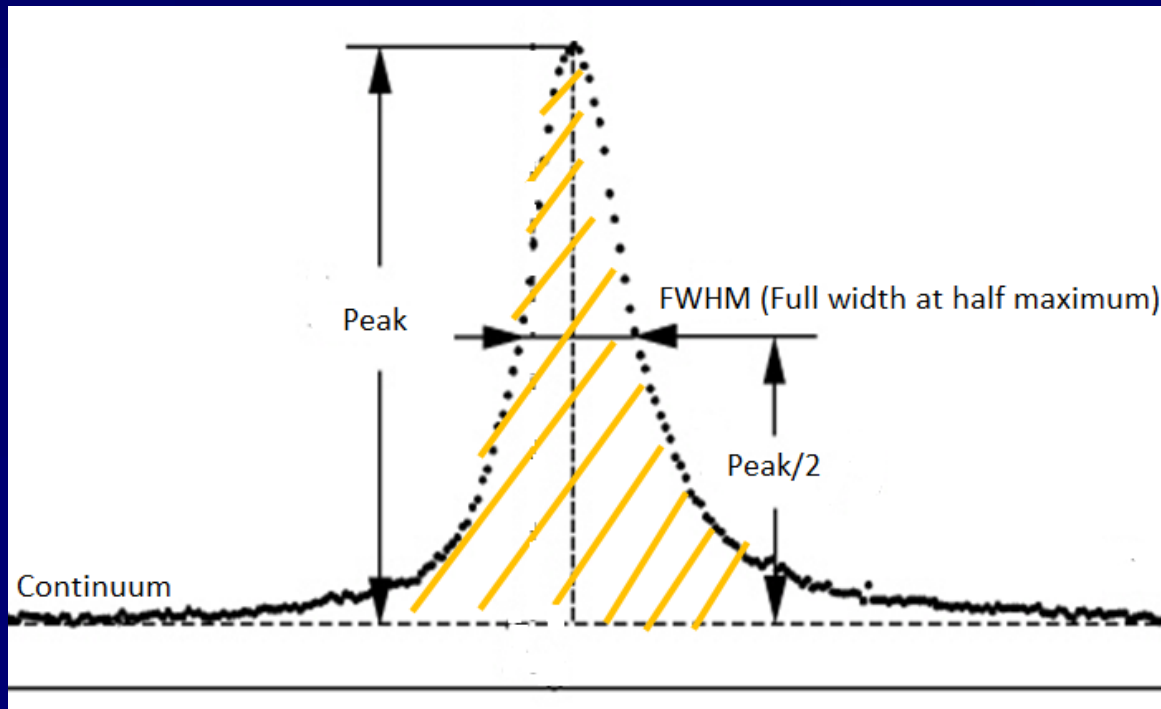
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# Transition probabilities of Nd III

Imperial College London



# Why Nd III?

- We can compare spectra measured at Imperial College (FTS,  $R=10^6$ ) with spectra measured in Valladolid (grating,  $R=10^5$ ) (see the real capability of our instrument).
- We can measure Nd II transition probabilities and compare with values from Lawler (Wisconsin)
- We can use work on energy levels carried out at Imperial (Milan Ding's thesis) to help us identify lines coming from an upper energy level.
- Use grating spectra for weak lines

For transition probabilities, on condition we are able to fit the line accurately, we are OK! (uncertainties don't depend on line width)



# OUTLINE

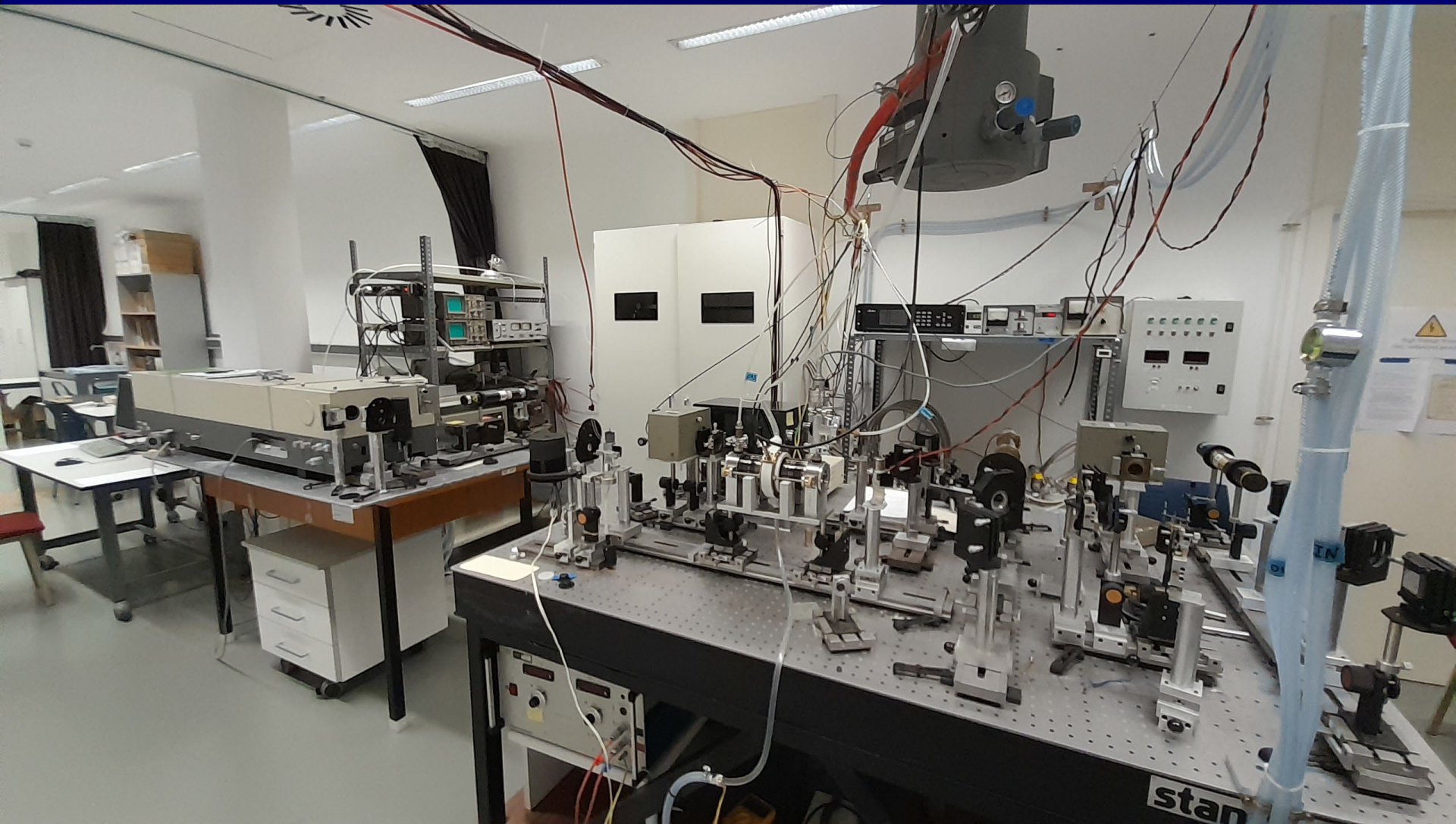
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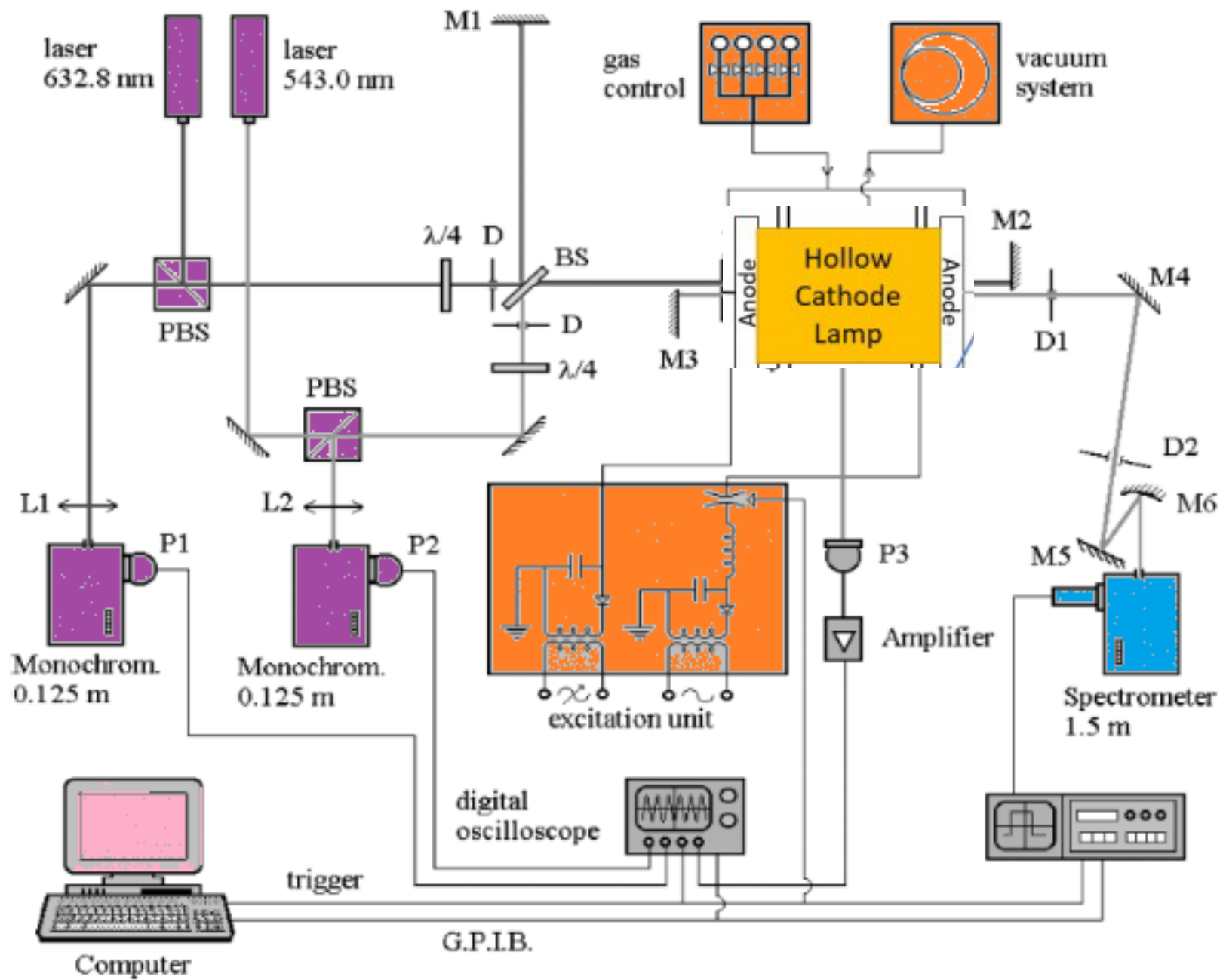
***4. Is there any equilibrium?***

# OUR LABORATORY

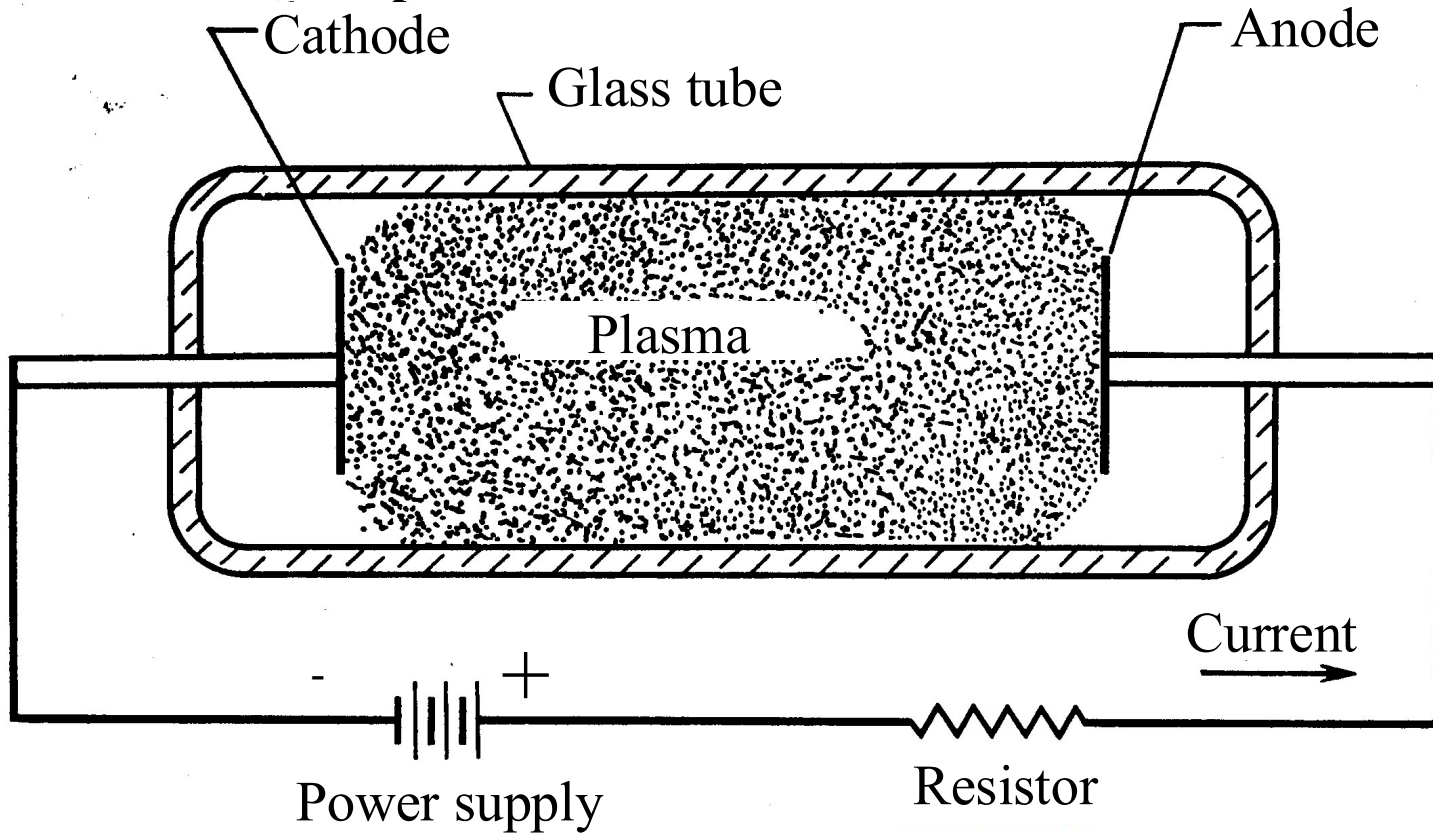


# OUR LABORATORY CAPABILITIES

- Neutral, singly and doubly ionised atomic spectra
- 1.5 m diffraction grating monochromator (Czerny-Turner)
- Diffraction grating: 2400 lines / mm
- Resolving power: 150 000 (at 450 nm)
- Setting-up a Fabry-Pérot interferometer
- Spectral range: UV-visible (200 – 800 nm)

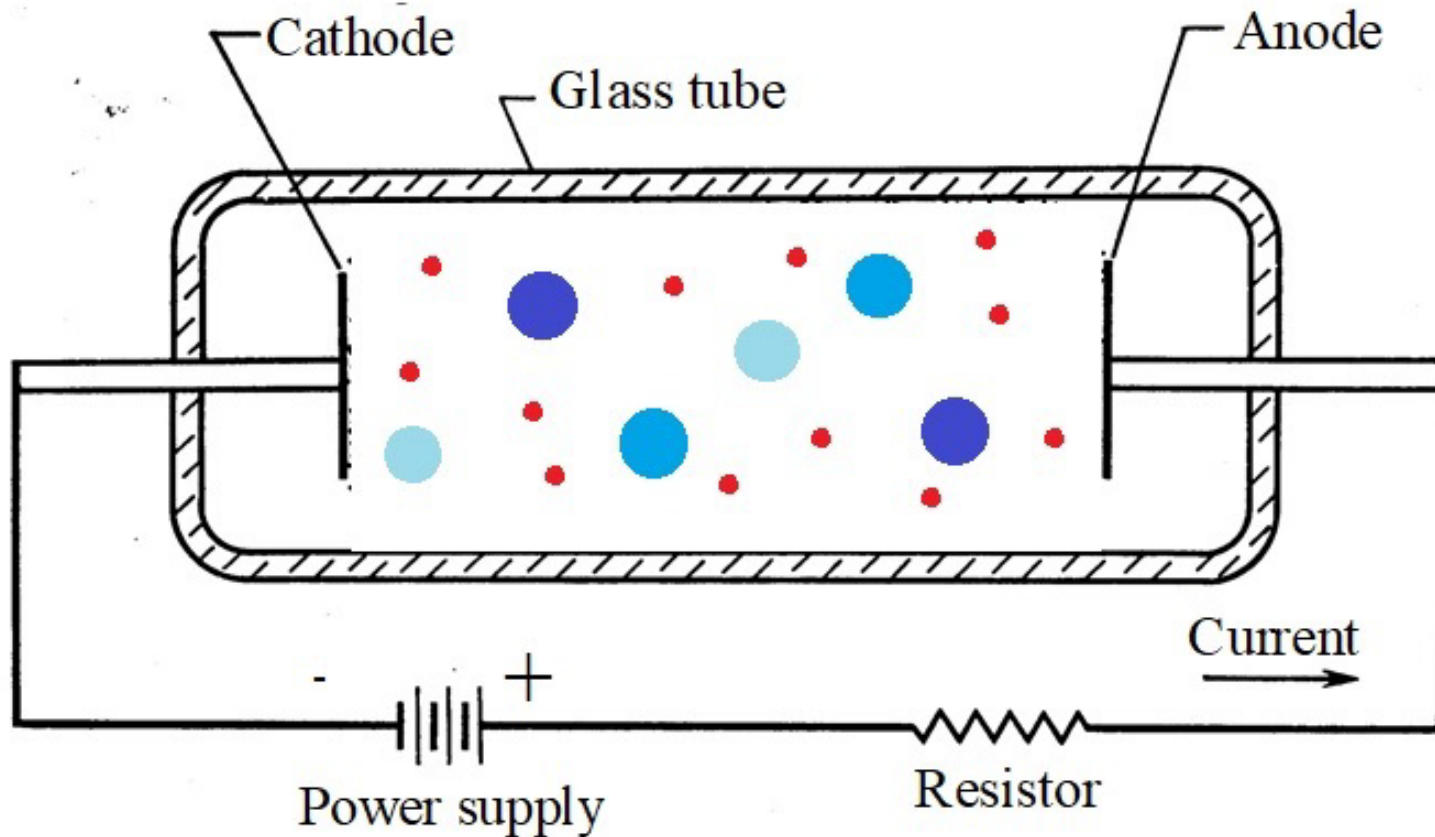


# Producing light: the LAMP

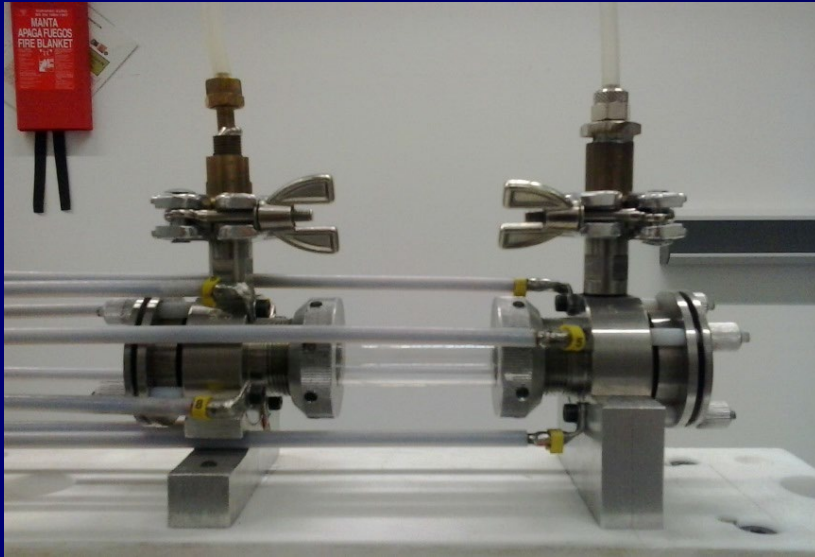




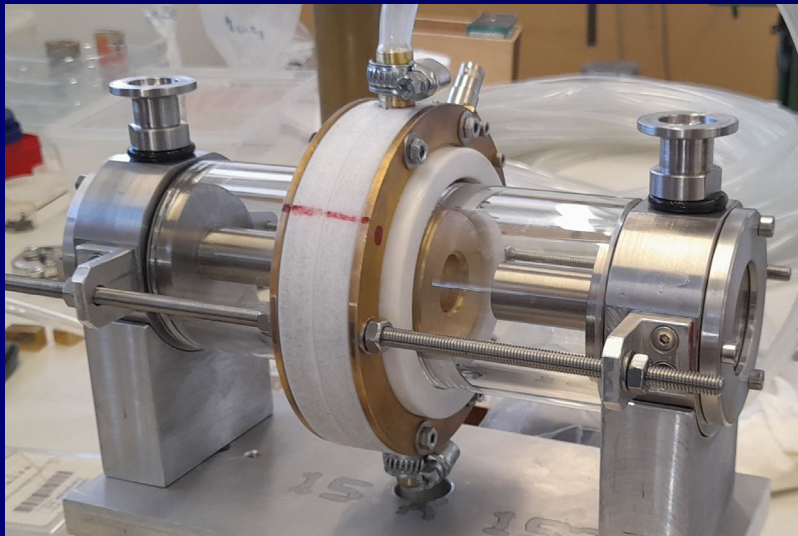
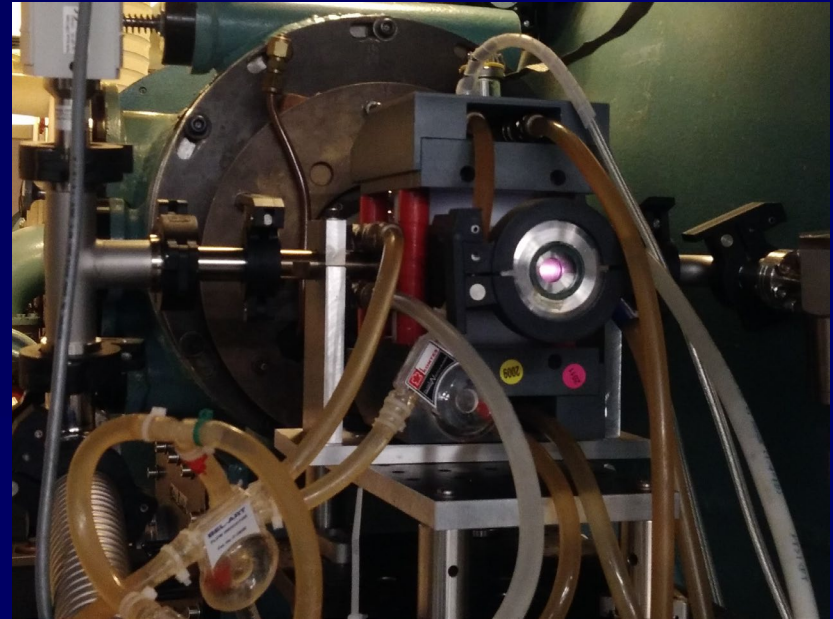
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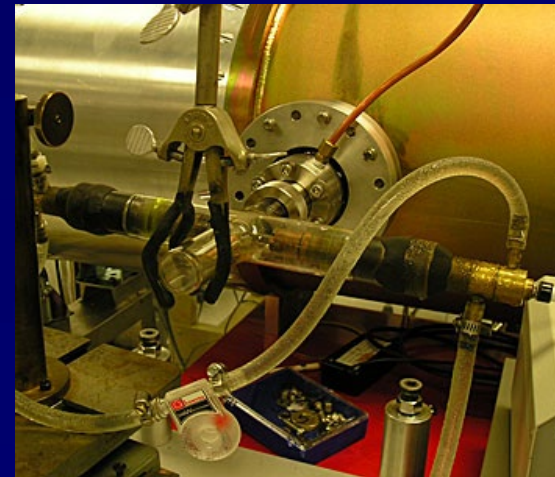
***Pulsed-discharge***



***Penning lamp***



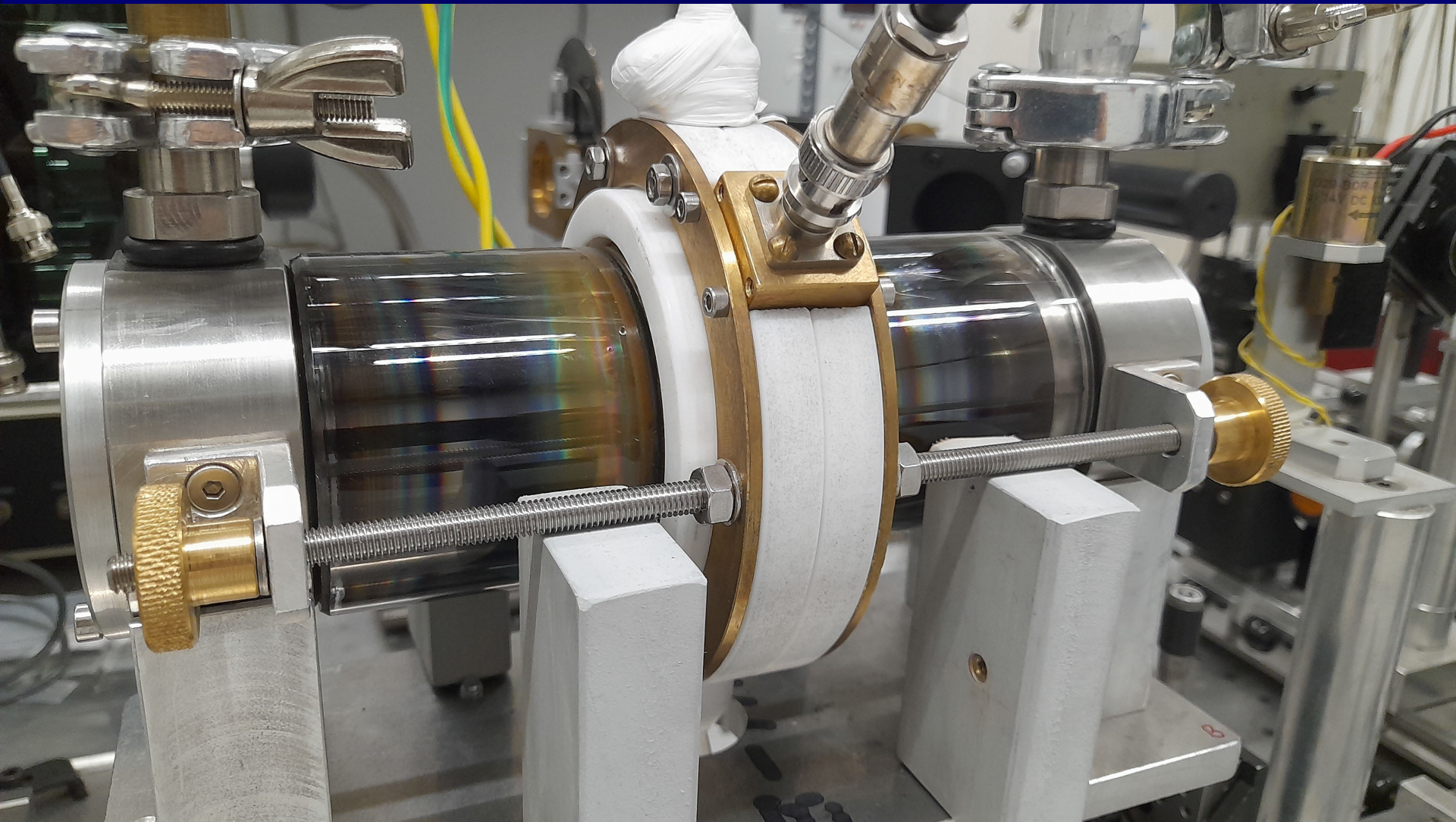
***Hollow-cathode lamp***



***Sliding spark***

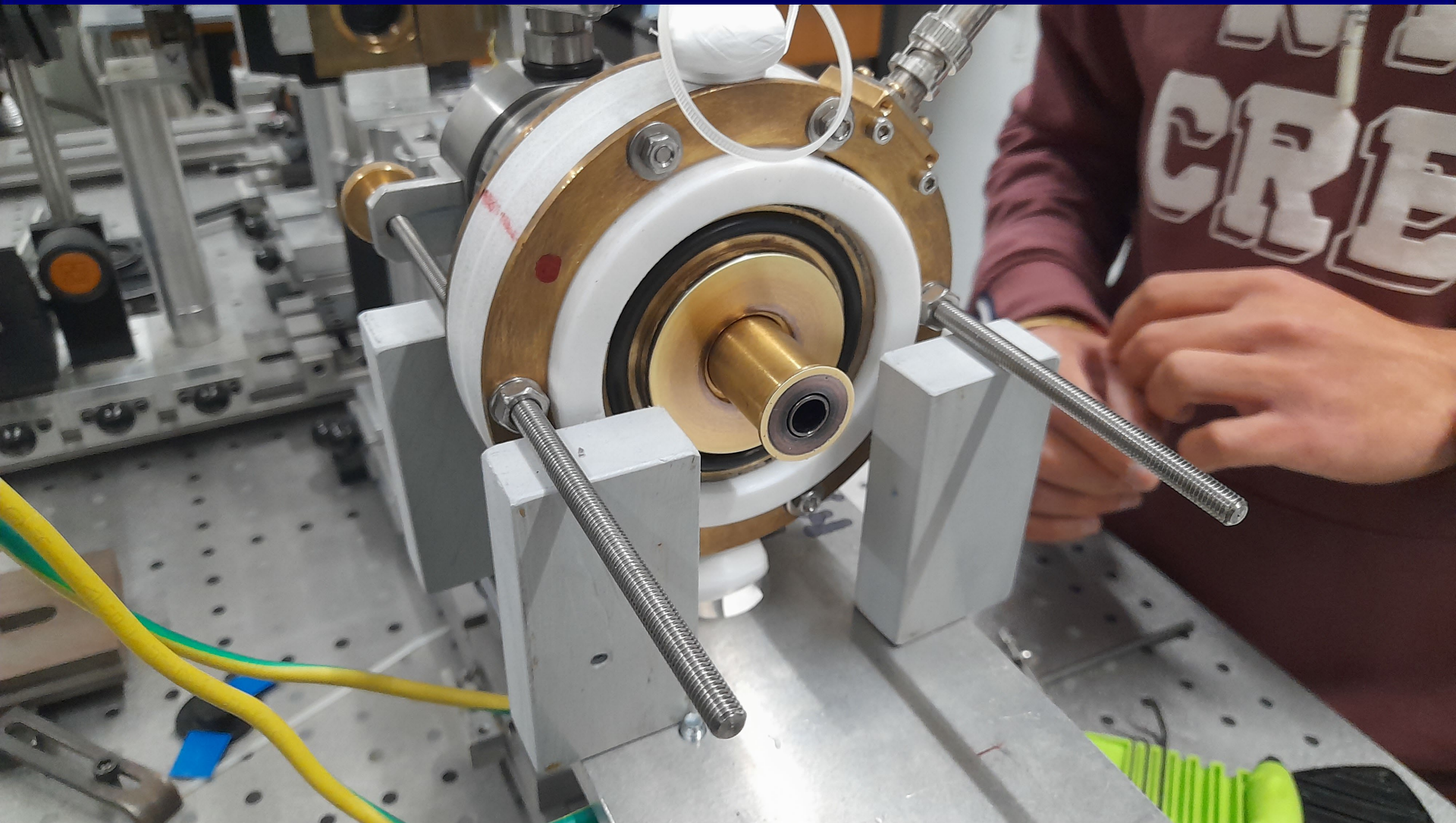


# Hollow-cathode lamp



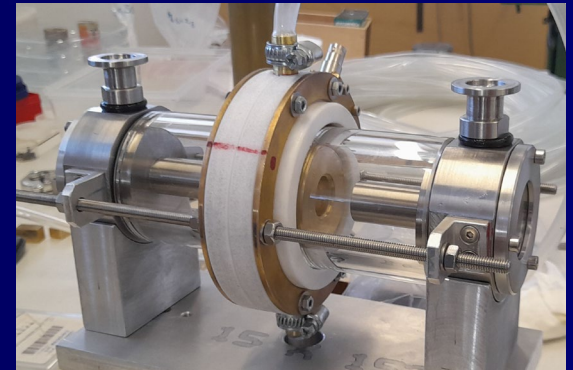


# Hollow-cathode lamp



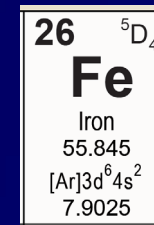
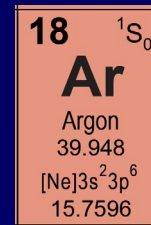
# We are characterising our hollow-cathode lamp

- Iron cathode
- Argon (Ar) as a Carrier gas
- Pressure Ar between 60 – 160 Pa
- Currents up to 750 mA



## Advantages:

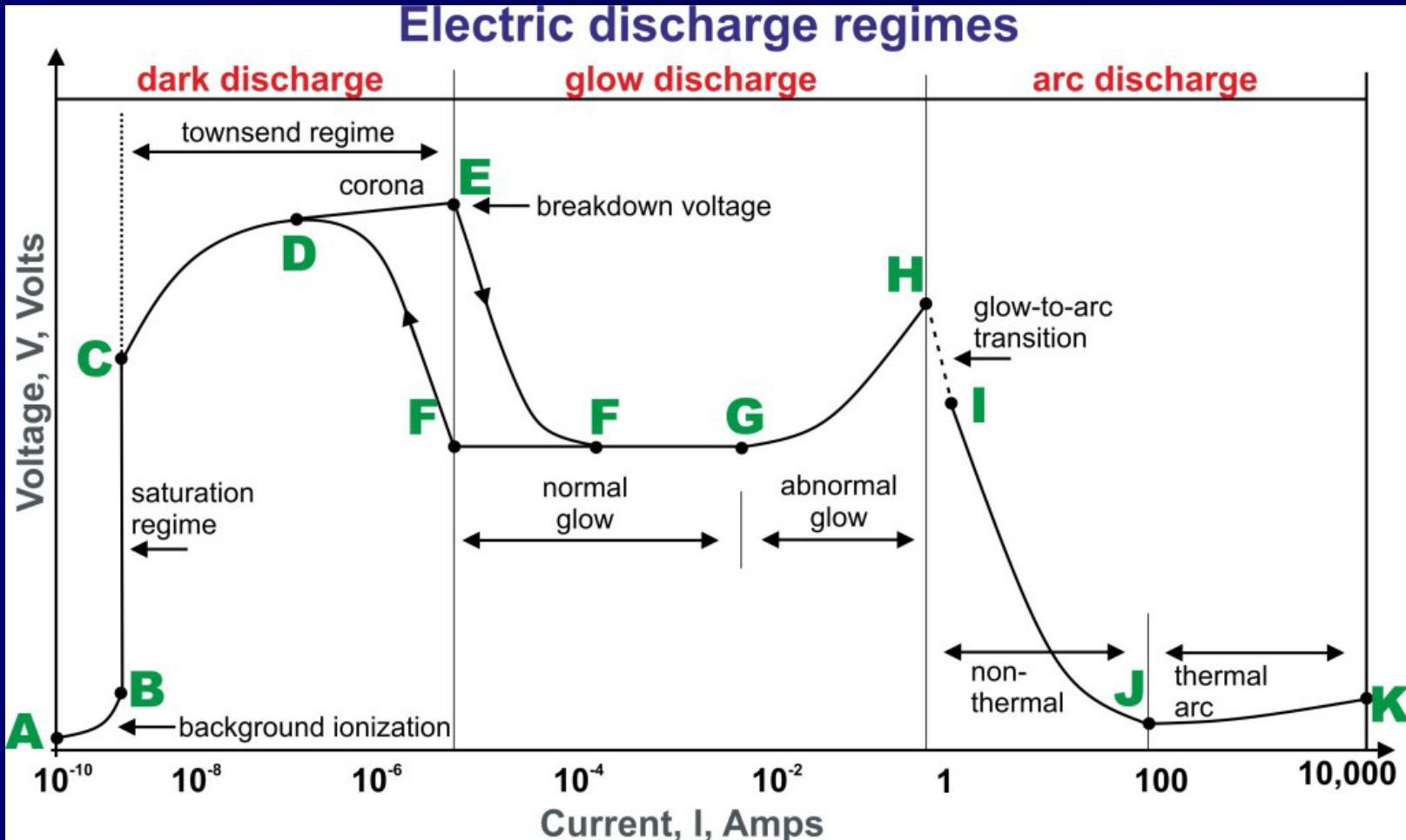
- A lot of information on wavelengths for line identification
- Good quality transition probabilities for many lines
- Branching ratios available for lines of many upper energy levels (Whaling, W., M. T. Carle, and M. L. Pitt. **JQSRT** 50.1 (1993): 7-18.)





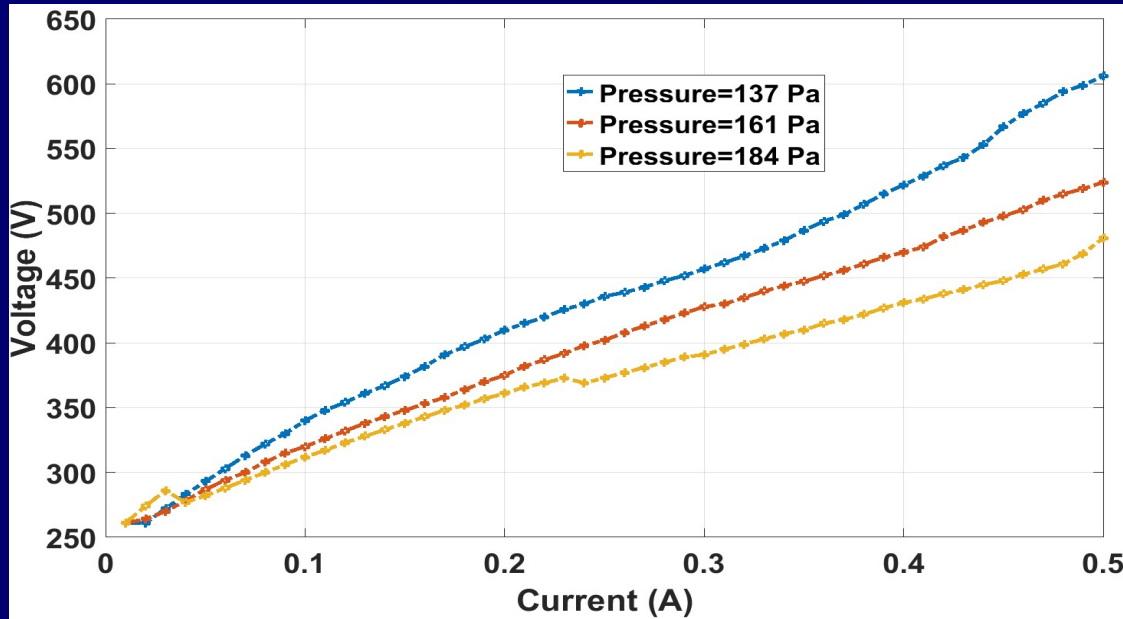


# Hollow-cathode lamp characterization

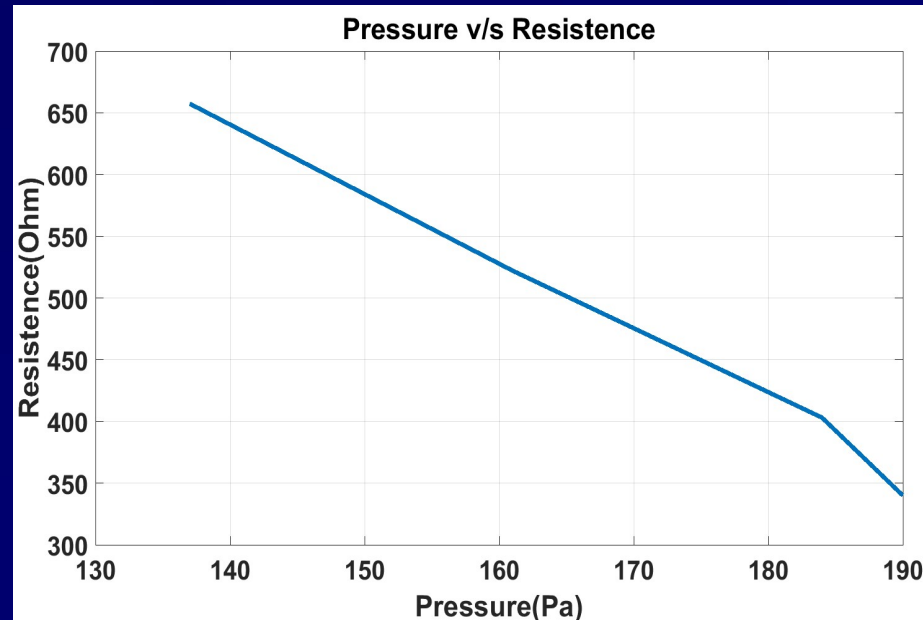


Structure of a Glow Discharge Princeton Plasma Physics Laboratory

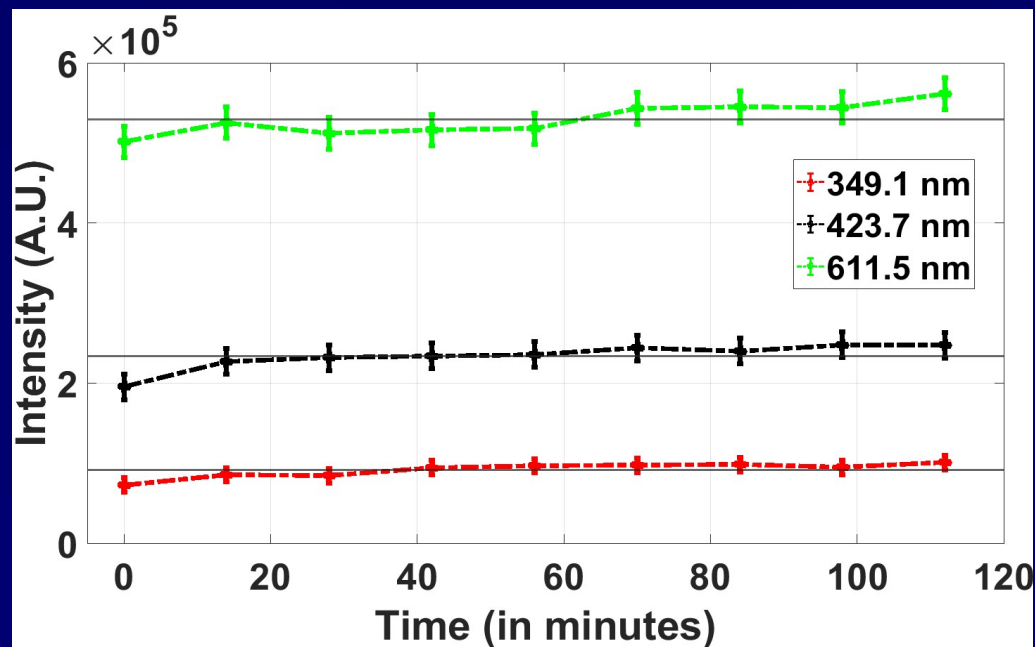
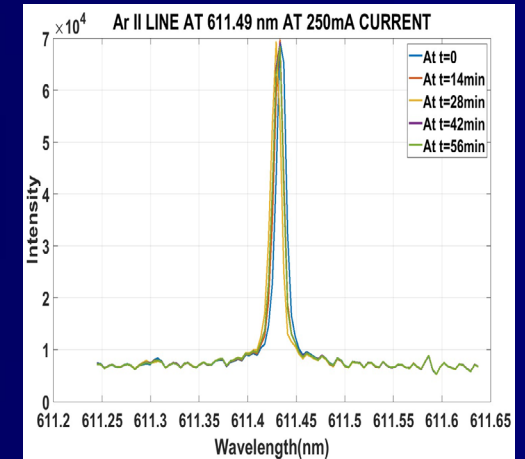
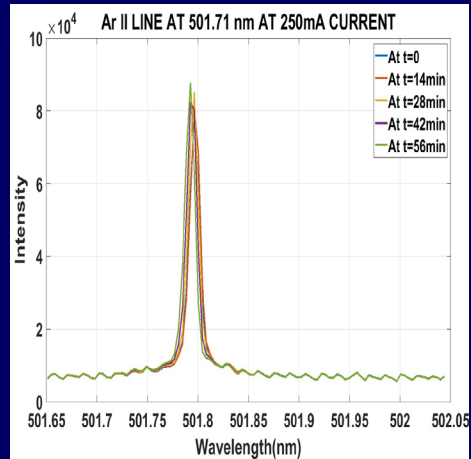
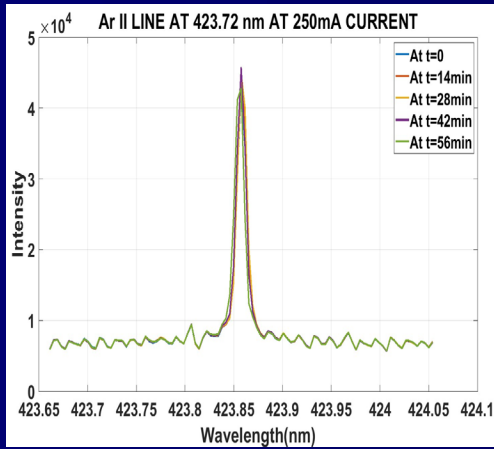
# Hollow-cathode lamp characterization



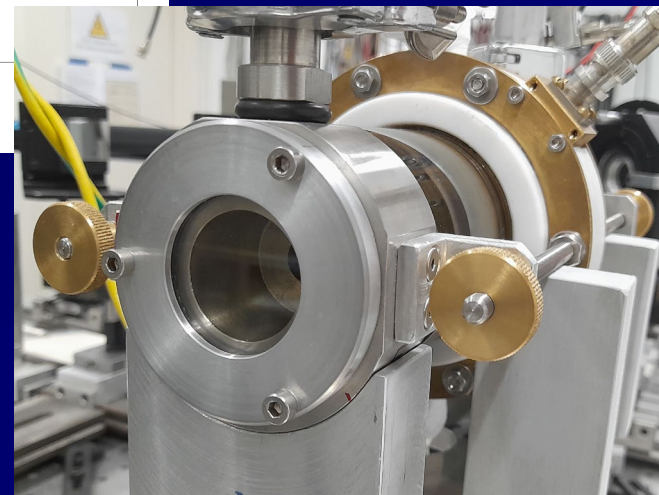
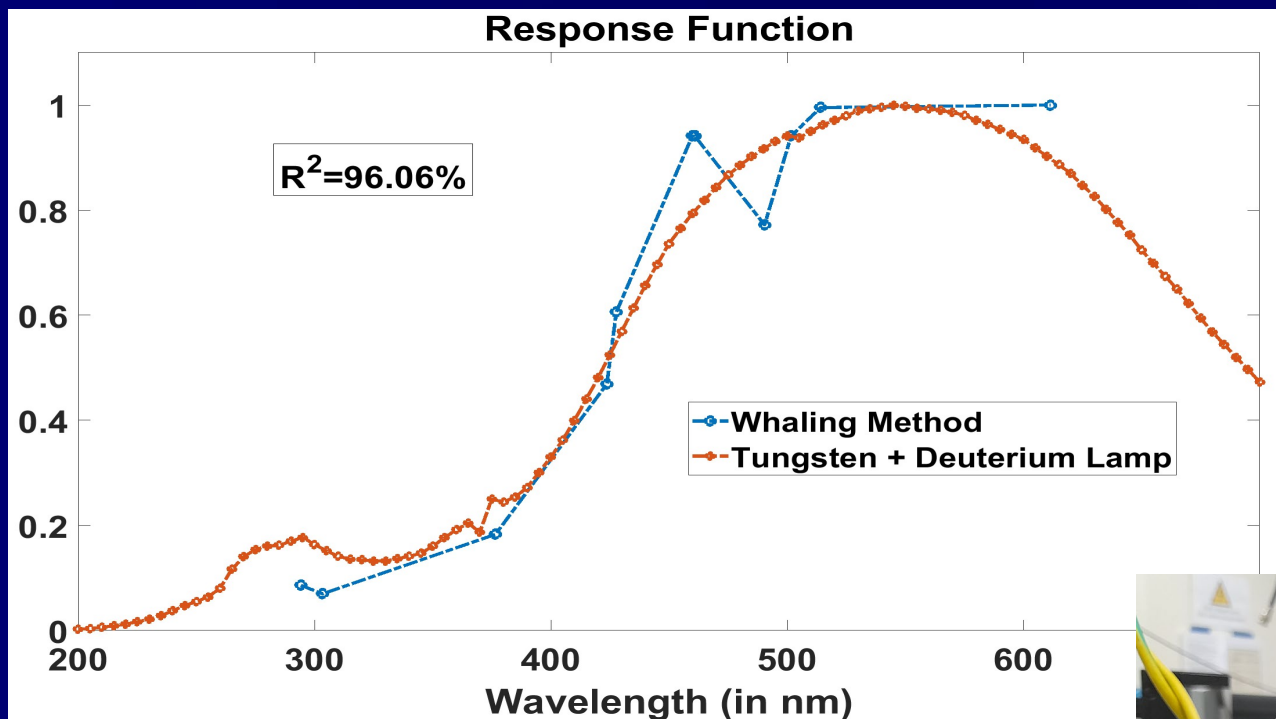
(poster P5)



# Hollow-cathode lamp characterization



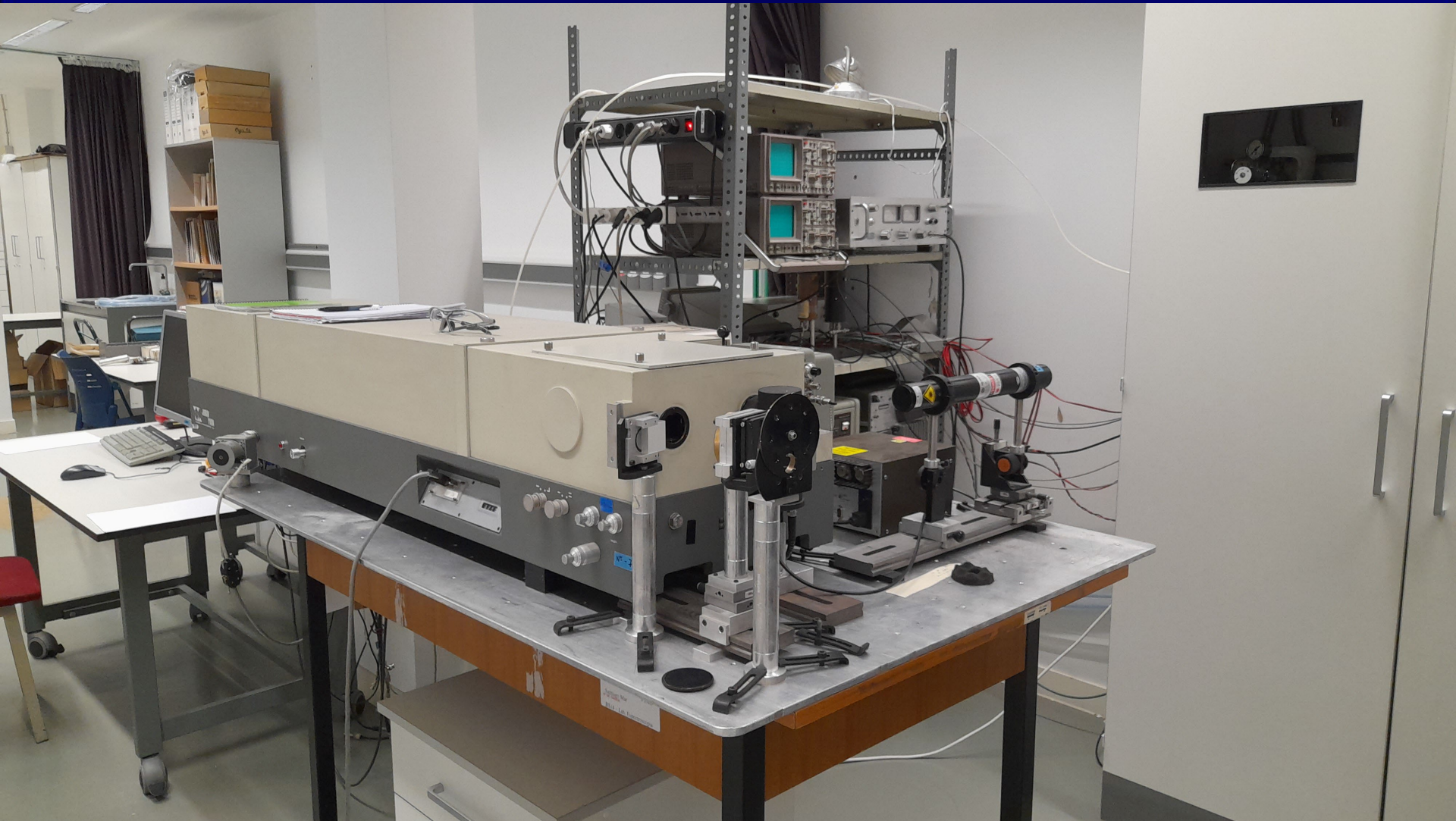
# Hollow-cathode lamp characterization



Whaling, W., M. T. Carle, and M. L. Pitt. **JQSRT** 50.1 (1993): 7-18.



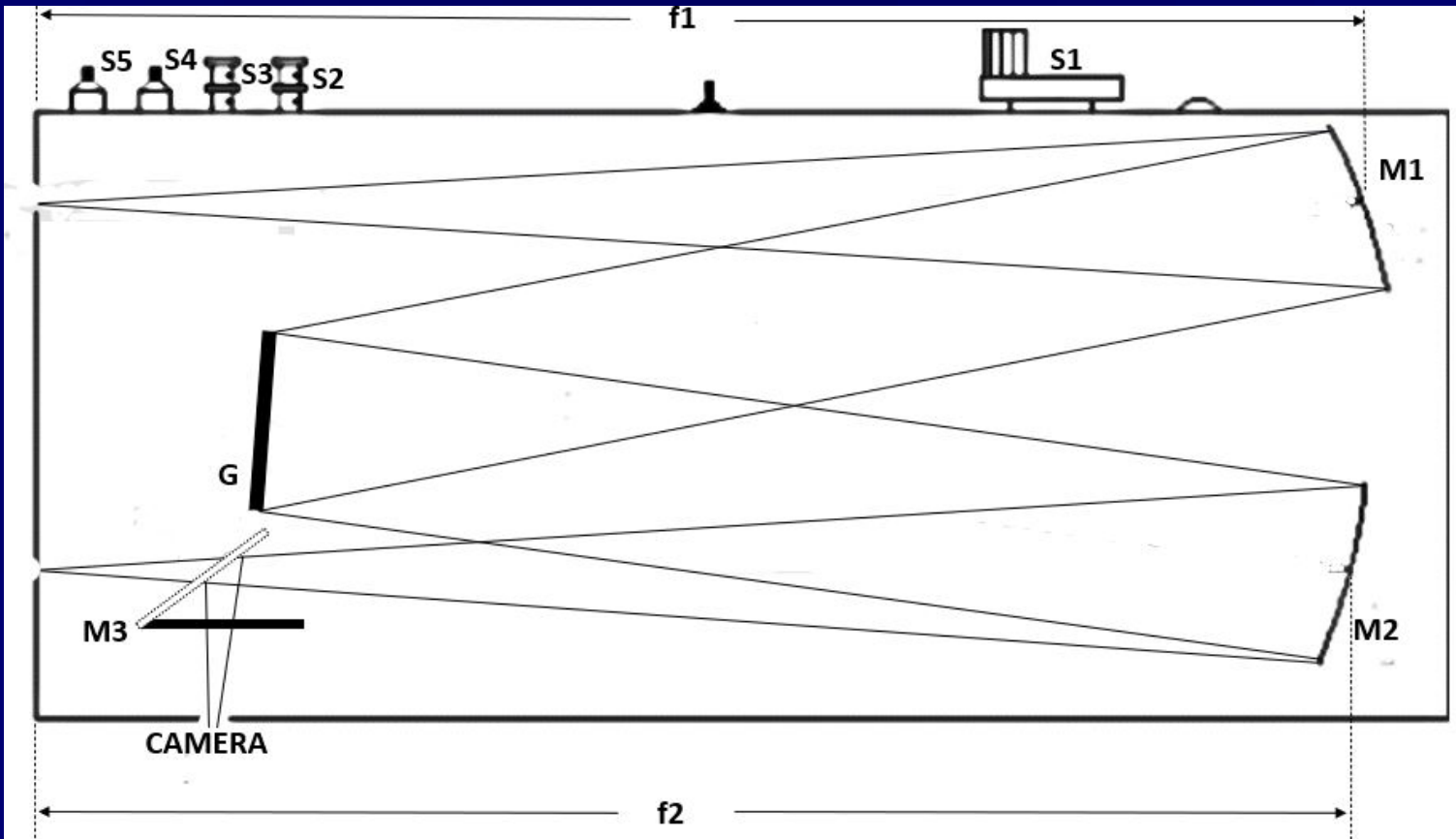
# 1.5 Jobin-Yvon HR1500 (diffraction grating 2400 lines/mm, size = 11 cm)





# 1.5 Jobin-Yvon HR1500

(diffraction grating 2400 lines/mm, size = 11 cm)



**Can I measure accurate transition probabilities  
of rare-earths?**

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**Can I measure accurate AREAS of rare-earths?**

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**Can I measure accurate AREAS of rare-earths?**



**What do I need to be able to measure areas of  
rare-earths accurately?**

# What do I need to be able to measure areas of rare-earths accurately?

- **Be able to determine the REAL number of photons emitted for a particular transition**
  - Lamp stability
  - Intensity calibration
  - Self-absorption
  - Transmittance of front window

$$I_{ul} \propto A_{ul} N_u$$

# What do I need to be able to measure areas of rare-earths accurately?

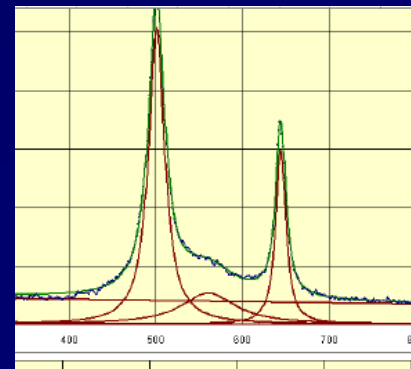
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## • **Be able to IDENTIFY lines**

Possible problems:

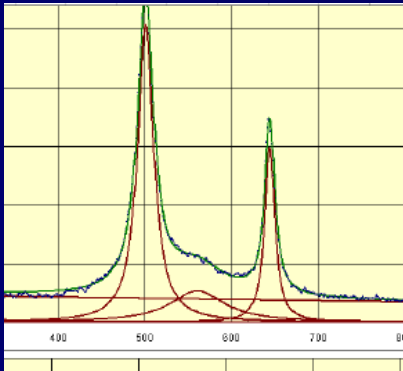
- Blends
- Weak lines (small signal-to-noise ratio)





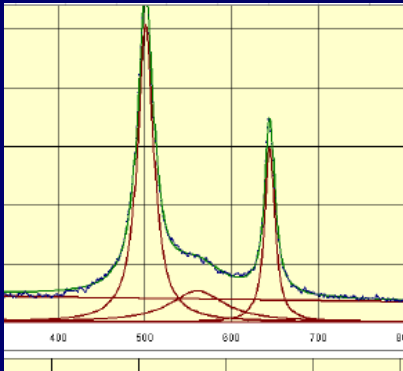


Can we RESOLVE  
different spectral lines in rare-earth  
spectra with our instrument...?





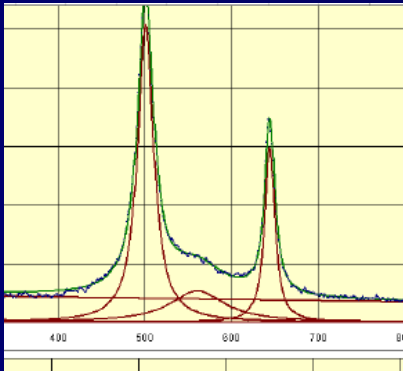
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**It depends...**



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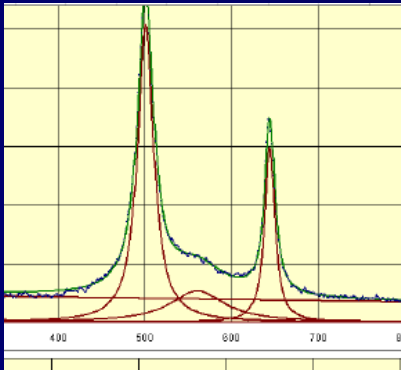
It depends...



What is the  
“intrinsic” width of  
the lines?



Can we RESOLVE  
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spectra with our instrument...?



**It depends...**

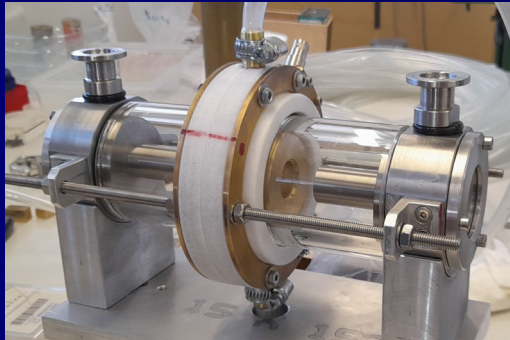


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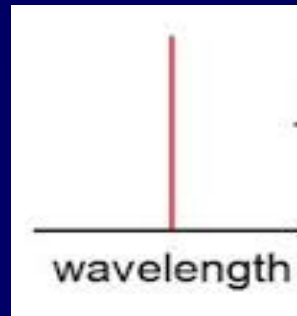
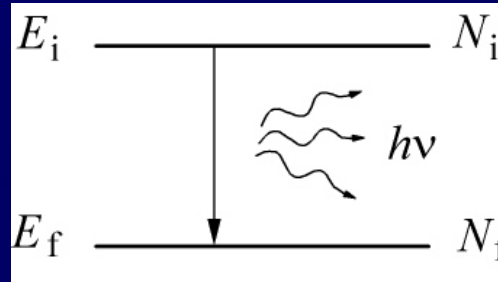
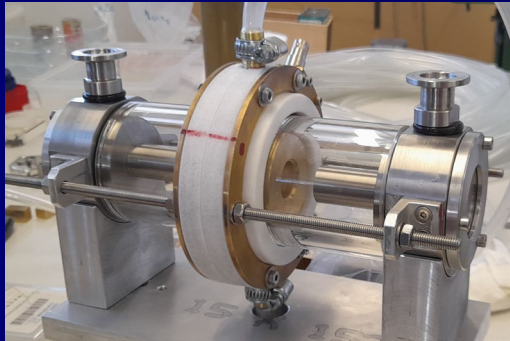


What is the  
instrumental width  
of our setup?

# LINE BROADENING: the “intrinsic width”

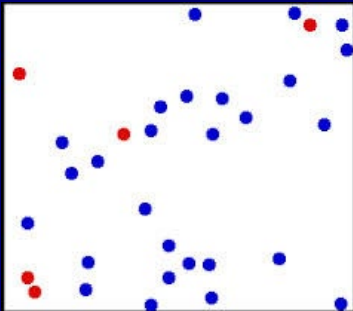
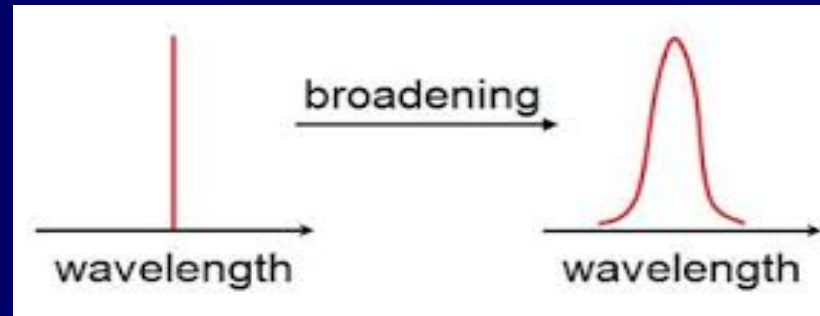
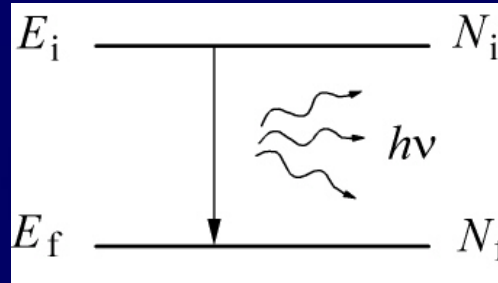
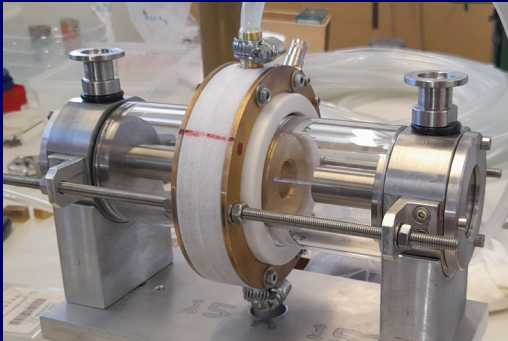


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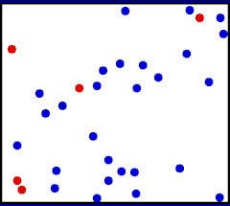




# LINE BROADENING: the “intrinsic width”



- Natural broadening (lorentzian)
- Doppler broadening (Gaussian)
- Pressure broadening (lorentzian)  
(VDW, resonance, Stark)



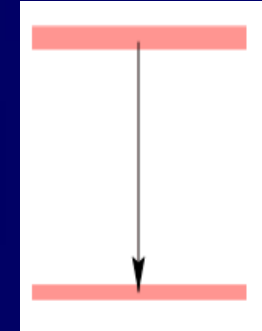
# LINE BROADENING MECHANISMS

- **Natural broadening (lorentzian)**

“INTRINSIC”  
W

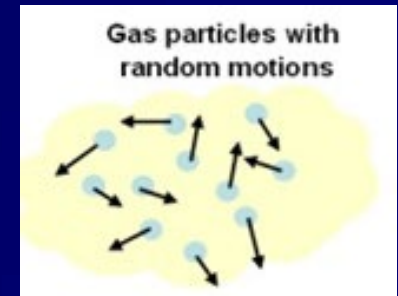
$$\Delta E \Delta t \sim \hbar$$

$$\Delta \nu \sim \frac{\Delta E}{h} \sim \frac{1}{2\pi\Delta t}$$



- **Doppler broadening (Gaussian)**

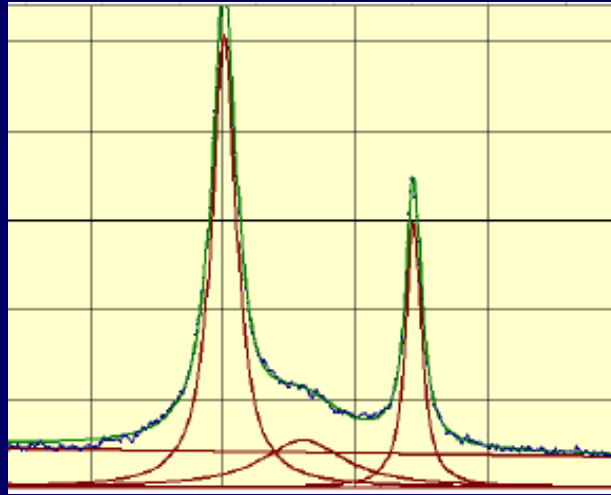
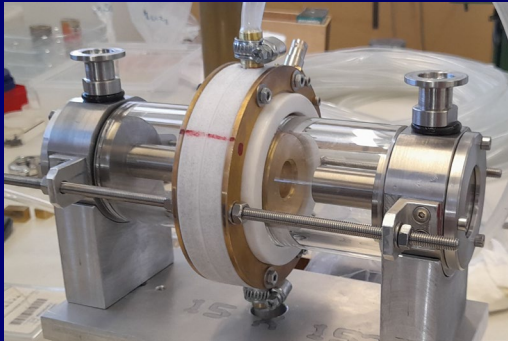
$$\Delta \lambda_D = \left( \frac{8 \ln 2 kT}{Mc^2} \right)^{\frac{1}{2}} \lambda_0 = 7.162 \cdot 10^{-7} \lambda_0 \sqrt{\frac{T}{M}}$$



- **Pressure broadening (lorentzian)**

- Van der Waals (emitter- neutral → induced dipole)
- Resonance
- Stark (emitter surrounded by charged particles)

# LINE BROADENING: the “intrinsic width”



If two lines “leave the lamp” already blended, there is nothing I can do about it, regardless of the instrument I use.



Assuming Nd III spectral lines leave the lamp unblended,

can we RESOLVE (separate) different spectral lines in rare-earth spectra  
WITH our instrument...?



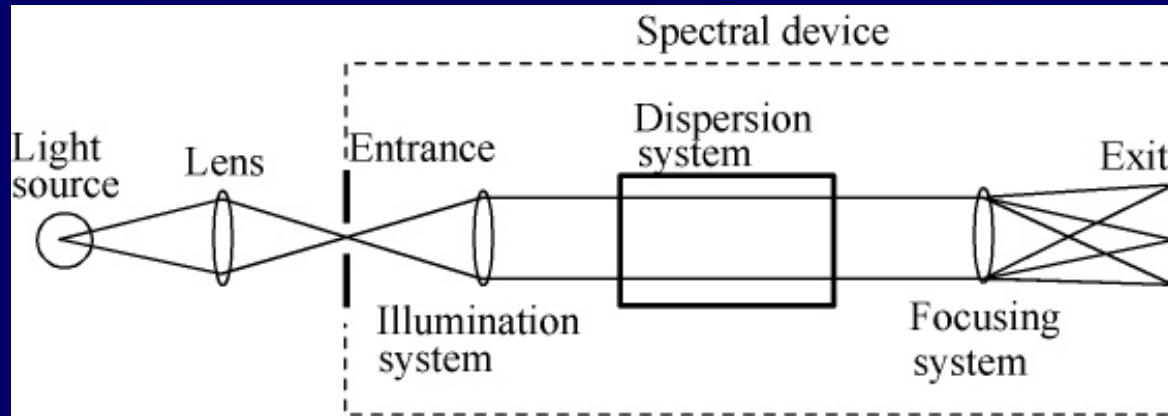
Assuming Nd III spectral lines leave the lamp unblended,

can we RESOLVE (separate) different spectral lines in rare-earth spectra WITH our instrument...?



**What is the INSTRUMENTAL WIDTH of our experiment?**

# Instrumental width (Gaussian)



- **Entrance slit (diffraction pattern one slit)**

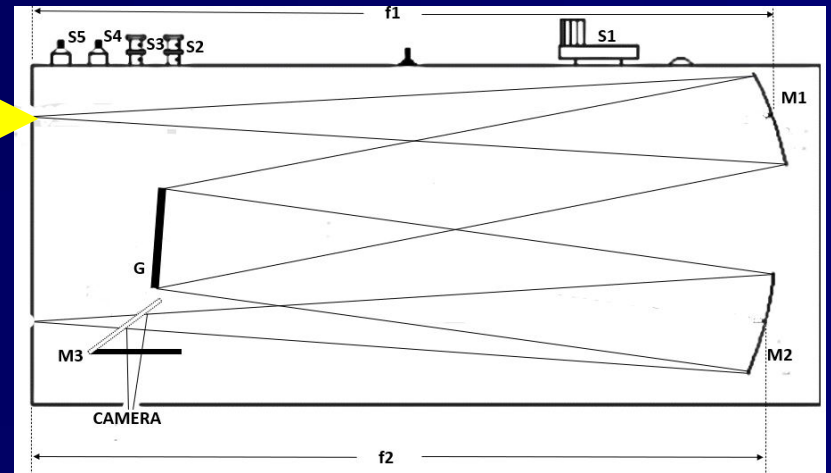
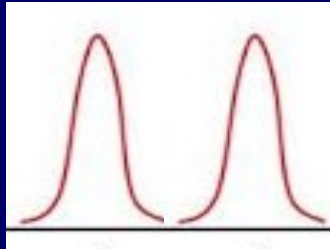
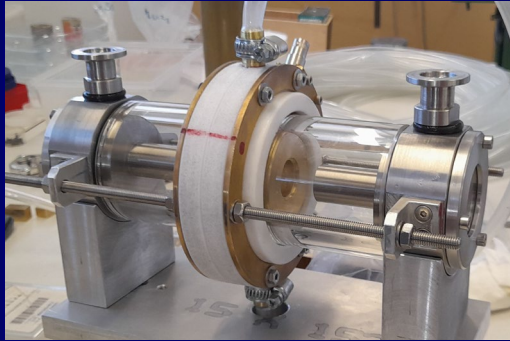
- **Resolving power diffraction grating**  
(  $R = 264\,000$ ,  $0.001\text{ nm}$  at  $260\text{ nm}$  )

$$R = \frac{\lambda}{(\Delta\lambda)_{\min}} = m N$$

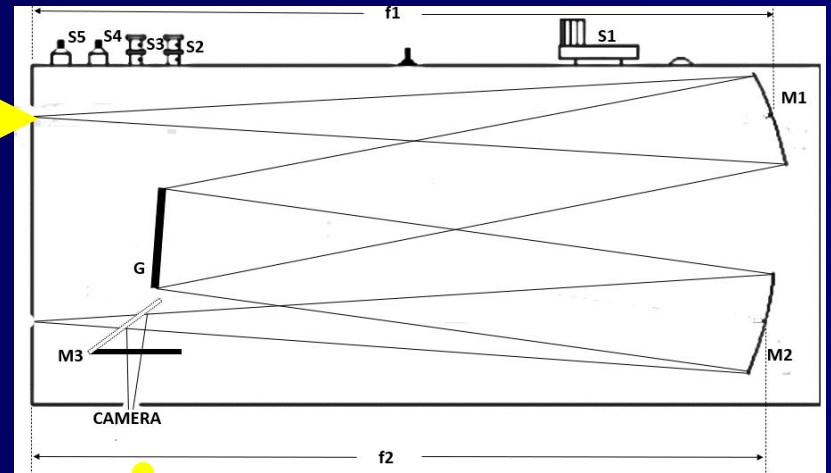
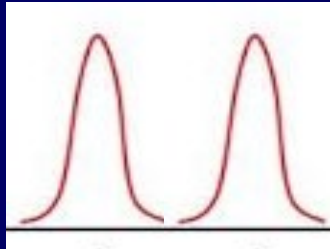
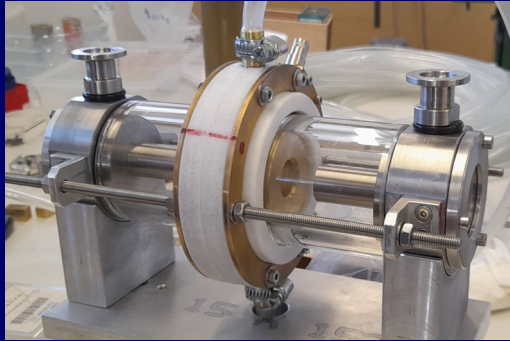
- **Diffraction pattern circular aperture (Airy)**



# INSTRUMENTAL WIDTH

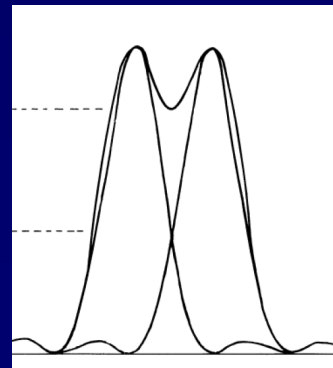
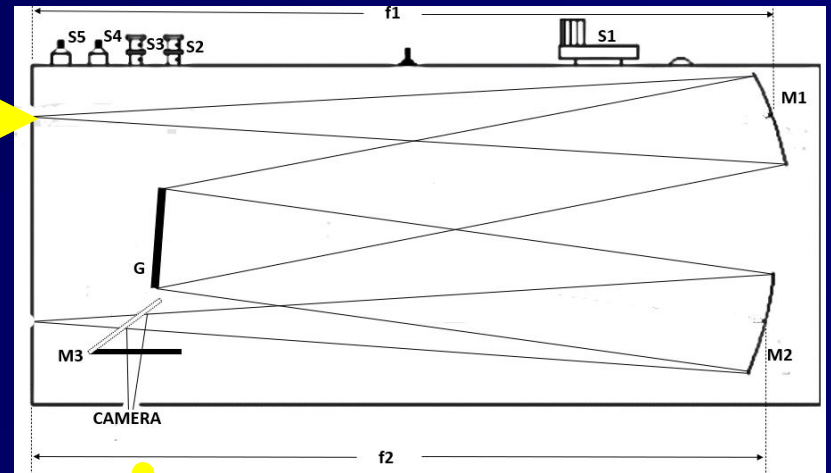
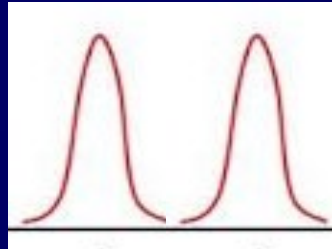
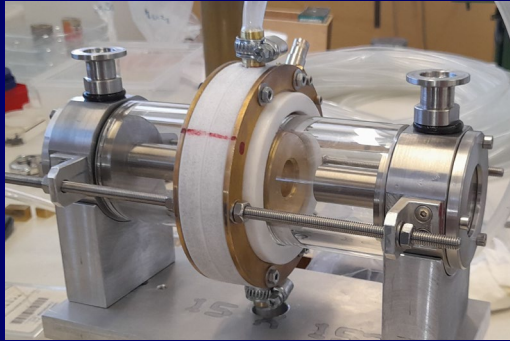


# INSTRUMENTAL WIDTH



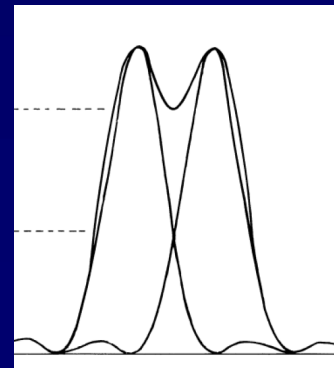
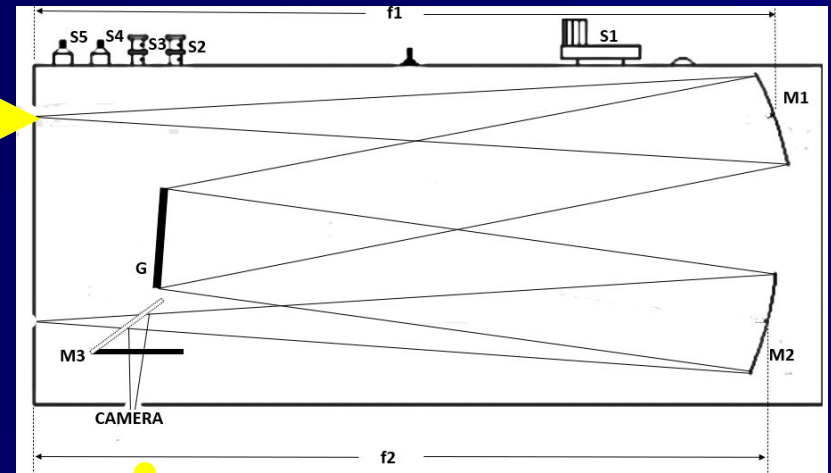
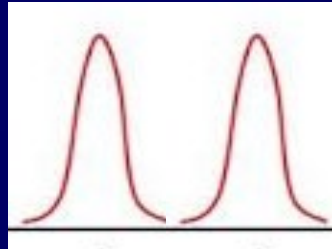
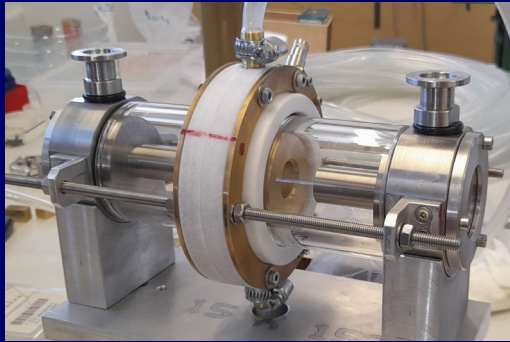
??

# INSTRUMENTAL WIDTH



??

# INSTRUMENTAL WIDTH

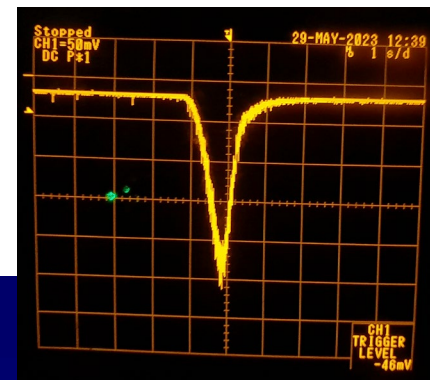
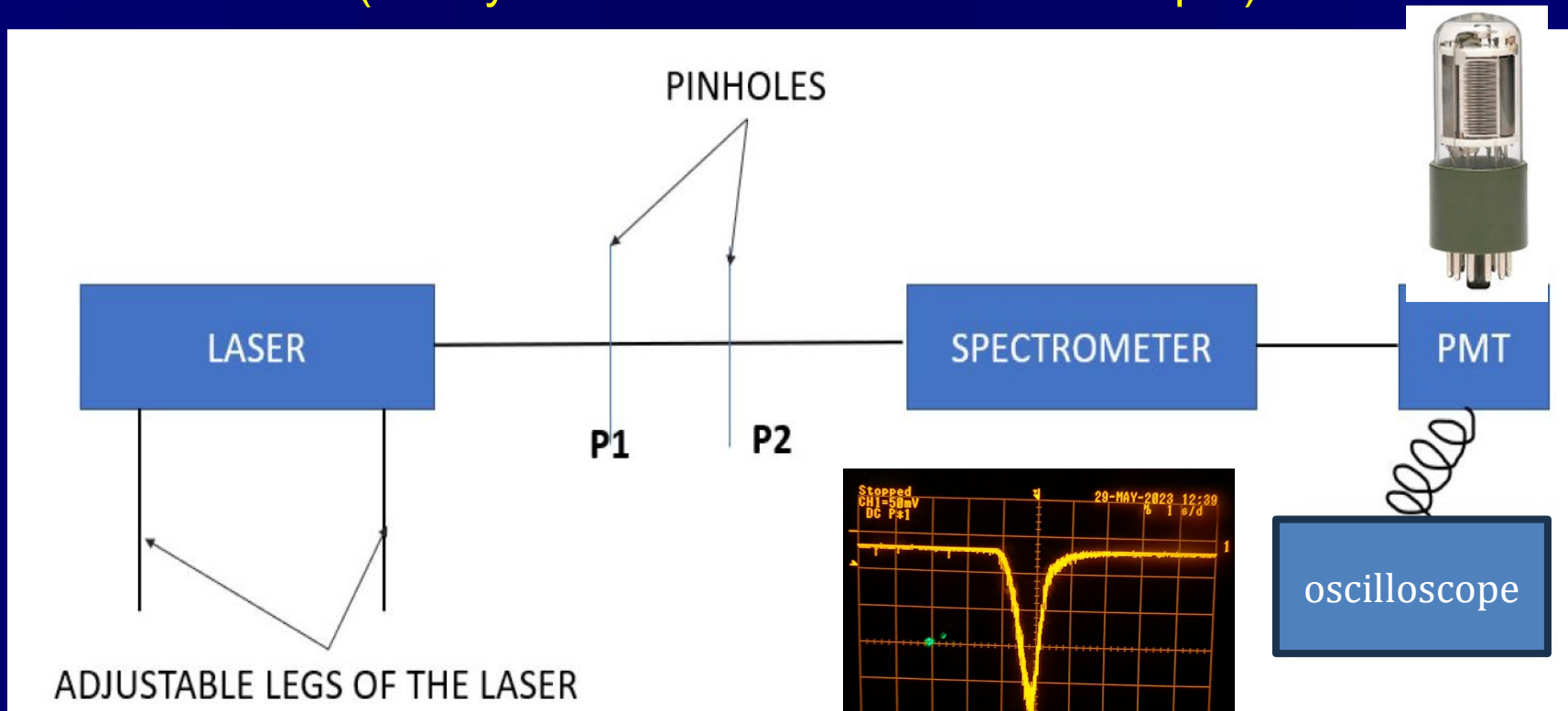


??

**This is what we want  
to avoid!**

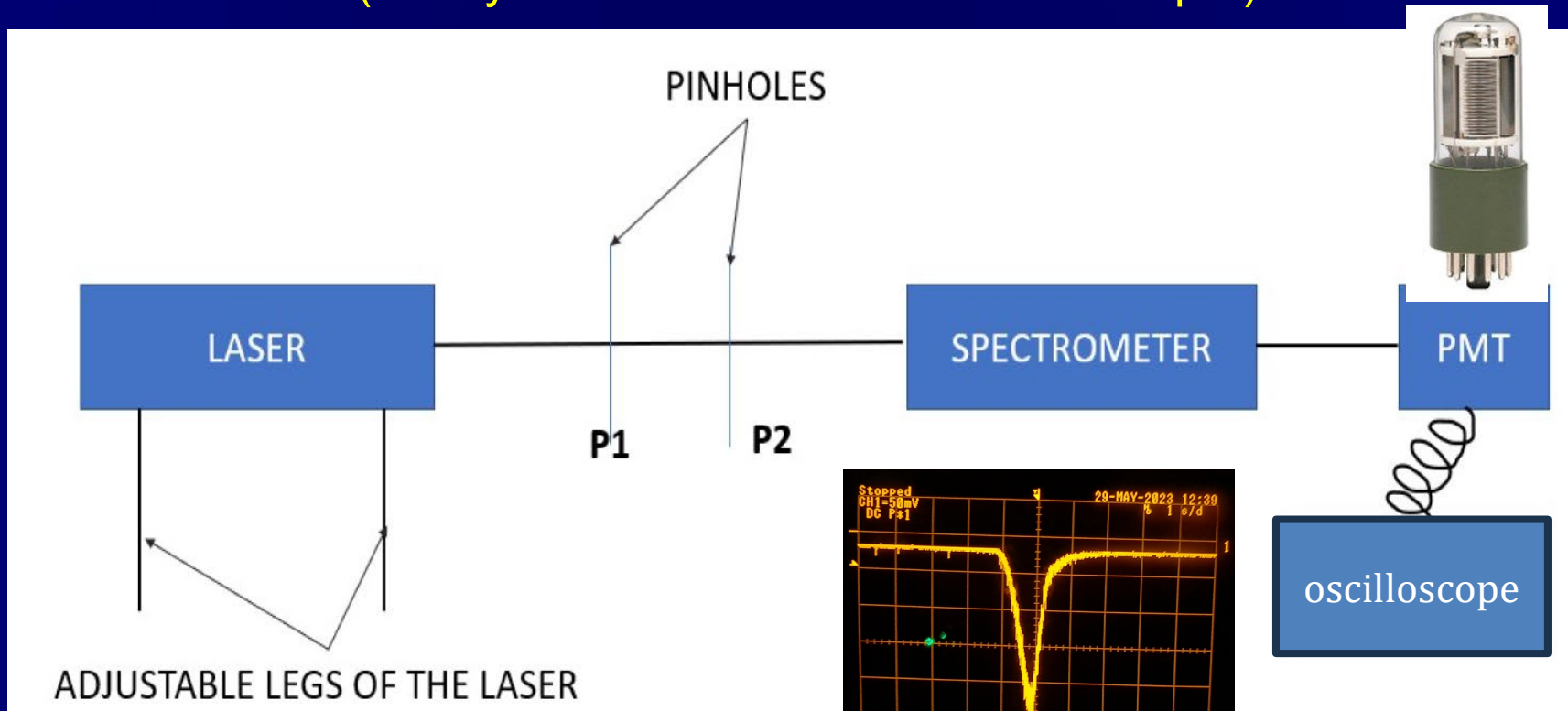
# Measuring the instrumental width of our monochromator

(theory told us instrumental width is 4 pm)



# Measuring the instrumental width of our monochromator

(theory told us instrumental width is 4 pm)



**Great influence of alignment!**

You can reduce your instrumental width from 8 to 4 pm by aligning!



## Using photomultiplier tube (PMT) as detector

Green laser	543.5 nm	4 pm
Ar II (from HCL)	460 nm	10 pm

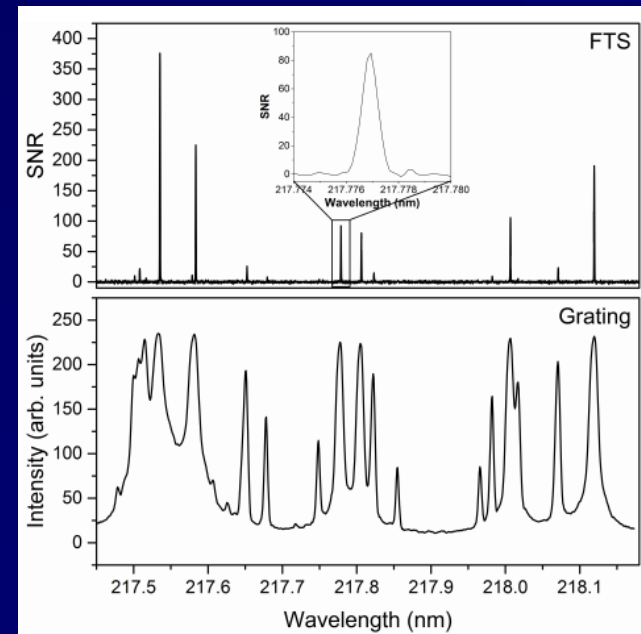
## Using OMA2 (pixel size = 25 $\mu\text{m}$ ) as detector

Green laser	543.5 nm	4 pm
Ar II (from HCL)	460 nm	36 pm

- **Importance of the characteristics of the detector (pixel size, blooming). →**

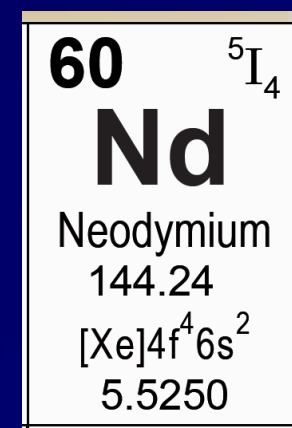
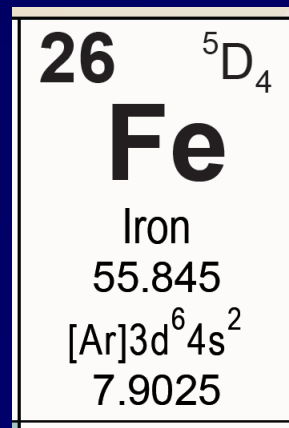
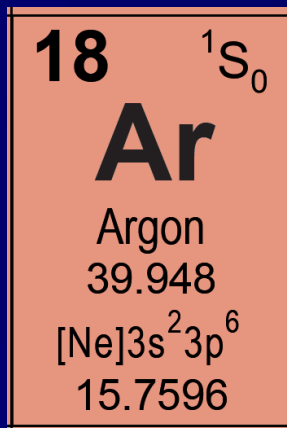
**We are upgrading to a new CMOS camera (pixel size = 6.5  $\mu\text{m}$ )**

*Clear, C.P., The Spectrum and Term Analysis of Singly Ionised Nickel. Ph.D. Thesis, Imperial College London, 2018.*

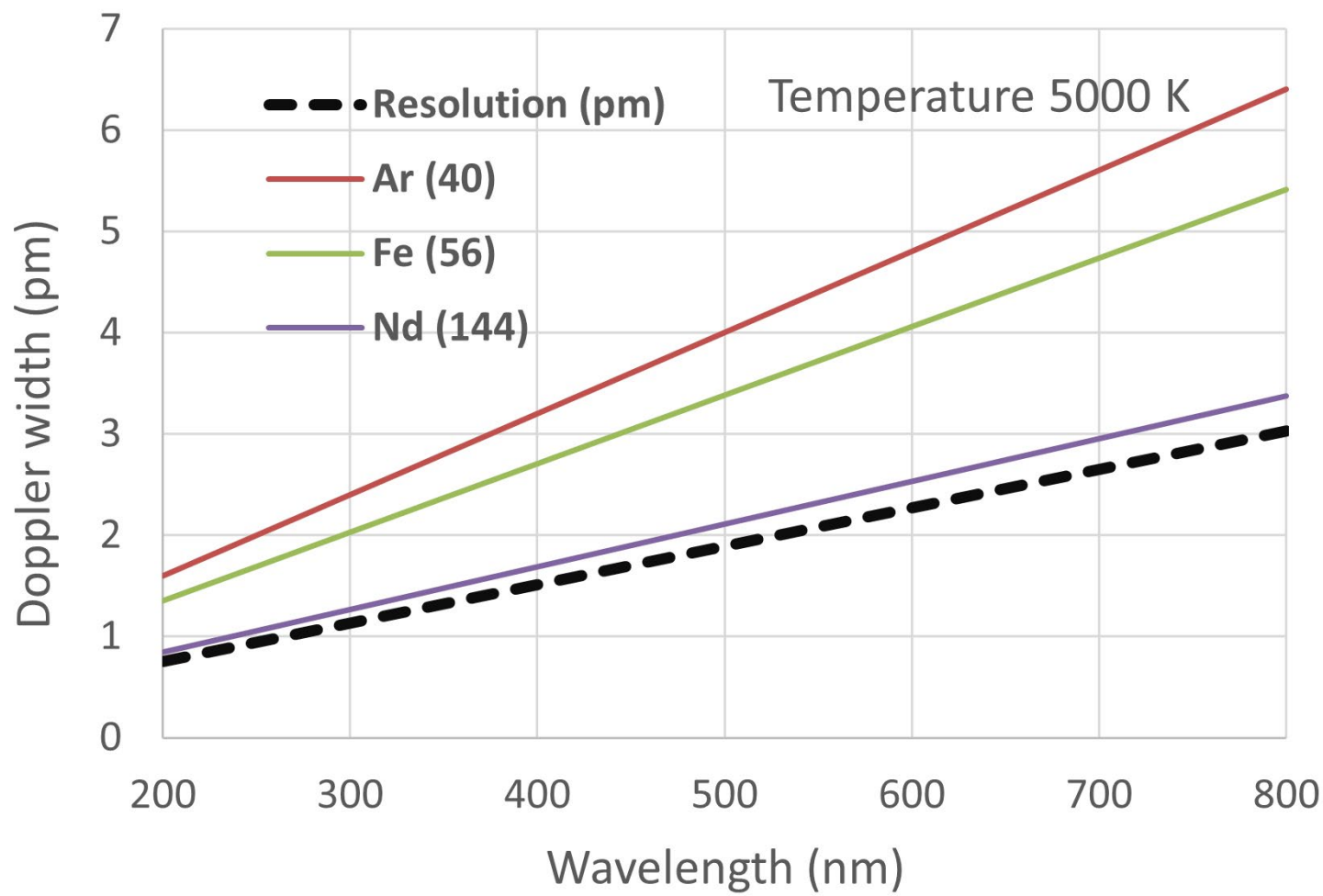


# Doppler width for rare-earths

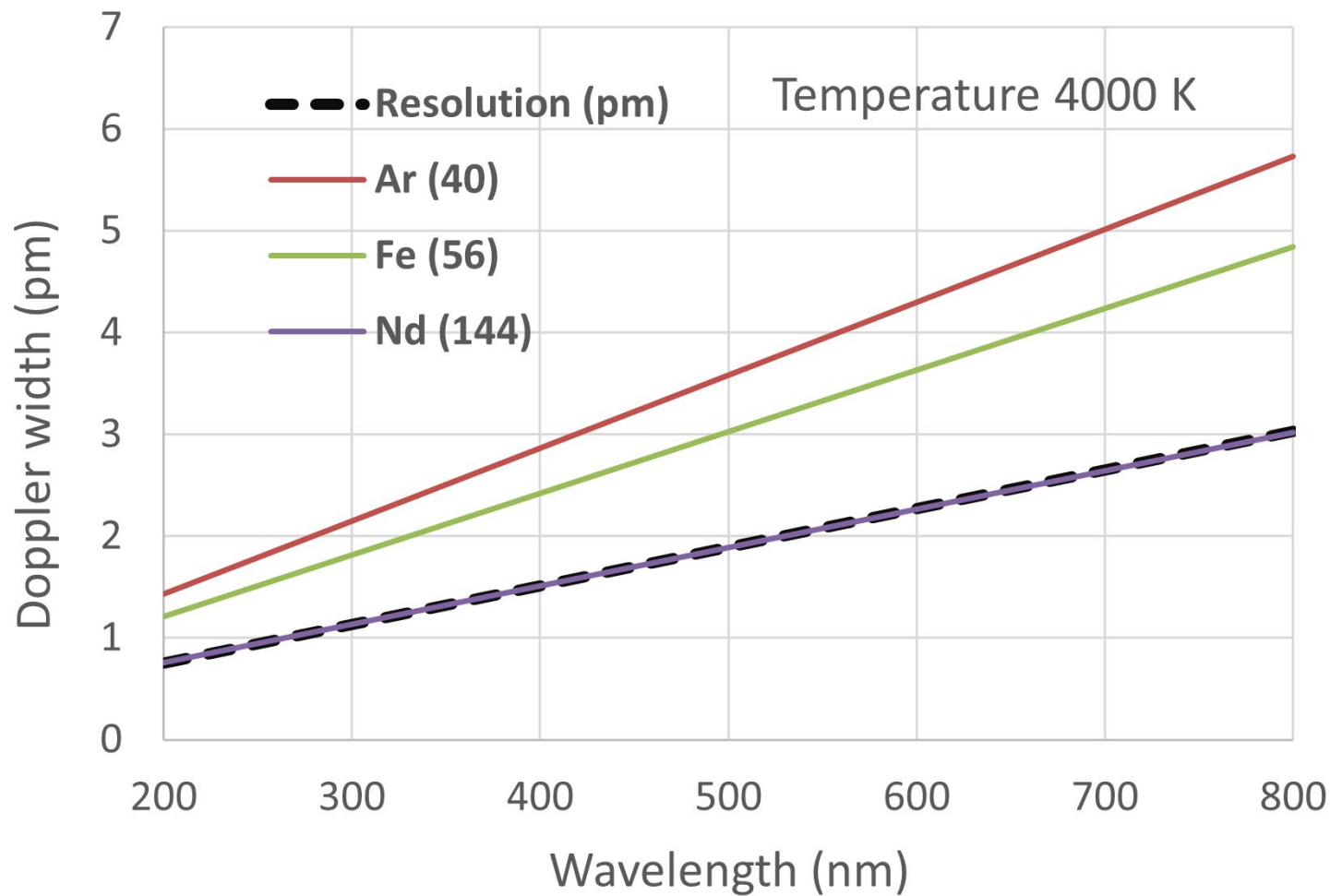
$$\Delta\lambda_D = \left( \frac{8 \ln 2 kT}{Mc^2} \right)^{\frac{1}{2}} \lambda_0 = 7.162 \cdot 10^{-7} \lambda_0 \sqrt{\frac{T}{M}}$$



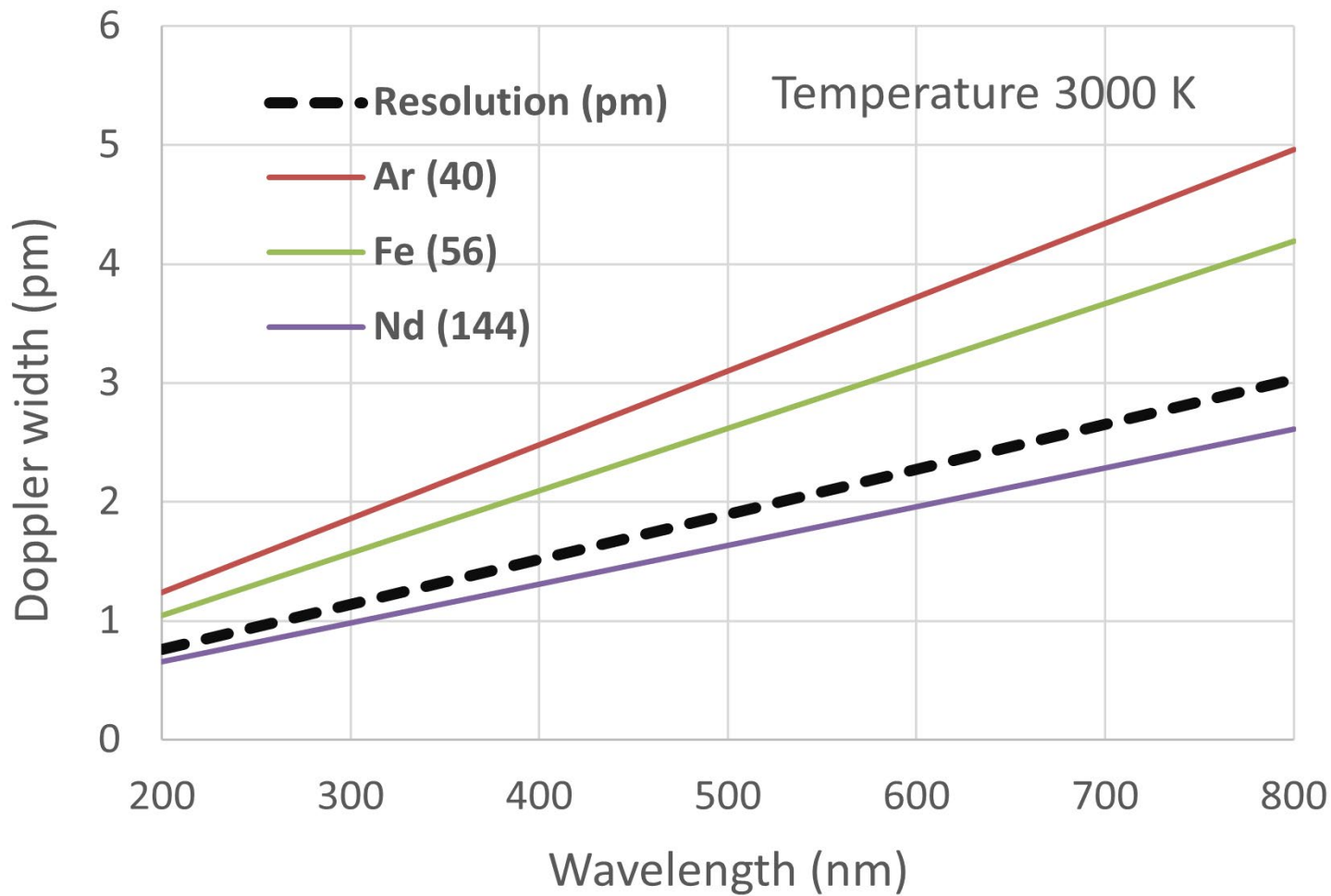
# Doppler width



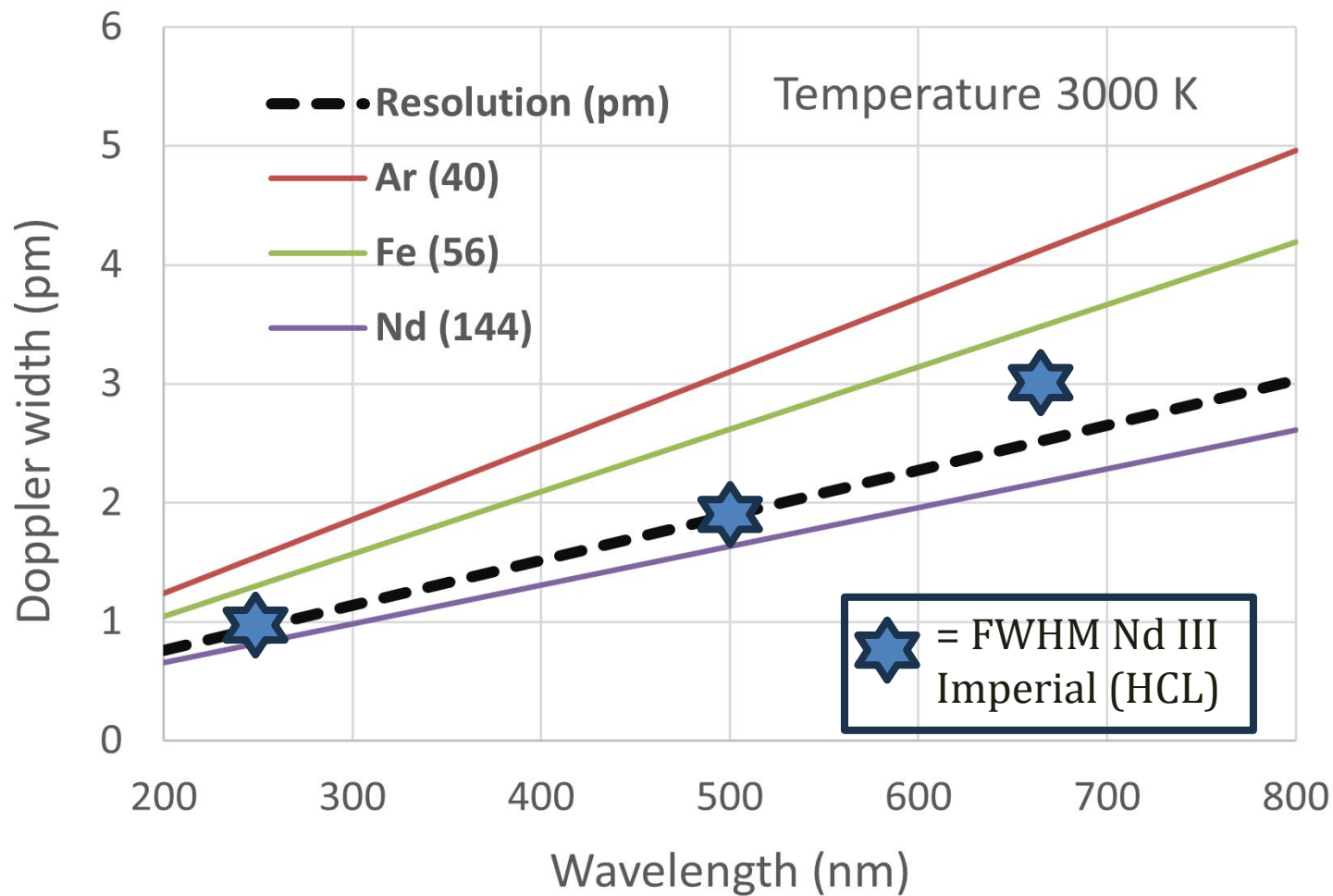
# Doppler width



# Doppler width



# Doppler width





# Atomic Properties of the Elements

Physical Measurement Laboratory [www.nist.gov/pml](http://www.nist.gov/pml)  
Standard Reference Data [www.nist.gov/srd](http://www.nist.gov/srd)

FREQUENTLY USED FUNDAMENTAL PHYSICAL CONSTANTS<sup>1</sup>

1 second = 9 192 631 770 periods of radiation corresponding to the transition between the two hyperfine levels of the ground state of <sup>133</sup>Cs

speed of light in vacuum	<i>c</i>	299 792 458 m s <sup>-1</sup>	(exact)
Planck constant	<i>h</i>	6.626 070 15 × 10 <sup>-34</sup> J Hz <sup>-1</sup>	(exact)
elementary charge	<i>e</i>	1.602 176 634 × 10 <sup>-19</sup> C	(exact)
Avogadro constant	<i>N<sub>A</sub></i>	6.022 140 76 × 10 <sup>23</sup> mol <sup>-1</sup>	(exact)
Boltzmann constant	<i>k</i>	1.380 649 × 10 <sup>-23</sup> J K <sup>-1</sup>	(exact)
electron volt	eV	1.602 176 634 × 10 <sup>-19</sup> J	(exact)
electron mass	<i>m<sub>e</sub></i>	9.109 383 70 × 10 <sup>-31</sup> kg	(exact)
energy equivalent	<i>m<sub>e</sub>c<sup>2</sup></i>	0.510 998 950 MeV	(exact)
proton mass	<i>m<sub>p</sub></i>	1.672 621 9 × 10 <sup>-27</sup> kg	(exact)
energy equivalent	<i>m<sub>p</sub>c<sup>2</sup></i>	938.272 088 MeV	(exact)
fine-structure constant	<i>α</i>	7.297 352 5698 × 10 <sup>-3</sup>	(exact)

<sup>2</sup>For the most accurate values of these and other constants, visit [pml.nist.gov/constants](http://pml.nist.gov/constants).

**CHALLENGE WITH RARE-EARTHS!**  
**(crowded spectra, narrow lines!)**

Group 1 IA	1 <sup>1</sup> H Hydrogen 1.008 1s 13.5984	2 IIA	FREQUENTLY USED FUNDAMENTAL PHYSICAL CONSTANTS <sup>1</sup>																13	14	15	16	17 VIIA	18 VIII A																													
	3 <sup>3</sup> Li Lithium 6.94 1s <sup>2</sup> 2s 5.3917	4 <sup>4</sup> Be Beryllium 9.0122 1s <sup>2</sup> 2s <sup>2</sup> 9.3227	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36																			
3	11 <sup>11</sup> Na Sodium 22.98976928 [Ne]3s <sup>1</sup>	12 <sup>12</sup> Mg Magnesium 24.304694 [Ne]3s <sup>2</sup>	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54									
4	19 <sup>19</sup> K Potassium 39.0983 [Ar]4s <sup>1</sup>	20 <sup>20</sup> Ca Calcium 40.078 [Ar]4s <sup>2</sup>	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71
5	37 <sup>37</sup> Rb Rubidium 85.468 [Kr]5s <sup>1</sup>	38 <sup>38</sup> Sr Strontium 87.62 [Kr]5s <sup>2</sup>	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86			
6	55 <sup>55</sup> Cs Cesium 132.91 [Xe]6s <sup>1</sup>	56 <sup>56</sup> Ba Barium 137.33 [Xe]6s <sup>2</sup>	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100	101	102	103				
7	87 <sup>87</sup> Fr Francium (223) [Rn]7s <sup>1</sup> 4.0727	88 <sup>88</sup> Ra Radium (226) [Rn]7s <sup>2</sup> 5.2784	89	90	91	92	93	94	95	96	97	98	99	100	101	102	103	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118	119	120	121	122	123	124	125	126	127	128	129	130	131	132	133	134	135	136	137	138	
			Lanthanides	57 <sup>57</sup> La Lanthanum 138.91 [Xe]5d <sup>1</sup> 6s <sup>2</sup>	58 <sup>58</sup> Ce Cerium 140.12 [Xe]4f <sup>1</sup> 5d <sup>1</sup> 6s <sup>2</sup>	59 <sup>59</sup> Pr Praseodymium 140.91 [Xe]4f <sup>3</sup> 6s <sup>2</sup>	60 <sup>60</sup> Nd Neodymium 144.24 [Xe]4f <sup>4</sup> 6s <sup>2</sup>	61 <sup>61</sup> Pm Promethium (145) [Xe]4f <sup>5</sup> 6s <sup>2</sup>	62 <sup>62</sup> Sm Samarium 150.36 [Xe]4f <sup>6</sup> 6s <sup>2</sup>	63 <sup>63</sup> Eu Europium 151.96 [Xe]4f <sup>7</sup> 6s <sup>2</sup>	64 <sup>64</sup> Gd Gadolinium 157.25 [Xe]4f <sup>7</sup> 5d <sup>1</sup> 6s <sup>2</sup>	65 <sup>65</sup> Tb Terbium 158.93 [Xe]4f <sup>9</sup> 6s <sup>2</sup>	66 <sup>66</sup> Dy Dysprosium 162.50 [Xe]4f <sup>10</sup> 6s <sup>2</sup>	67 <sup>67</sup> Ho Holmium 164.93 [Xe]4f <sup>11</sup> 6s <sup>2</sup>	68 <sup>68</sup> Er Erbium 167.26 [Xe]4f <sup>12</sup> 6s <sup>2</sup>	69 <sup>69</sup> Tm Thulium 168.93 [Xe]4f <sup>13</sup> 6s <sup>2</sup>	70 <sup>70</sup> Yb Ytterbium 173.05 [Xe]4f <sup>14</sup> 6s <sup>2</sup>	71 <sup>71</sup> Lu Lutetium 174.97 [Xe]4f <sup>14</sup> 5d <sup>1</sup> 6s <sup>2</sup>	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100	101	102	103			
			Actinides	89 <sup>89</sup> Ac Actinium (227) [Rn]6d <sup>1</sup> 7s <sup>2</sup>	90 <sup>90</sup> Th Thorium 232.04 [Rn]6d <sup>2</sup> 7s <sup>2</sup>	91 <sup>91</sup> Pa Protactinium 231.04 [Rn]5f <sup>2</sup> 6d <sup>1</sup> 7s <sup>2</sup>	92 <sup>92</sup> U Uranium 238.03 [Rn]5f <sup>3</sup> 6d <sup>1</sup> 7s <sup>2</sup>	93 <sup>93</sup> Np Neptunium (237) [Rn]5f <sup>4</sup> 6d <sup>1</sup> 7s <sup>2</sup>	94 <sup>94</sup> Pu Plutonium (244) [Rn]5f <sup>6</sup> 7s <sup>2</sup>	95 <sup>95</sup> Am Americium (243) [Rn]5f <sup>7</sup> 7s <sup>2</sup>	96 <sup>96</sup> Cm Curium (247) [Rn]5f <sup>8</sup> 6d <sup>1</sup> 7s <sup>2</sup>	97 <sup>97</sup> Bk Berkelium (247) [Rn]5f <sup>9</sup> 7s <sup>2</sup>	98 <sup>98</sup> Cf Californium (251) [Rn]5f <sup>10</sup> 7s <sup>2</sup>	99 <sup>99</sup> Es Einsteinium (252) [Rn]5f <sup>11</sup> 7s <sup>2</sup>	100 <sup>100</sup> Fm Fermium (257) [Rn]5f <sup>12</sup> 7s <sup>2</sup>	101 <sup>101</sup> Md Mendelevium (258) [Rn]5f <sup>13</sup> 7s <sup>2</sup>	102 <sup>102</sup> No Nobelium (259) [Rn]5f <sup>14</sup> 7s <sup>2</sup>	103 <sup>103</sup> Lr Lawrencium (266) [Rn]5f <sup>14</sup> 7p <sup>1</sup> 7s <sup>2</sup>	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118	119	120	121	122	123	124	125	126	127	128	129	130	131	132	133	134	135	136	137	138

Atomic Number: 58  
Ground State: 1G<sub>4</sub>  
Symbol: Ce  
Name: Cerium  
Standard Atomic Weight (u): 140.12  
Ground-state Configuration: [Xe]4f<sup>1</sup>5d<sup>1</sup>6s<sup>2</sup>  
Ionization Energy (eV): 5.5386

<sup>1</sup>Based upon <sup>12</sup>C. (.) indicates the mass number of the longest-lived isotope.

For the most precise values and uncertainties visit [ciaaw.org](http://ciaaw.org) and [pml.nist.gov/data](http://pml.nist.gov/data).

# OUTLINE

***1. Who are we?***

***2. Transition probabilities*** (what are they, why are they important, how do I measure them?)

***3. Experimental requirements and challenges***

***4. Is there any equilibrium?***

$$I_{ul} \propto A_{ul} N_u$$

**Assume  
Thermodynamic  
equilibrium**



**Boltzmann Population  
of energy levels**

$$N_u \propto e^{-\frac{E_u}{kT}}$$

**Eliminate  $N_u$ !**



**Ratios of lines coming  
from the same upper  
energy level**

**(Branching Fractions)**

$$A_{ul} = \frac{BF}{\tau_u}$$

$$I_{ul} \propto A_{ul} N_u$$



**Boltzmann-Plot  
technique**



**What I need:**

- **Assume pLTE**  
(partial local thermodynamic equilibrium)
- **Some lines with  
known  $A_{ul}$**

**Branching fraction  
technique**

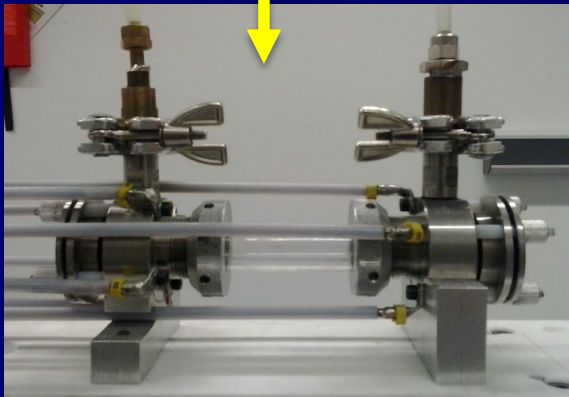


**What I need:**

- **Measure ALL lines  
coming from an  
upper energy level**
- **The lifetime**

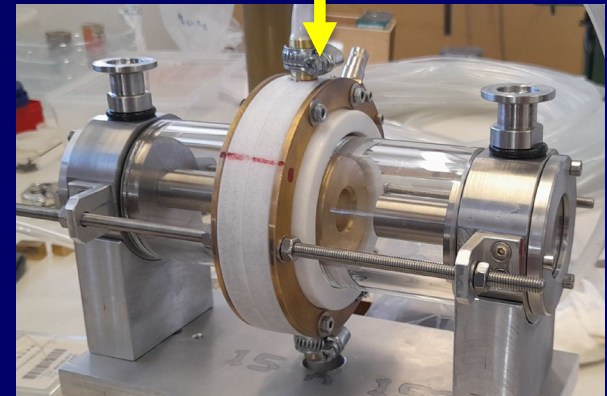
$$I_{ul} \propto A_{ul} N_u$$

**Assume  
Thermodynamic  
equilibrium**



**Pulsed-discharge lamp  
(Noble gases)**

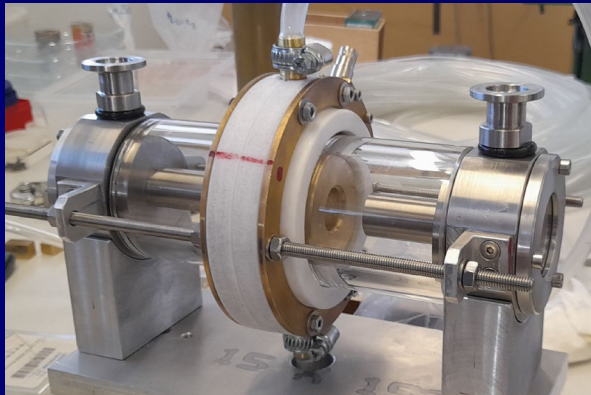
**No equilibrium:  
Eliminate  $N_u$ !**



**Hollow-cathode lamp  
(Heavy elements)**

$$I_{ul} \propto A_{ul} N_u$$

**Assume  
Thermodynamic  
equilibrium**



**Hollow cathode lamp  
(Heavy elements)**

**No equilibrium:  
Eliminate  $N_u$ !**



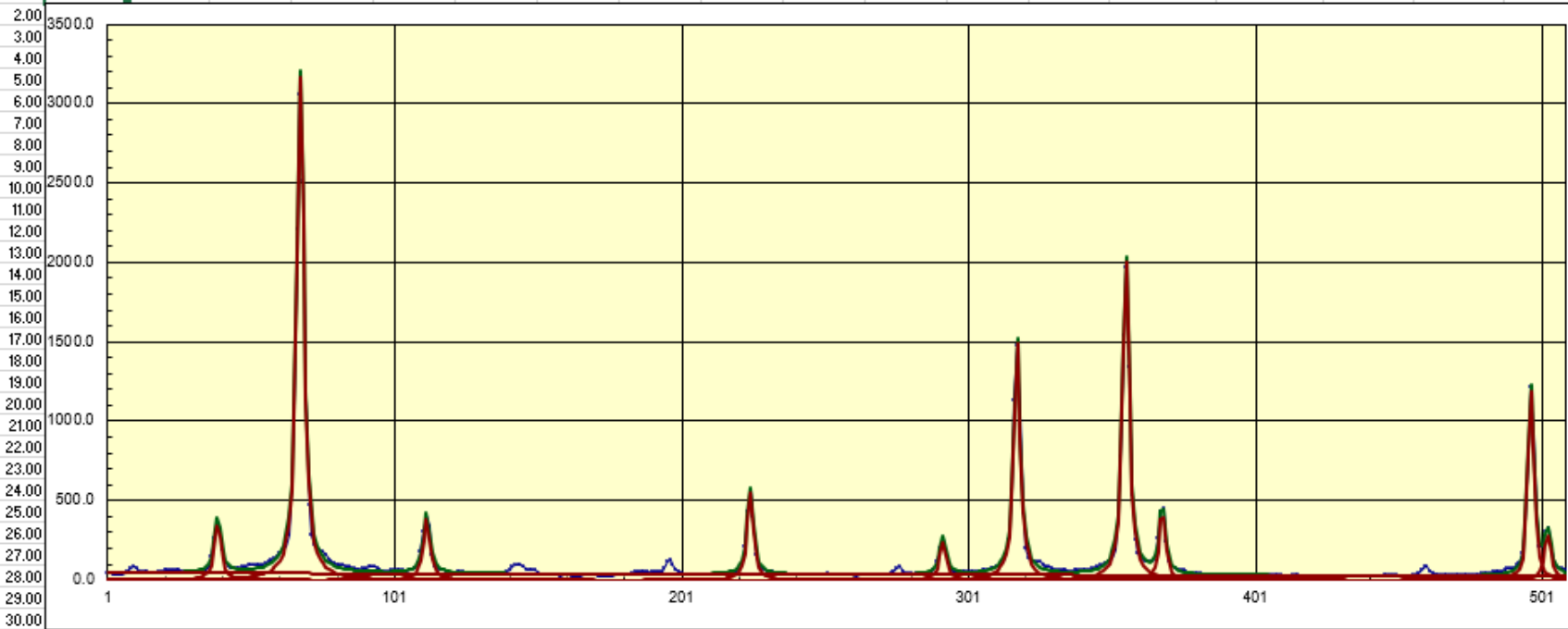
**??**

Nitz, Curry et al.. Transition Probabilities of Ce I Obtained from Boltzmann Analysis of Visible and Near-Infrared Emission Spectra. Journal of Physics B: Atomic, Molecular and Optical Physics, 51, 1 2018.



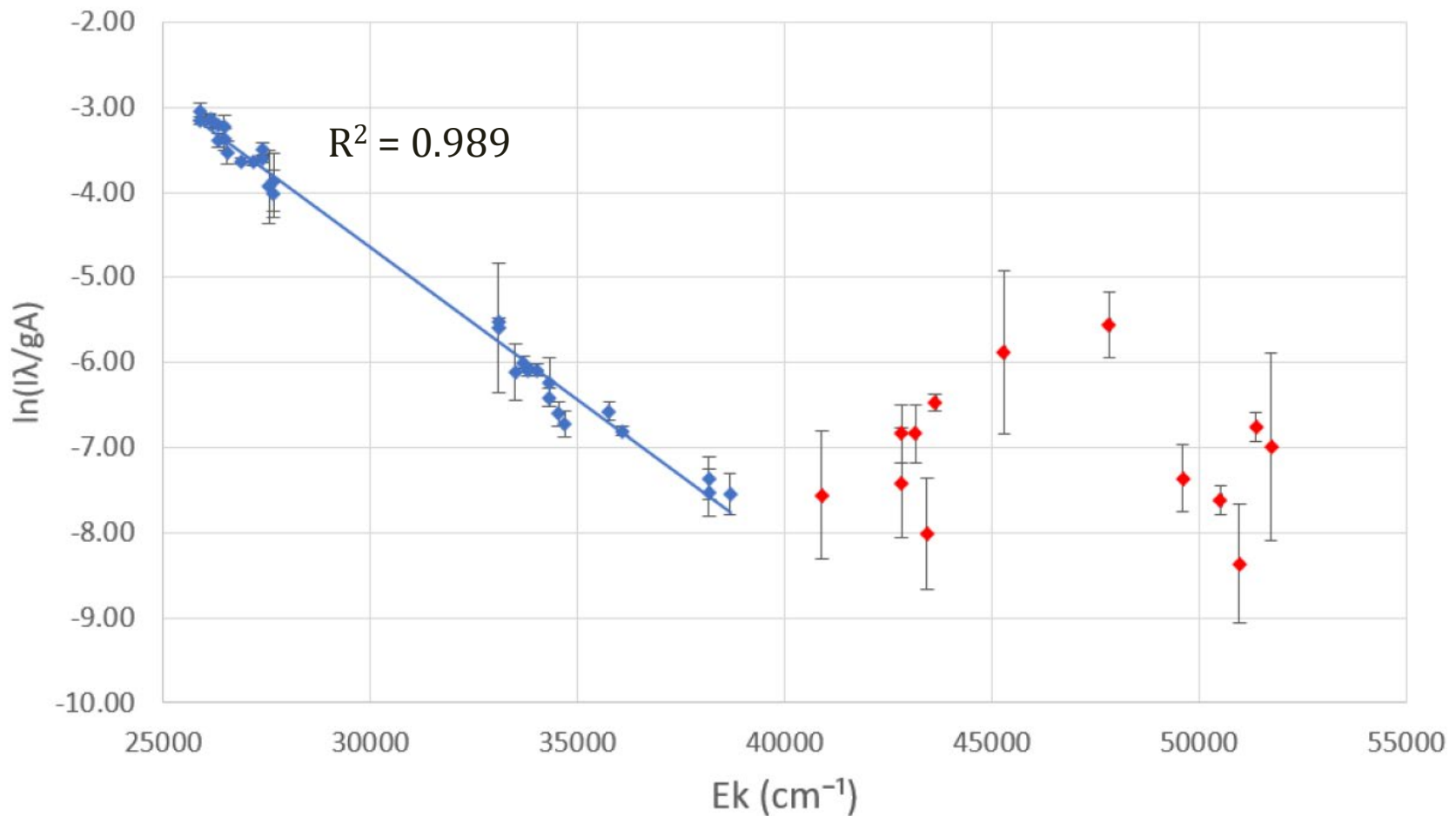
# Fe I

HELP													Profile	Factor	Weight	Read	C:\Userstusuario\OneDrive - UWat_T	
													29	1	100		COR-2D-IRONBP-RSP.009	
Height	<input checked="" type="checkbox"/> A0	45.28	352.3543	3174.348	380.1452	550.9221	237.4021	1499.444	2027.423	458	1192	279		<b>Remove</b>	<b>Fixed</b>		Save	C:\Userstusuario\OneDrive - UWat_T
Width	<input checked="" type="checkbox"/> A1	-0.04	2.74	2.86	2.80	2.51	2.66	2.71	2.67	2.37	2.82	3.01		0	0			IRONEX6-B5.001
Center	<input type="checkbox"/> A2	0.00	39.2756	68.0918	112.0538	224.8977	292.0032	317.8987	355.8478	368.5246	497.06	502.83		<b>Include</b>	0		Delete	Invert
<input type="checkbox"/> Asymmetry	<input type="checkbox"/> A3	0.00	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000		0	509	0		1
<input type="checkbox"/> Gauss	<input type="checkbox"/> A4	0.00	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4606	0.1864		0	0	0		10
Comment														0	0	0	Start	Multiply
Height Exp.			352	3174	380	551	237	1499	2027	458	1192	279		0	0	0		0.70
Width Exp.			2.74	2.86	2.80	2.51	2.66	2.71	2.67	2.37	2.82	3.01		0	0	0	Fitting	Multiply
Center Exp.			39.28	68.09	112.05	224.90	292.00	317.90	355.85	368.52	497.06	502.83		0	0	0		1.40
Area Exp.			1515	14268	1673	2175	993	6378	8491	1703	4495	1237		<b>Time</b>	<b>Sigma</b>	<b>Serie</b>	Next	Zoom
Xmax Exp.			39.28	68.09	112.05	224.90	292.00	317.90	355.85	368.52	497.06	502.83		180.6	27.3	193		1
Height*Factor			352	3174	380	551	237	1499	2027	458	1192	279					Autoscale	509
																		1
X	Y	Backgr.	Loren 1	Loren 2	Loren 3	Loren 4	Loren 5	Loren 6	Loren 7	Loren 8	Loren 9	Loren10	Sum	Deviation	Dev.Fized	Difference	Fixed	2300
1.00	45.0	45.24	0.45	1.44	0.06	0.02	0.00	0.03	0.03	0.00	0.01	0.00	47.28	5.22	5.22	-2.28	-1000.00	X Min

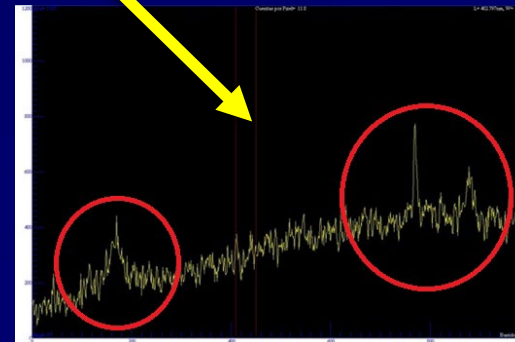
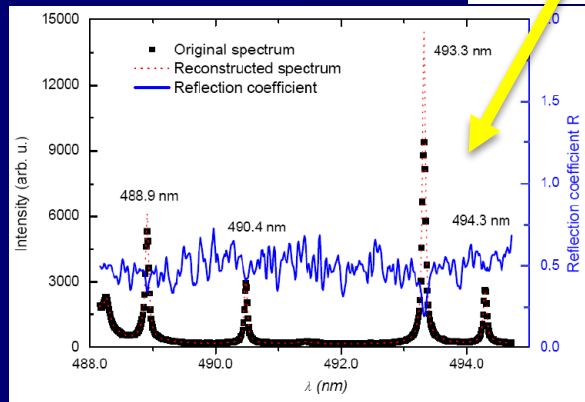
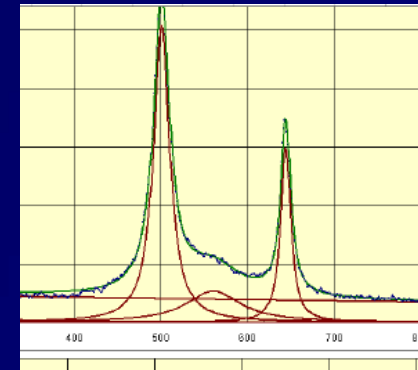
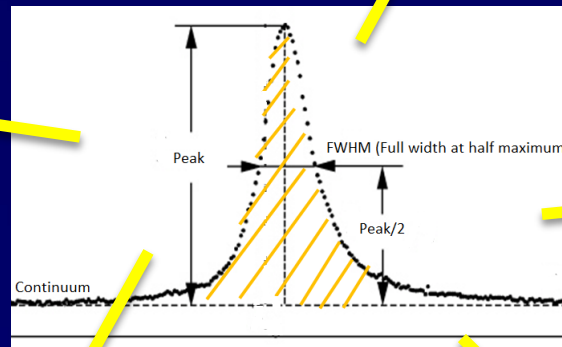
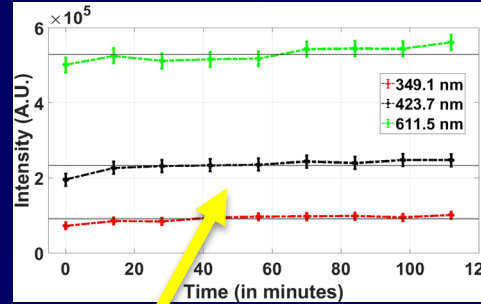
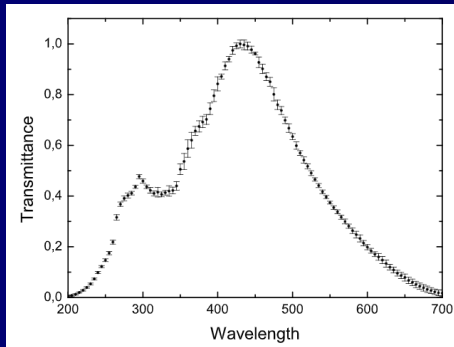


# Can I assume pLTE? Boltzmann-plot

$$\ln \left( \frac{I_{ki} \lambda}{g_k A_{ki}} \right) = \ln \left( \frac{\hbar c M N(T)}{2Z(T)} \right) - \frac{E_k}{kT}$$



# Sources of uncertainty (everything that affects the determination of the intensity/area of the spectral line...)



# International School on Atomic and Molecular Data Evaluation and Curation

## Organising committee:

- María Teresa Belmonte (UVa, Spain)
- Gabriel Pérez-Callejo (UVa, Spain)
- Yuri Ralchenko (NIST)
- Christian Hill (IAEA)

Faculty of Sciences, University of Valladolid (Spain),  
22-25 October 2023

## TOPICS

- Training of data producers (both experimental and theoretical) on critical compilation and curation of atomic and molecular data.
- Developing skills for atomic and molecular data description and classification (metadata descriptors, FAIR data principles).
- Networking, knowledge-exchange and capacity-building within the atomic and molecular data community.

Application deadline: 20 July 2023

[schoolatomicdata2023@gmail.com](mailto:schoolatomicdata2023@gmail.com)

More information on



SCAN ME







# Valladolid



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## Organising committee

- María Teresa Belmonte (UVa)
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- Christian Hill (IAEA)

## Confirmed speakers

- Alexander Kramida (NIST)
- Chris Fontes (Los Álamos)
- Christian Hill (IAEA)
- Yuri Ralchenko (NIST)
- María Teresa Belmonte (UVa)
- Gabriel Pérez-Callejo (UVa)

**Application deadline: 20 July 2023**

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SCAN ME



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In cooperation with



**IAEA**  
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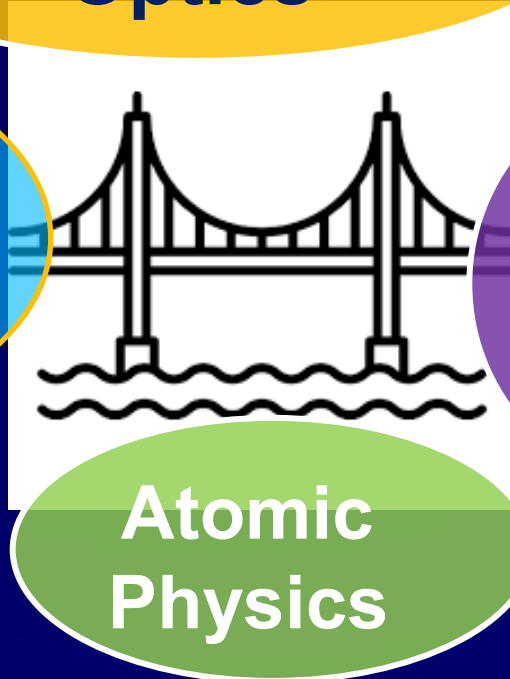
# THANK YOU VERY MUCH FOR YOUR ATTENTION!



**Spectroscopy  
Optics**

**Astronomy  
and  
astrophysics**

**Plasma  
physics**



**Atomic  
Physics**

**New data needed**

**New collaborations?**

**New funding proposals?**

**Please, come and talk with us!**

**[mariateresa.belmonte@uva.es](mailto:mariateresa.belmonte@uva.es)**