The Imperial College London Spectroscopy Group

Atomic Data Measured Using High Resolution Spectroscopy

Christian Clear (Research Fellow, Imperial College London)

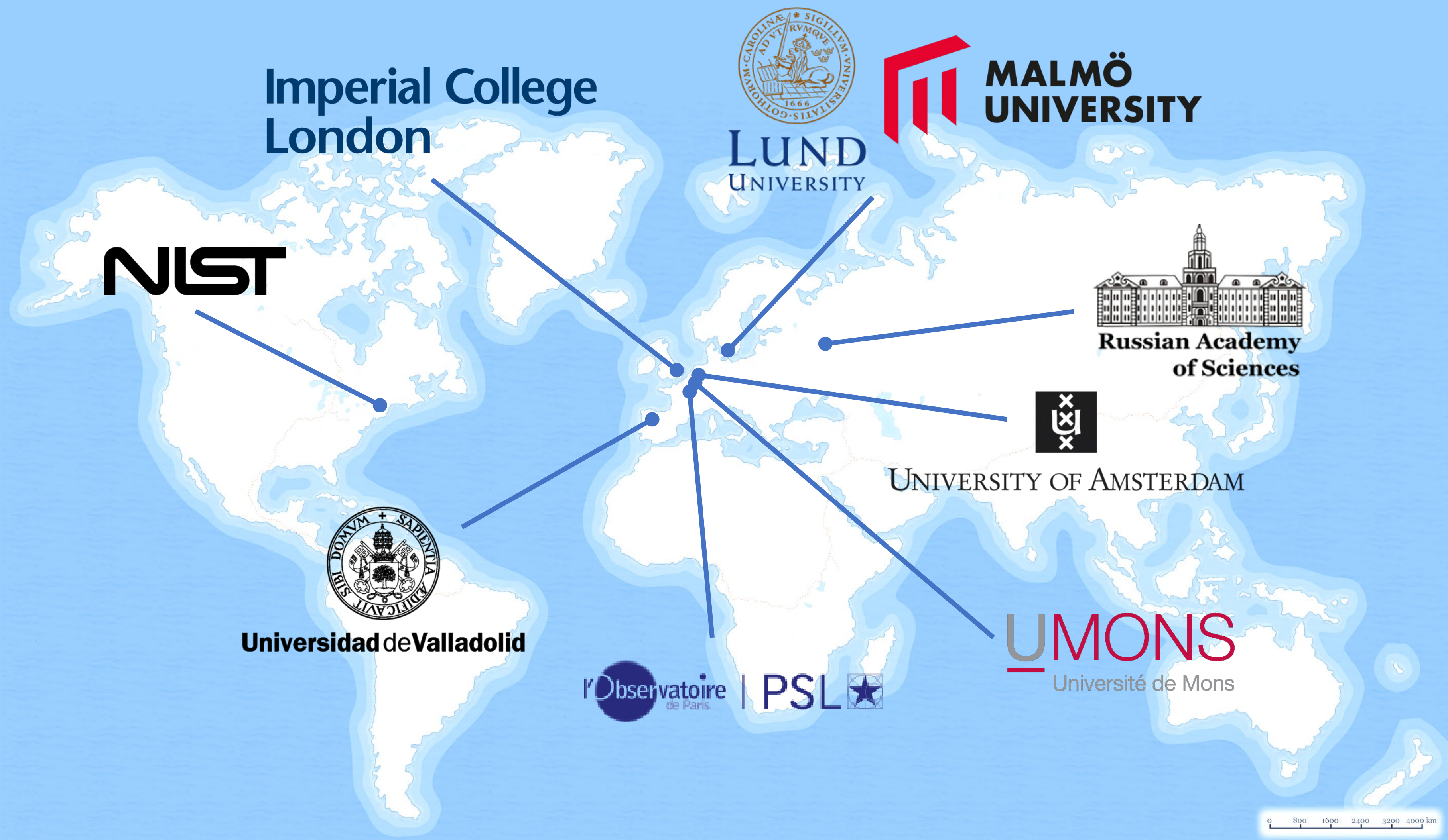
The 14th International Colloquium on Atomic Spectra and Oscillator Strengths for Astrophysical and Laboratory Plasmas (**ASOS14**), Paris, July 2023

The Imperial College Group

- People:
  - Prof. Juliet Pickering (PI)
  - Dr. Christian Clear (PDF)
  - Dr. Florence Concepcion (PDRA)
  - Milan Ding (PhD)
  - Ruairi Shannon (PhD – Oct 2023)
- Focus:
  - Measure atomic data
    - High-resolution, high-accuracy fundamental properties of atoms
  - Use high resolution spectroscopy to measure:
    - Transition wavelengths
    - Energy Levels
    - Transition probabilities, oscillator strengths, f-values
    - Nuclear effects - hyperfine & isotope structure
  - Regularly collaborate with other experimental and theoretical groups.



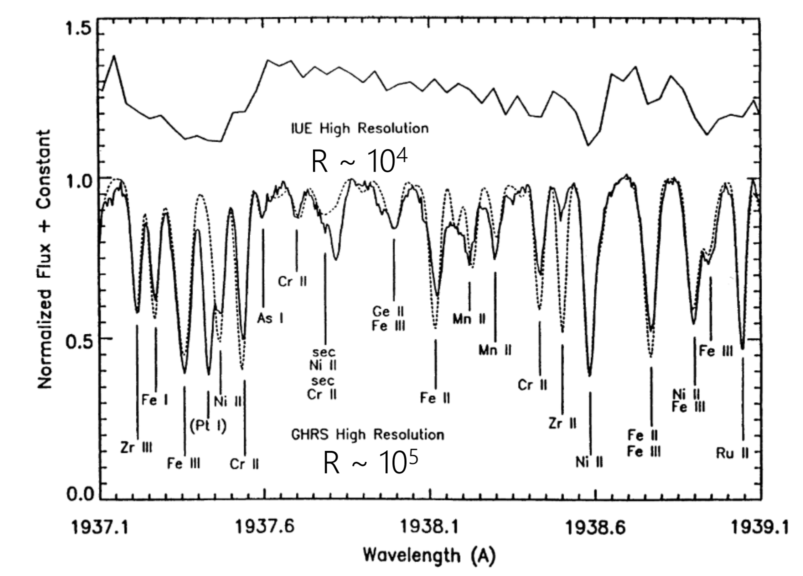




Collaborations

Why Atomic Physics?

- Atomic data is vital for many fields:
  - Astrophysical spectra
  - Laboratory plasmas
  - Medical
  - Industrial
  - Fundamental physics in general
- 99% of observable universe in plasma form
  - Atomic data is vital to understanding the processes involved
- Very high accuracy needed
  - no other field of science places such higher demands on atomic data



High dispersion spectra of χ Lupi [1]

[1] Leckrone, D. S. et al, 1993, PhyS, **T47**, 149-156

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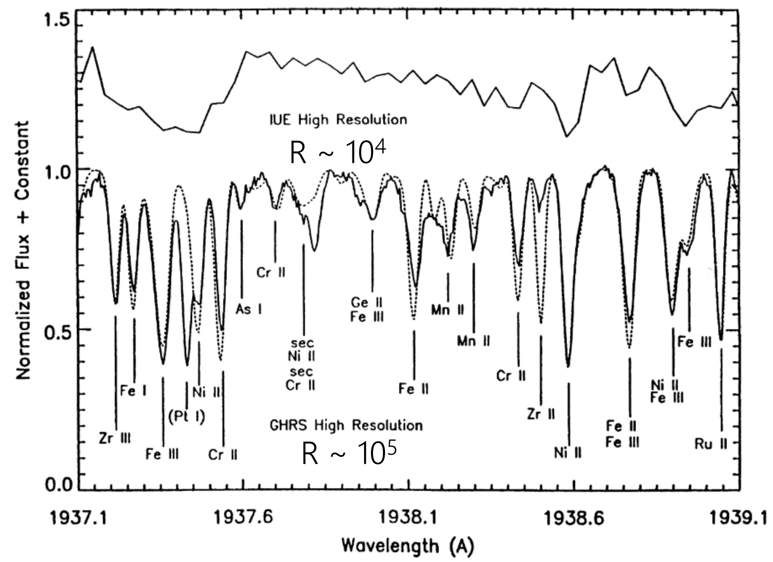
  - Measured a long time ago
  - Using lower resolution techniques than are available now
- Our group focuses on astrophysically important elements:
  - Iron group (scandium to copper)
  - Rare earth



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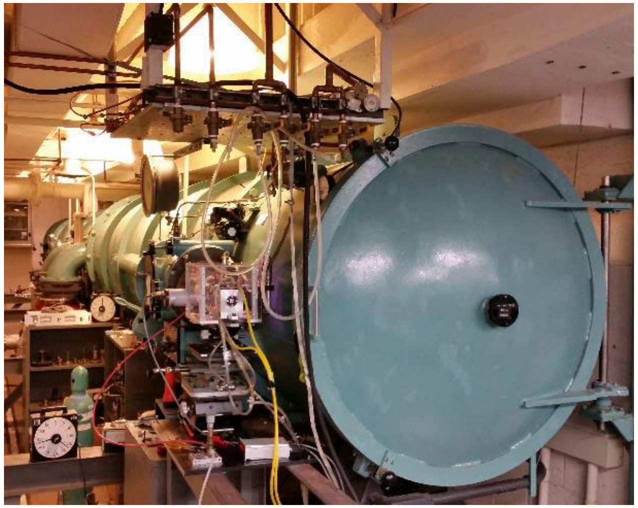

NIST 10.7m NIVS Grating Spectrometer – R ~ 150,000

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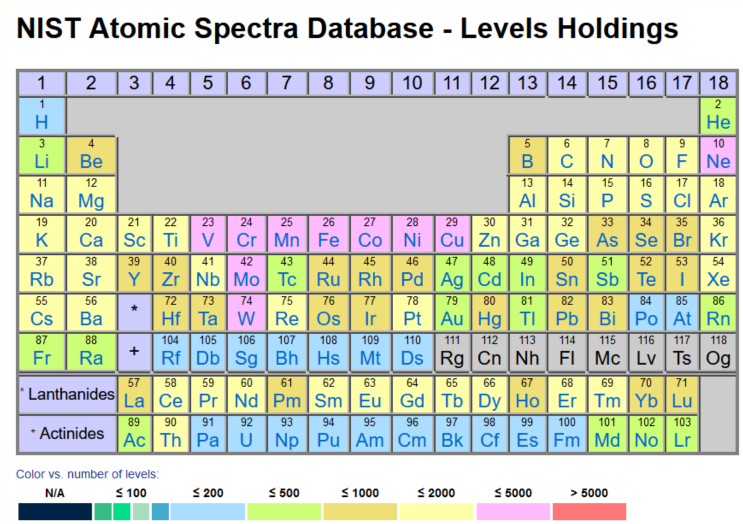
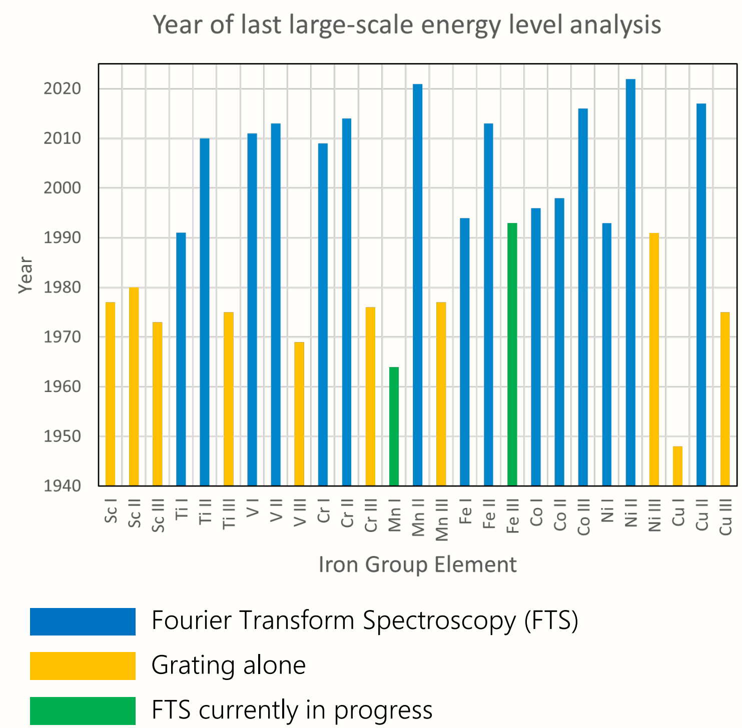


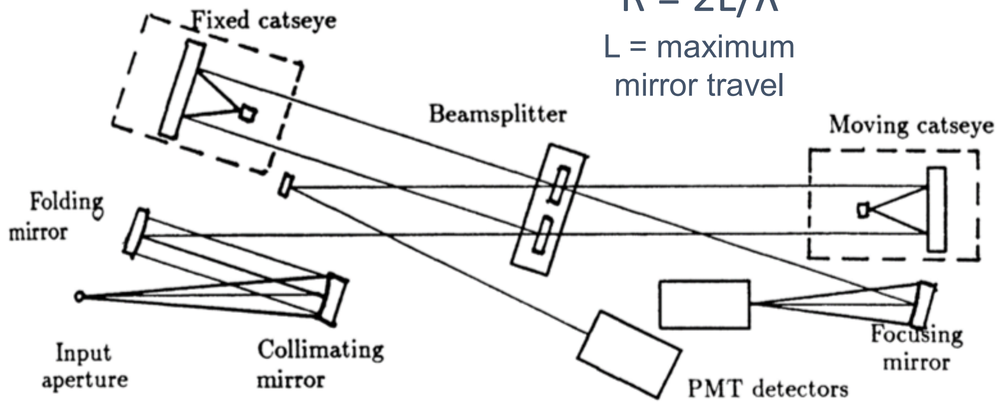


[1] Kramida, A. et al ,2021, *NIST Atomic Spectra Database* (version 5.9), [Online]

Fourier Transform Spectroscopy (FTS)

$$R = 2L/\lambda$$

L = maximum mirror travel



Schematic of a Fourier transform spectrometer

- 1 fixed and 1 moving mirror
- Partially reflective beamsplitter
- Intensity recorded as function of path difference

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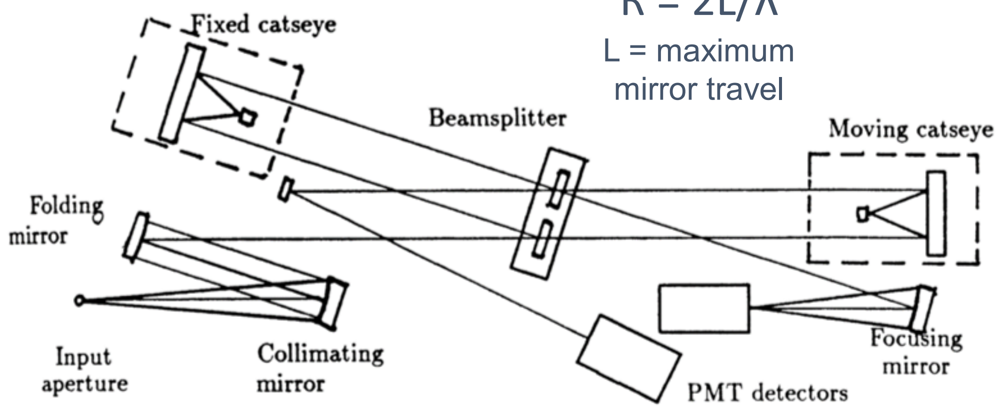

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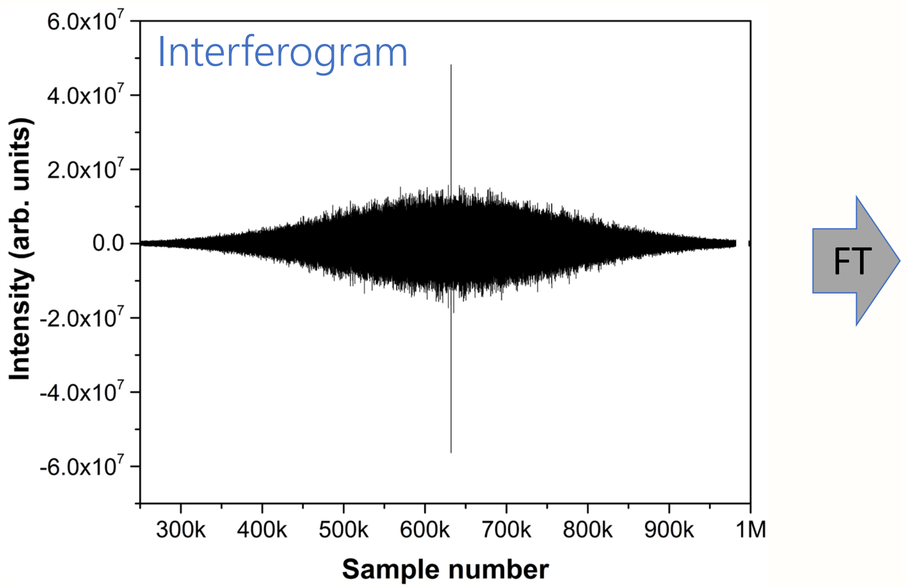

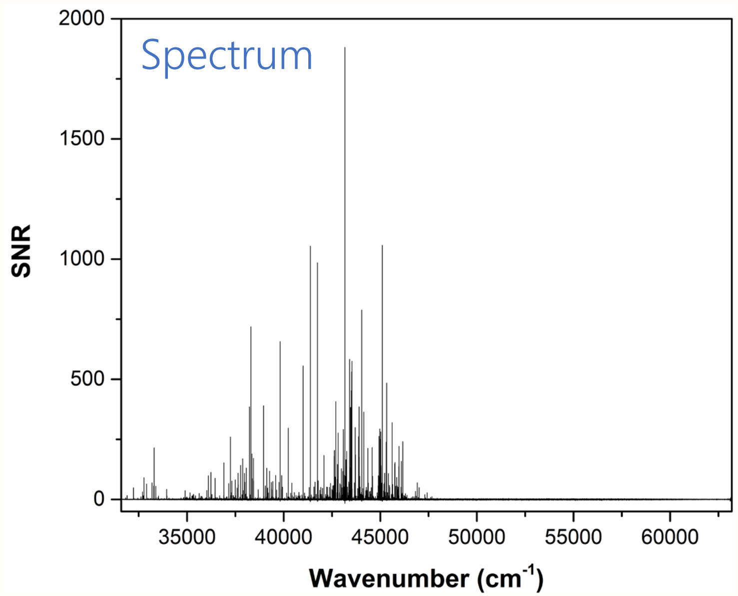

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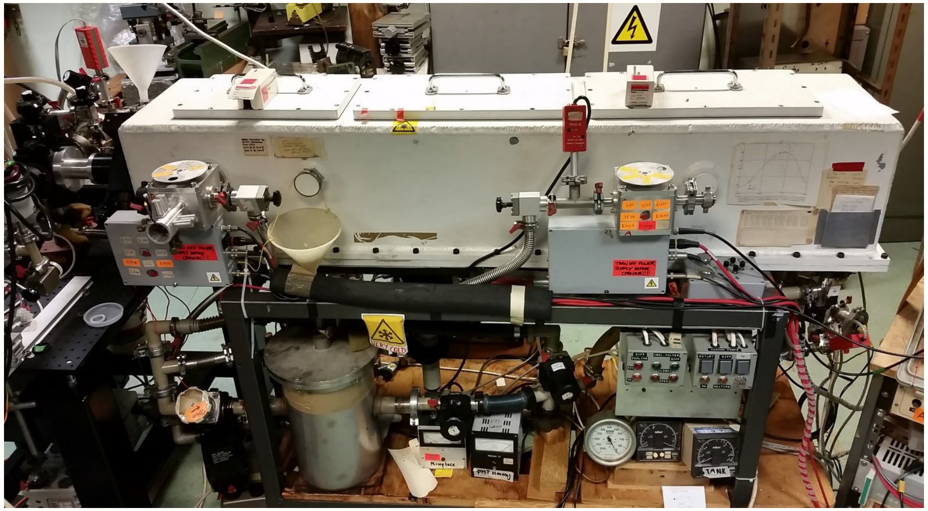
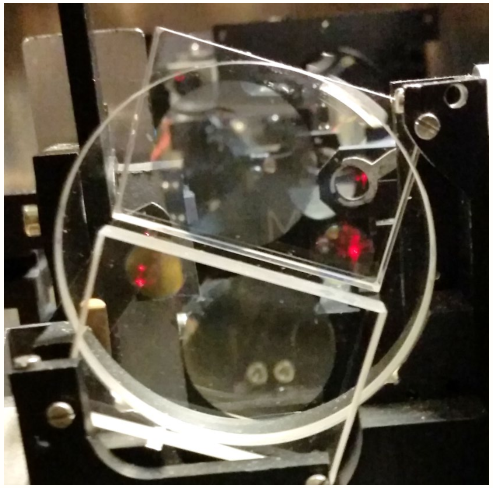
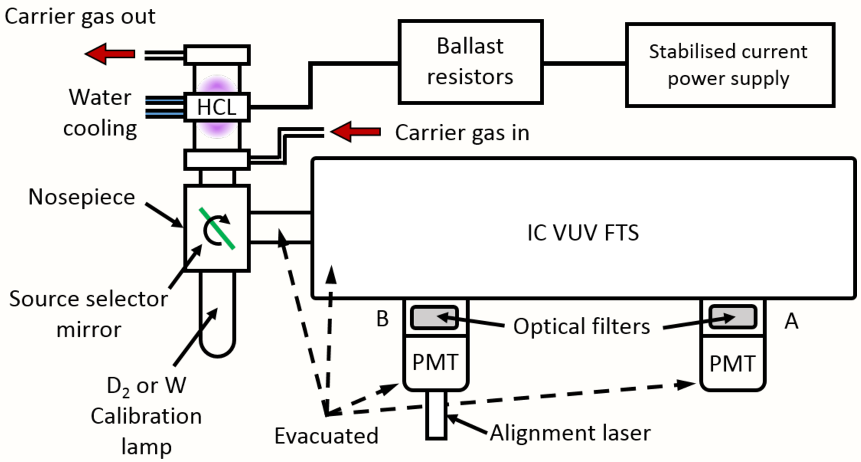


Imperial College VUV FTS



MgF_2 Beamsplitter

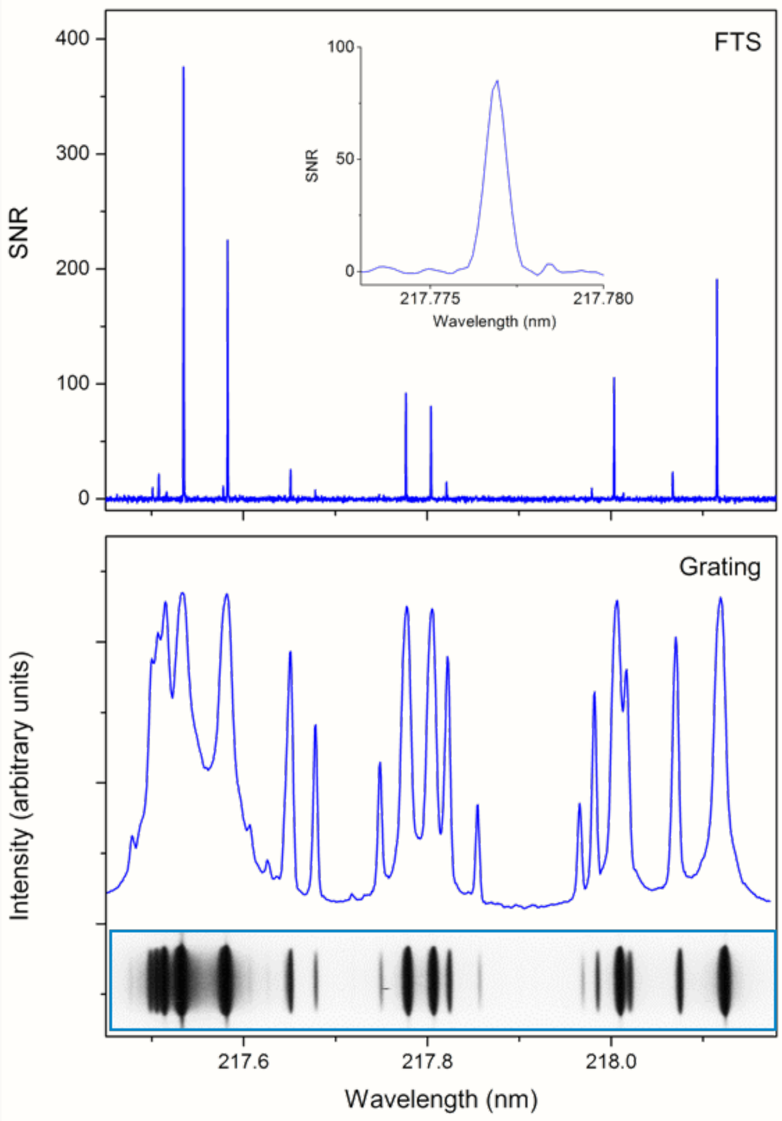


Imperial College VUV FTS – experimental setup

Max. path difference	20 cm
Resolving power	2 x 10^6 at 200 nm
Maximum resolution	0.025 cm^{-1}
Range	74,000 – 12,000 cm^{-1} (135 – 850 nm)
Wavenumber accuracy	±0.001 cm^{-1}

Fourier Transform Spectroscopy - Advantages

- High Resolving Power:
  - Doppler-limited resolving power – fully resolve 3d group line at 50,000cm^{-1} (widths are few hundredths of a wavenumber).
  - High enough for nuclear effects such as Hyperfine and Isotope Structure.
- Linear wavenumber scale and high wavenumber accuracy:
  - 1 part 10^8 achievable.
- Slowly-varying photometric response:
  - Reliable and accurate intensity calibration.
  - Comes from the fact that all elements are measured at once therefore small drifts in source won't affect relative intensities.
- Large and variable free spectral range:
  - V. important for large-scale studies.



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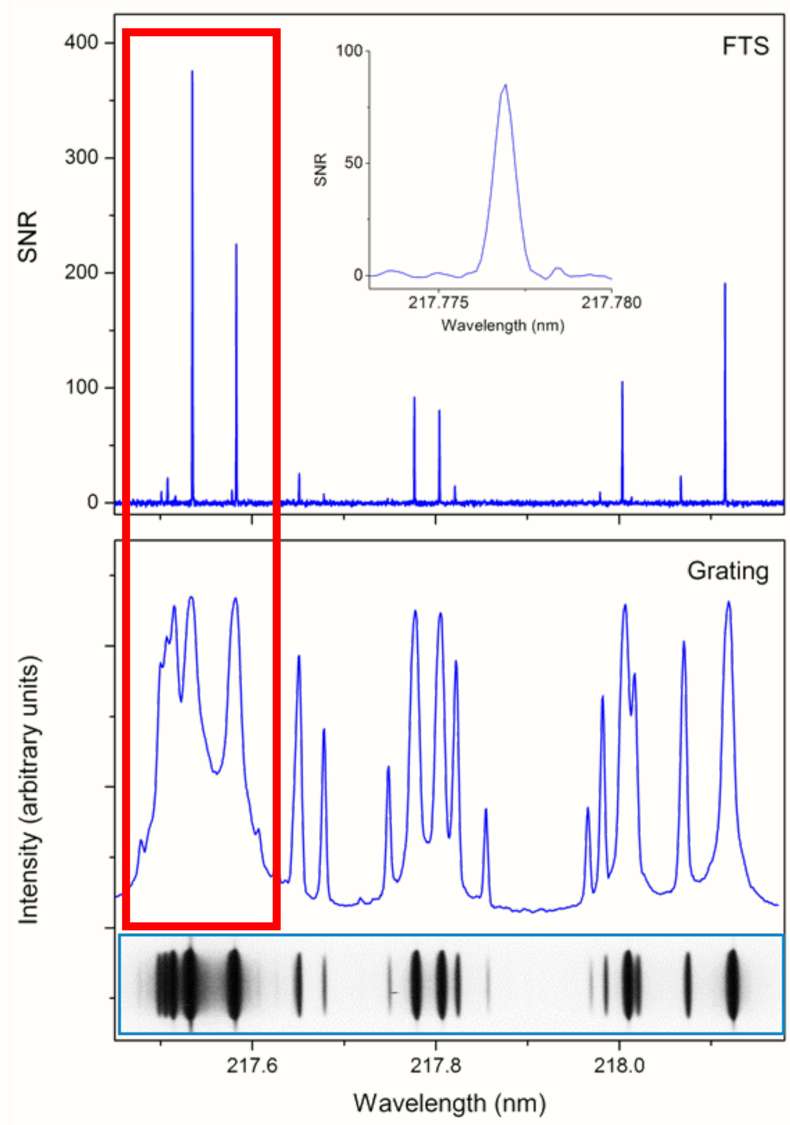

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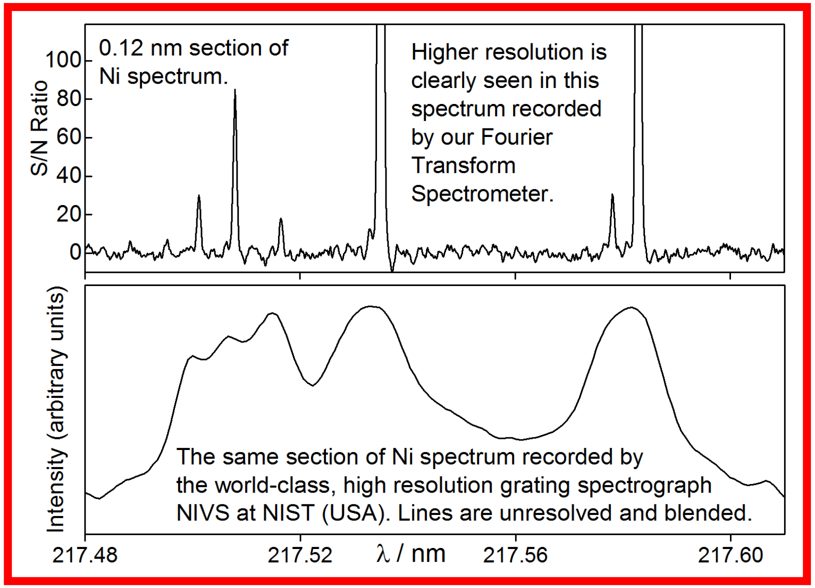

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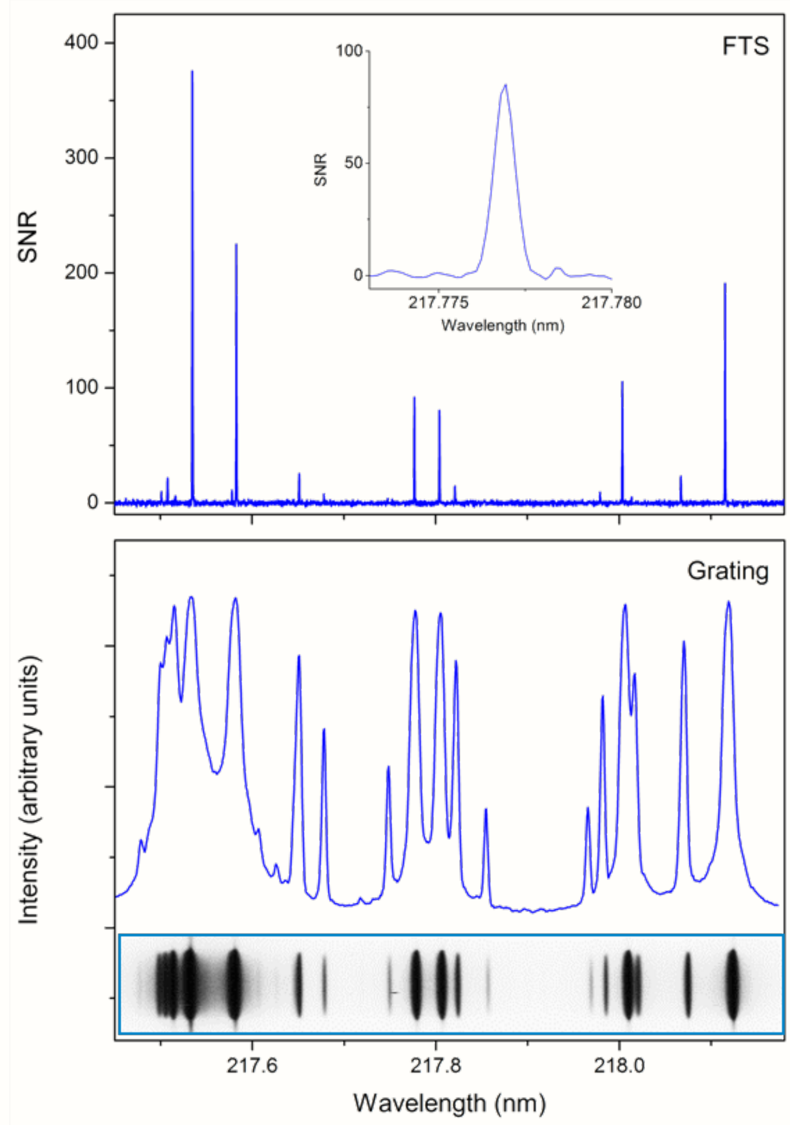

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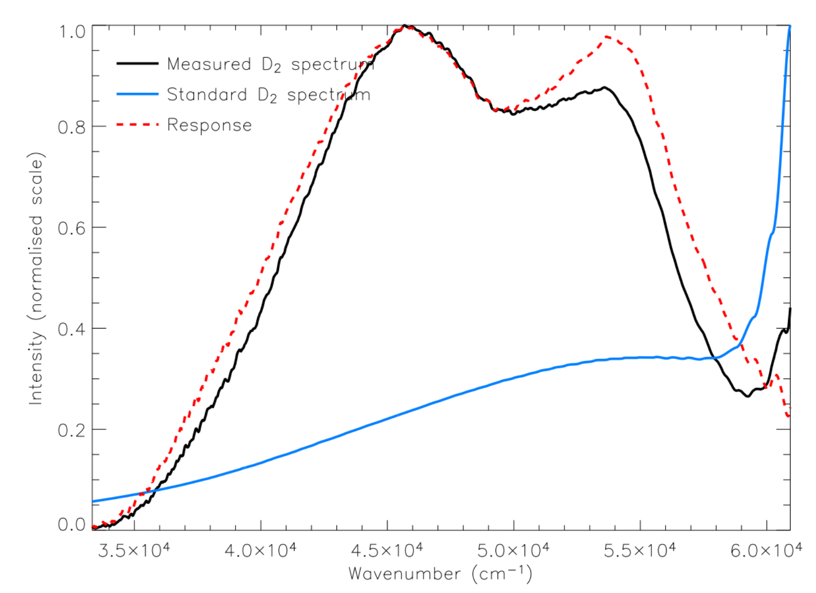

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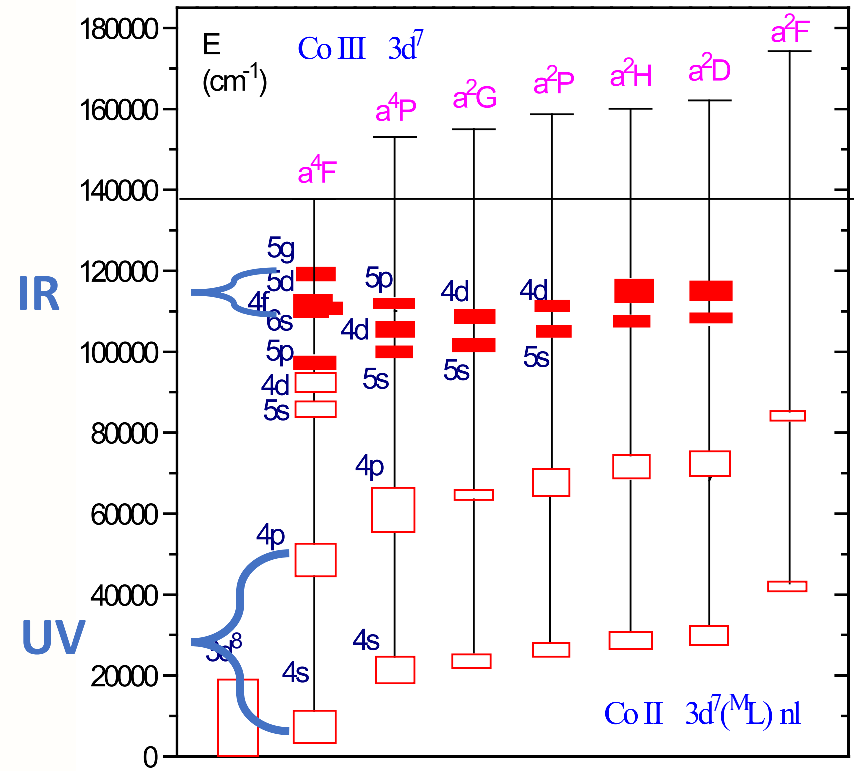

Term diagram of Co II [1]

[1] Pickering, J. C. et al., 1998, ApJS, **117**, 261-311

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Which other tools are available?

- Grating spectroscopy
  - Wide spectral ranges
  - Lower resolving powers
  - Lower accuracies
- Fabry-Perot interferometer and Laser spectroscopy
  - High resolution and accuracy
  - Line-by-line techniques
- Theoretical calculations
  - Extensive but with large uncertainties
  - Provide essential data for experimentalists as well

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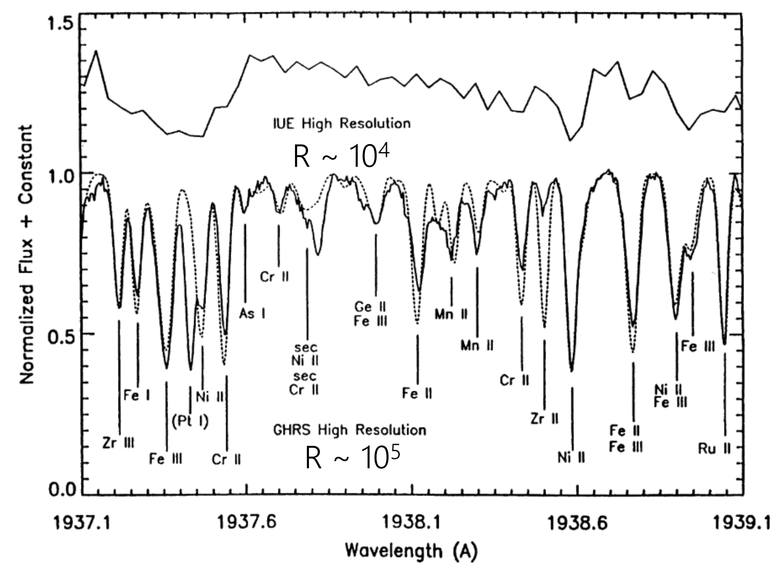

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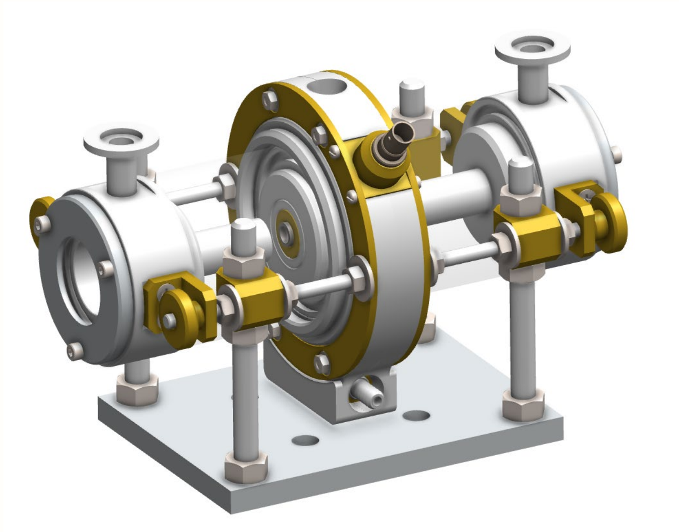
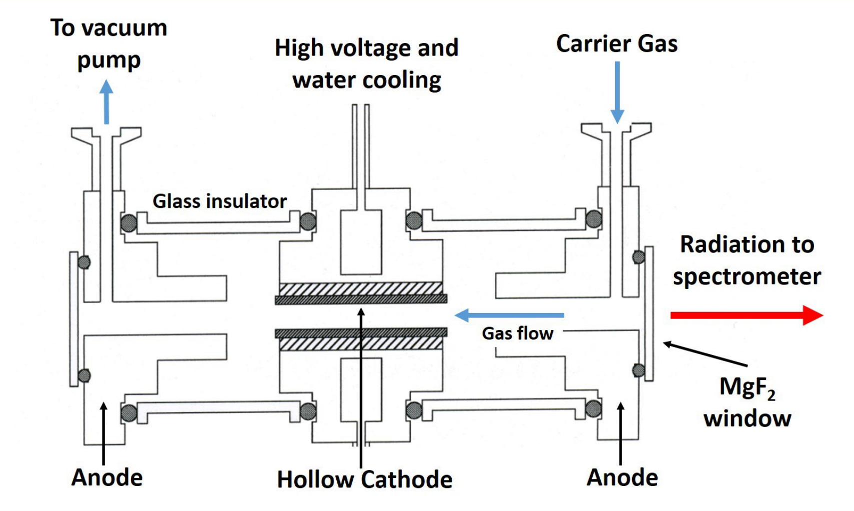
Sources – Hollow Cathode Discharge





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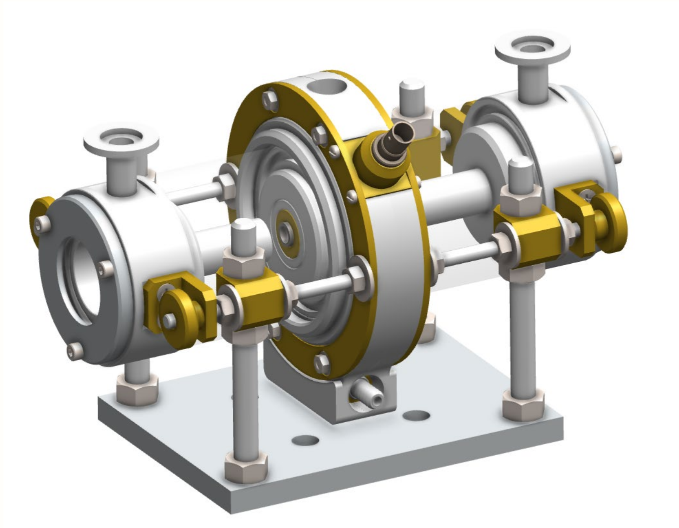
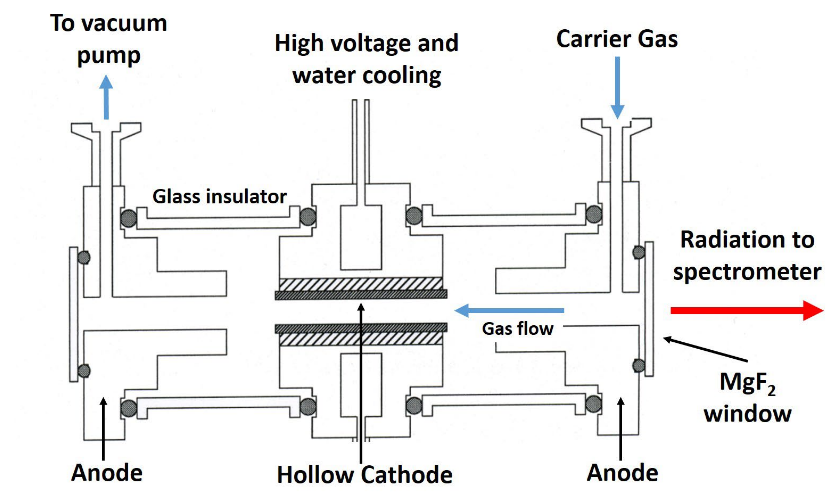
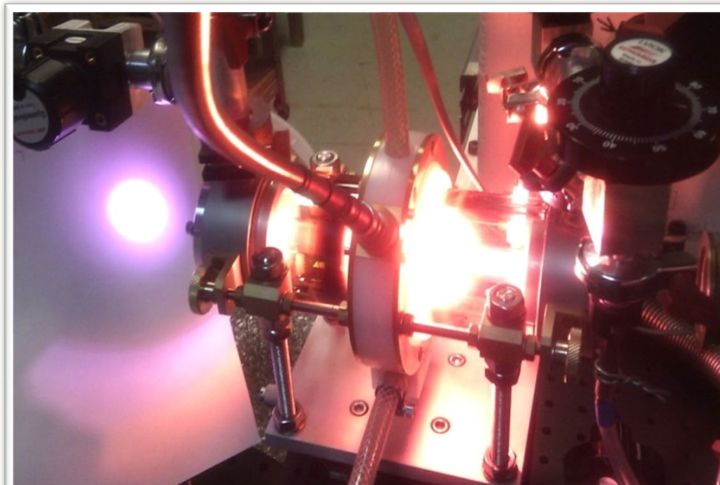




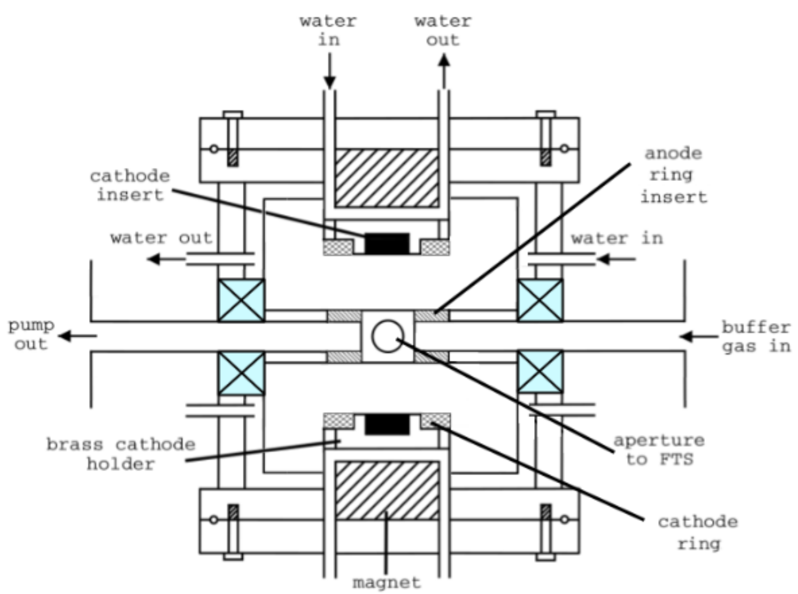
Noble carrier gas ionised → Gas ions sputter cathode material → Metal atoms excited and ionised in plasma →



Predominantly <u>neutral</u> and <u>singly-ionised</u> species

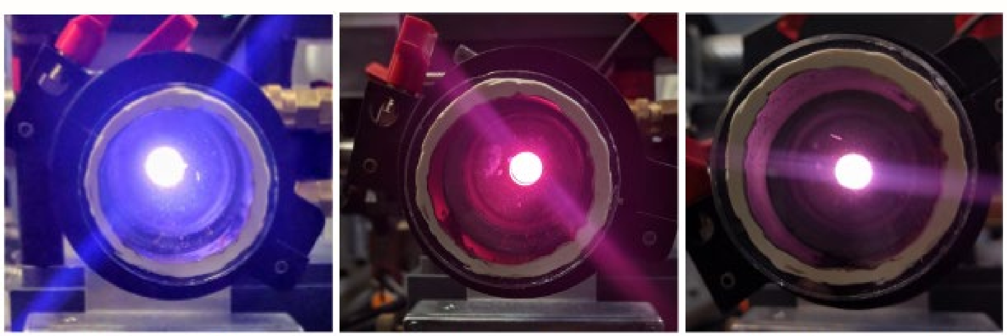
- High stability
- Water-cooled:
  - High currents
  - Reduction of Doppler widths

Sources – Penning Discharge



- Same excitation method as HCD with addition of static magnetic field
- Magnetic field confines plasma, leading to higher ionisations

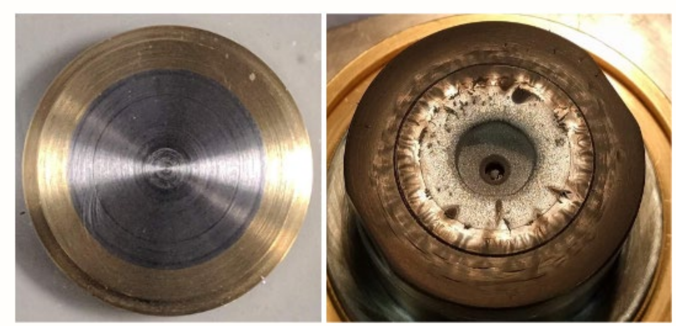
Predominantly singly- and doubly-ionised species



(b) PDL plasma with argon gas.

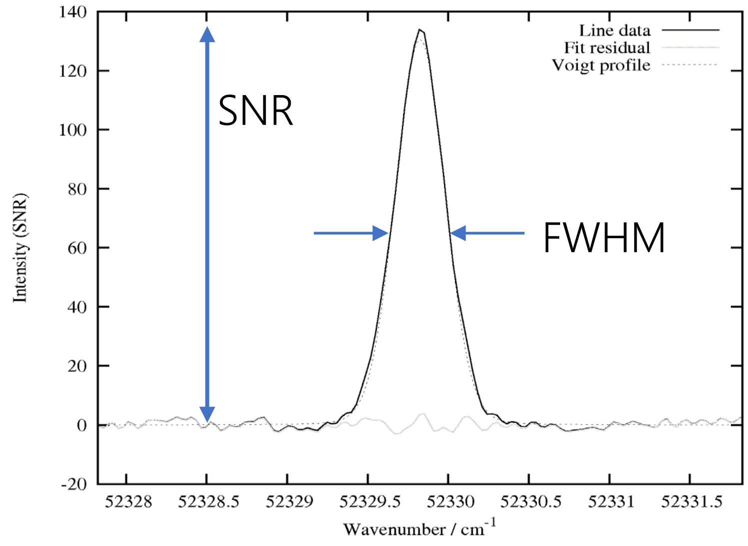
(c) PDL plasma with neon gas.

(d) PDL plasma with neon-helium gas mixture.



Wavelengths

- Record spectra. **Coadding** *n* spectra improves SNR by $\sqrt{n}$
- Fitting – Voigt or Centre of Gravity
- Extracted Parameters:
  - **Peak position** (σ in cm^{-1})
  - **Width of line** (FWHM)
  - Area under curve – **intensity**



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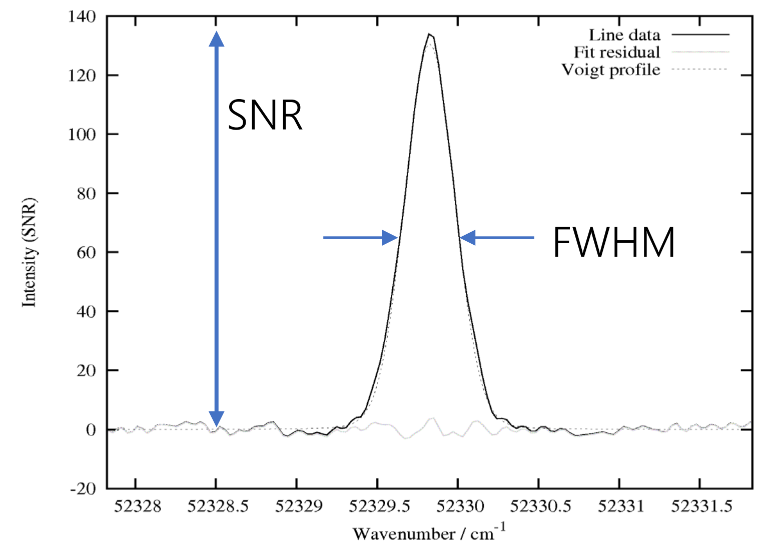
- Wavenumber uncertainties:
  - Both a statistical uncertainty, from fitting, and a calibration uncertainty.
  - FTS wavelength uncertainty: **few parts in 10^8**



$$\delta\sigma_{stat} = \frac{\sqrt{FWHM \times R_{spec}}}{SNR}$$

$$= \frac{FWHM}{\sqrt{N} \times SNR} \approx \boxed{\frac{FWHM}{2 \times SNR}}$$

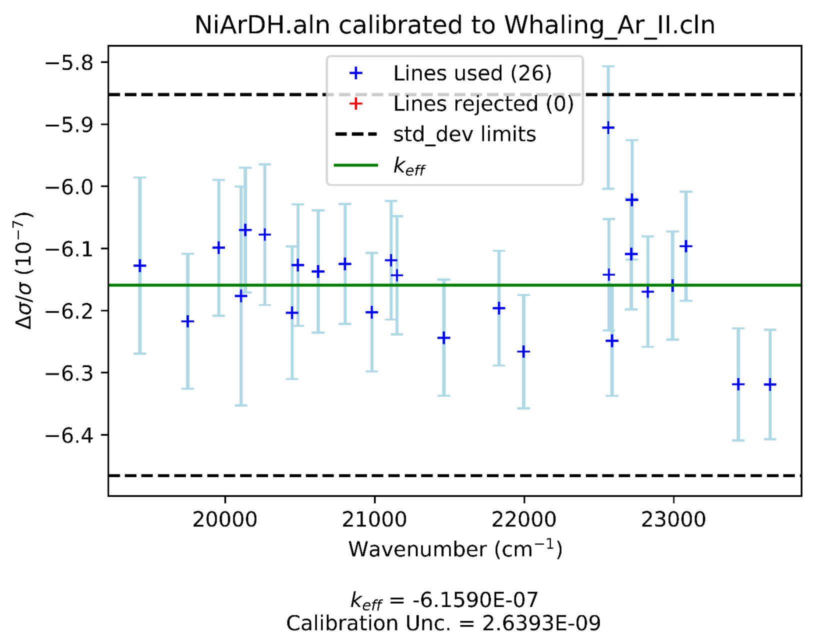
N = number of points across the line

Wavelengths - Calibration

- Small change in path of laser and source light through FTS gives linear wavenumber shift

$$\sigma_{corr} = (1 + K_{eff})\sigma_{obs}$$

- Match lines to standards (usually Ar II) or to lines in previously calibrated spectra to give K_{eff}



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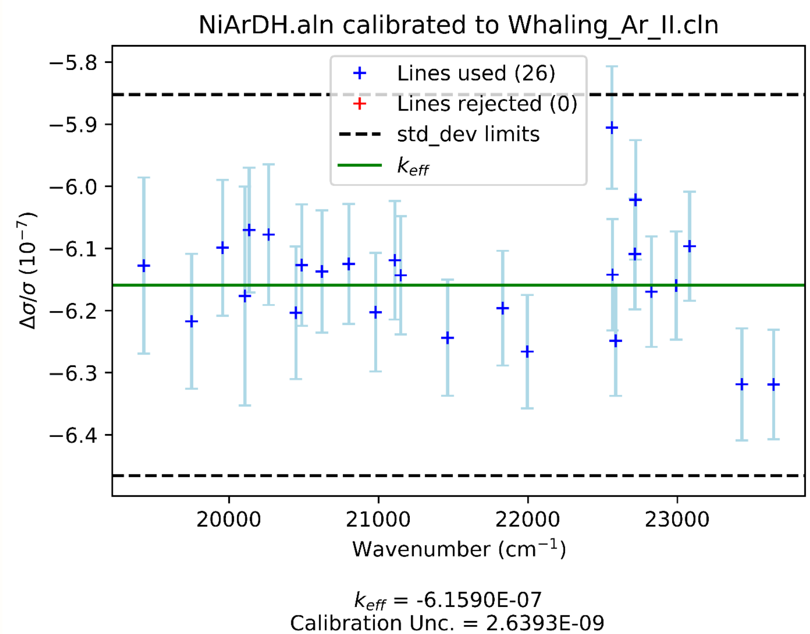
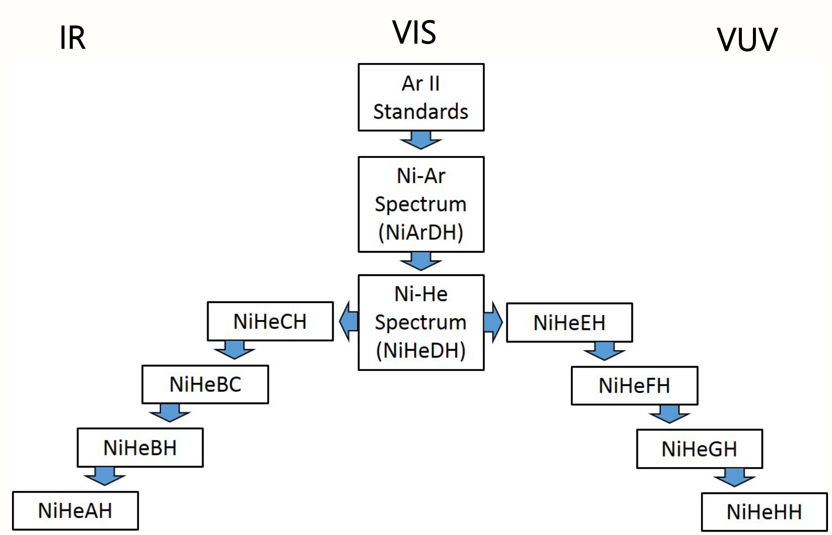
- Match lines to standards (usually Ar II) or to lines in previously calibrated spectra to give K_{eff}
- Total calibration uncertainty is then sum of all matched line differences:

$$\delta\sigma_{calib} = \delta\sigma_{prev} + \sum_i \delta k_i$$

- Finally get total uncertainty of a measured line:

$$\delta\sigma_{total} = \sqrt{\delta\sigma_{stat}^2 + \delta\sigma_{calib}^2}$$





Example wavenumber calibration schema for Ni II

Energy Levels – Term Analysis

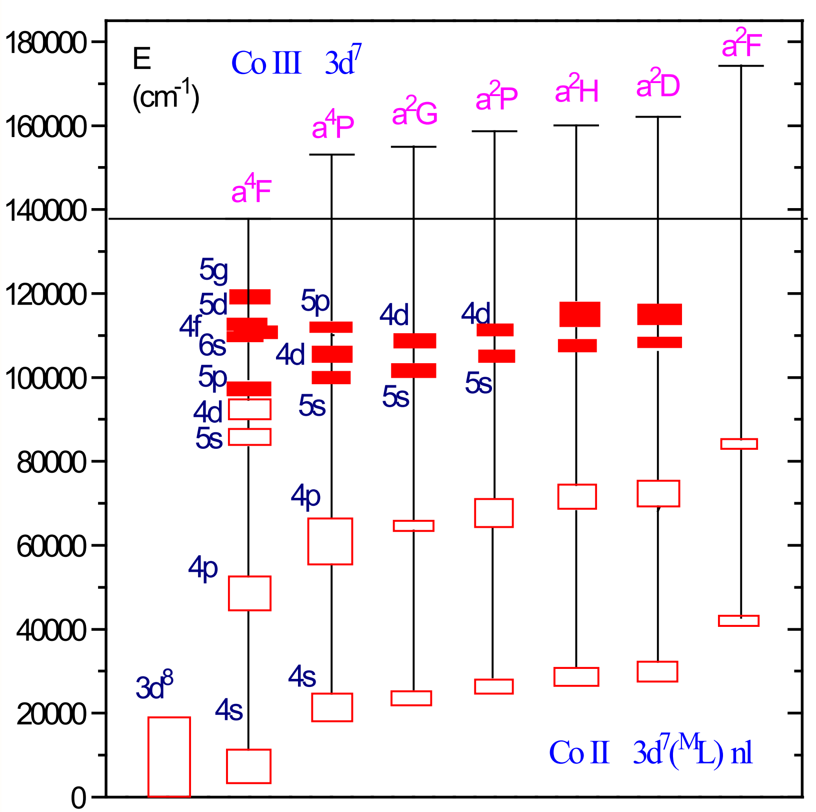
- Derivation of energy levels from observed spectral lines
- Energy levels give the fundamental atomic structure of nature

NO air correction applied to wavelengths.
INTENSITY CALIBRATION APPLIED.

line	wavenumber	peak	width	dmp	eq width	itn	H	tags	identification
26	25215.293478	.4397E+03	329.75	0.2514	0.7287E+06	-6	0	L	no id
27	25220.643674	.4226E+02	94.49	0.1981	0.1934E+05	-7	0	L	no id
28	25248.743844	.9900E+01	87.39	0.0000	0.3577E+04	-4	0	L	no id
29	25251.205389	.5493E+01	71.68	0.0000	0.1618E+04	-3	0	L	no id
30	25258.484244	.2700E+02	99.26	0.0000	0.1083E+05	-6	0	L	no id
31	25276.719294	.7098E+01	148.17	1.0000	0.6035E+04	-6	0	L	no id
32	25301.578648	.1512E+02	98.28	0.0000	0.5546E+04	-8	0	L	no id
33	25315.038229	.2976E+02	89.09	0.0000	0.9717E+04	-4	0	L	no id
34	25316.864134	.8872E+01	103.22	0.0000	0.3348E+04	-3	0	L	no id
35	25338.581944	.1724E+02	94.76	0.0000	0.5833E+04	-4	0	L	no id
36	25339.154692	.1118E+02	92.43	0.5325	0.4568E+04	-5	0	L	no id
37	25347.119072	.6398E+01	88.02	0.0000	0.1994E+04	-8	0	L	no id
38	25353.933531	.3200E+02	97.97	0.2494	0.1220E+05	-7	0	L	no id
39	25387.717456	.6439E+01	87.09	0.0000	0.1918E+04	-4	0	L	no id
40	25502.477609	.8526E+01	82.64	0.1060	0.2227E+04	-8	0	L	no id
41	25533.097702	.7833E+01	103.02	0.1369	0.2452E+04	-7	0	L	no id
42	25548.764946	.9801E+01	100.17	0.0000	0.2740E+04	-5	0	L	no id
43	25553.247984	.4252E+01	119.30	0.0000	0.1403E+04	-5	0	L	no id
44	25554.286312	.4420E+01	80.97	0.0000	0.9880E+03	-6	0	L	no id
45	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

Energy Levels – Term Analysis

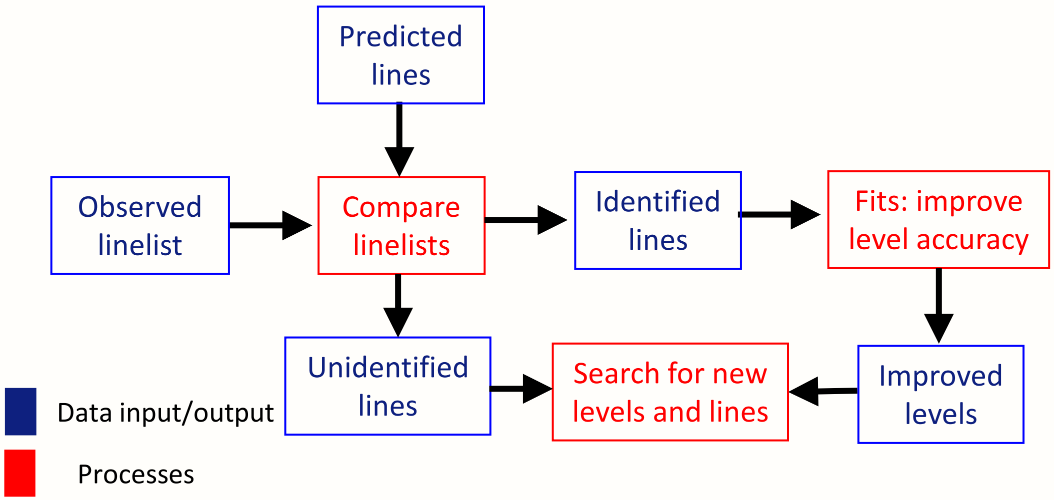
- Derivation of energy levels from observed spectral lines
- Energy levels give the fundamental atomic structure of nature
- Ritz wavelengths often more accurate than observed lines.
- Ritz wavelengths also provide data of experimental accuracy for lines not observed in the lab:
  - very weak lines or,
  - parity-forbidden transitions
- Levels also form one of the key inputs to semi-empirical calculations:
  - Allowing the "fine-tuning" of calculated eigenvalues to the experimental energy levels resulting in more accurate eigenvectors and therefore transition probabilities.

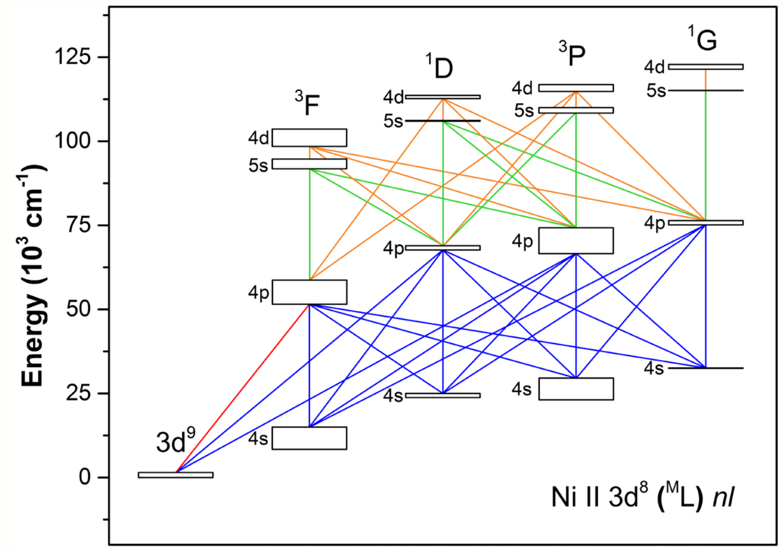


Term diagram of Co II [1]

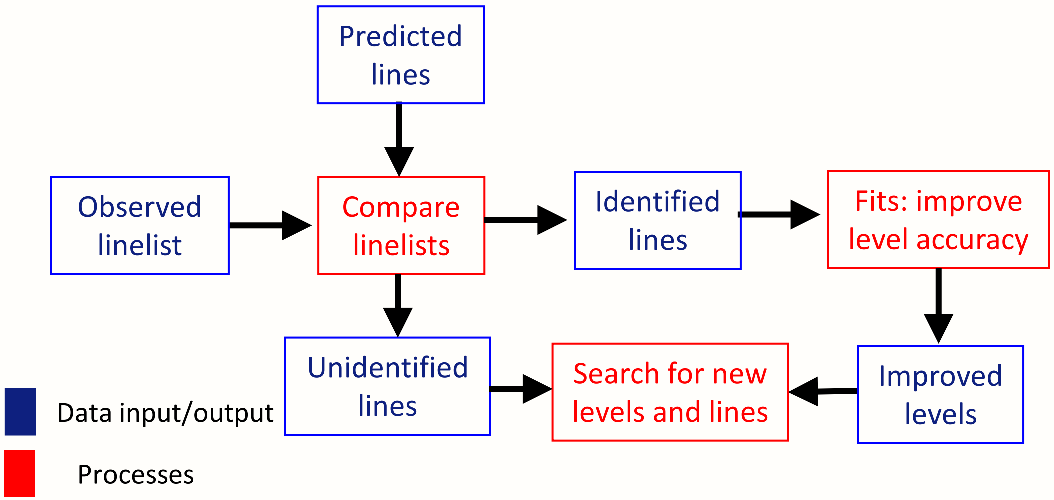
[1] Pickering, J. C. et al., 1998, ApJS, **117**, 261-311

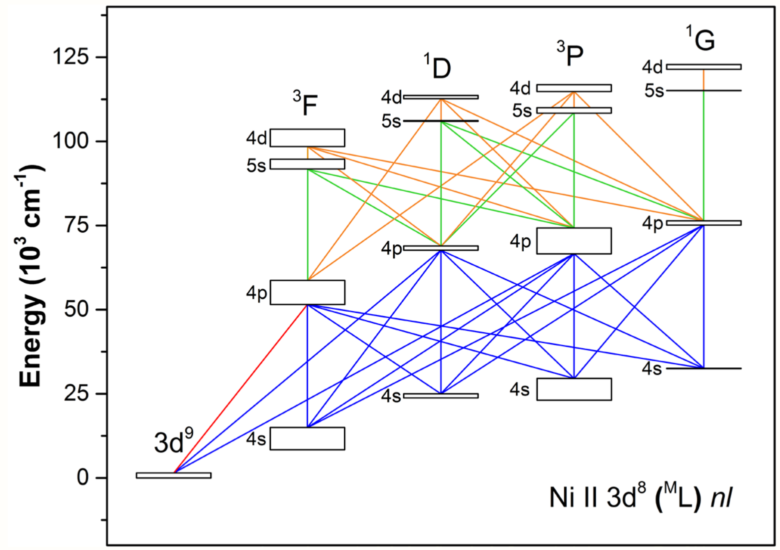
Energy Levels – Term Analysis





Energy Levels – Term Analysis

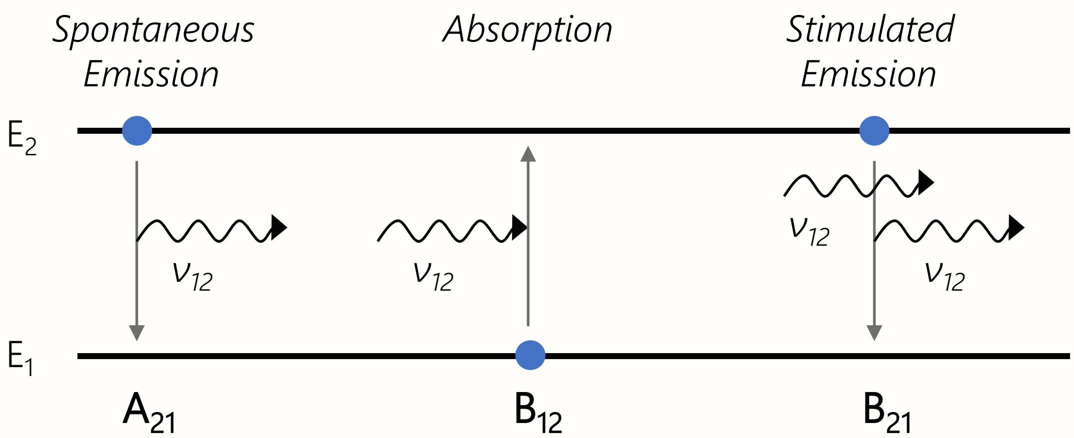




Spectral term analysis is like a complicated jigsaw, where:

The pieces never fit exactly - lines have finite uncertainties
Some pieces fit spuriously - accidental wavelength coincidences
Some crucial pieces are missing - missing lines (weak or blended)
There are pieces belonging to a completely different puzzle - impurities
And the picture on the box is not very clear - theory as a guide

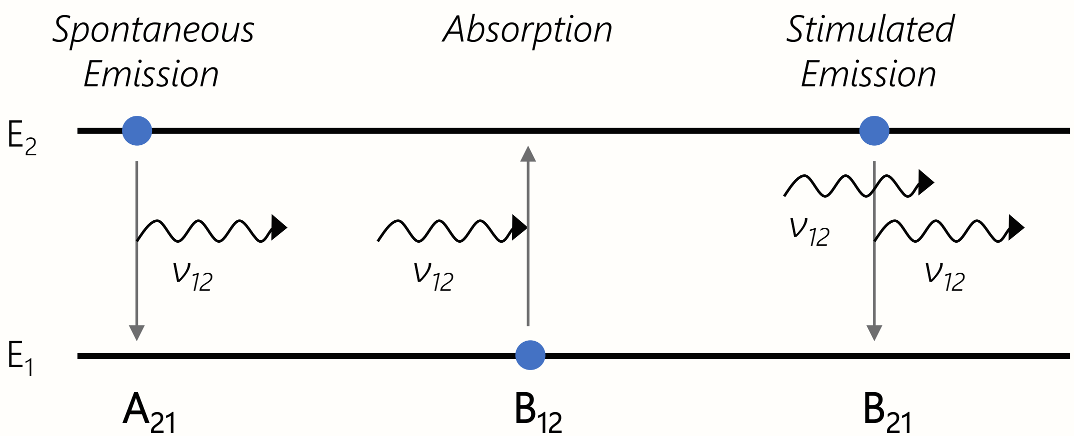
Transition Probabilities – Branching Fractions



Einstein coefficients

$$B_{12} = \frac{g_2}{g_1}\frac{c^3}{8\pi h v_{12}^3}A_{21}$$

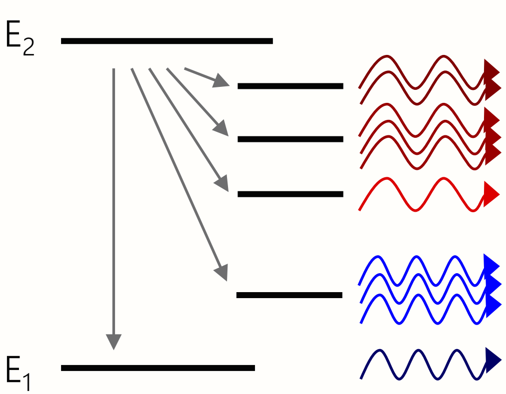
Transition Probabilities – Branching Fractions

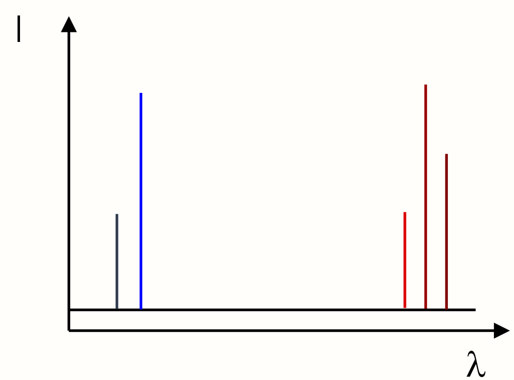


Einstein coefficients

$$B_{12} = \frac{g_2}{g_1}\frac{c^3}{8\pi h \nu_{12}^3}A_{21}$$

Decay to multiple levels





$$A_{21} = \frac{BF_{21}}{\tau_2}$$

$$BF_{21} = \frac{I_{21}}{\sum_i I_{2i}} = \frac{EW_{21}}{\sum_i EW_{2i}}$$

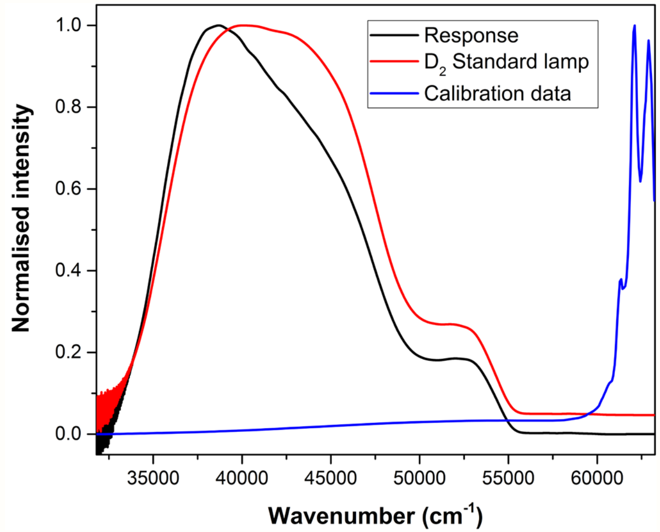
BF = Branching fraction
EW = Line equivalent width
τ = Level lifetime (s)

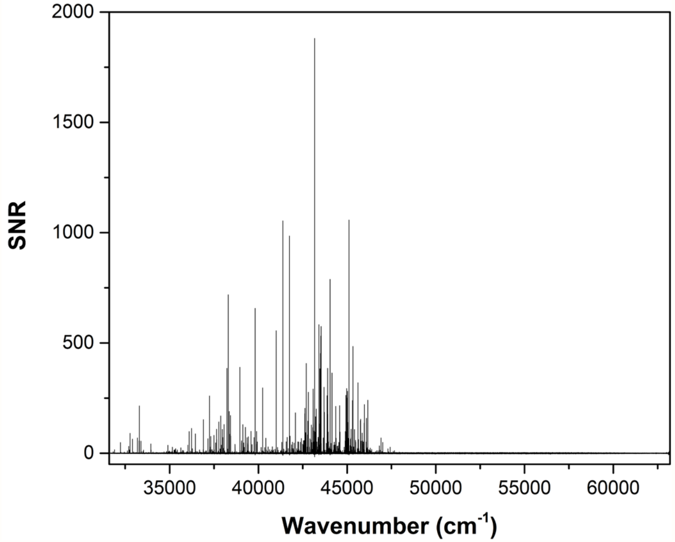
Transition Probabilities – Intensity Calibration

- Branching fraction:

$$BF_{21} = \frac{I_{21}}{\sum_i I_{2i}} = \frac{EW_{21}}{\sum_i EW_{2i}}$$

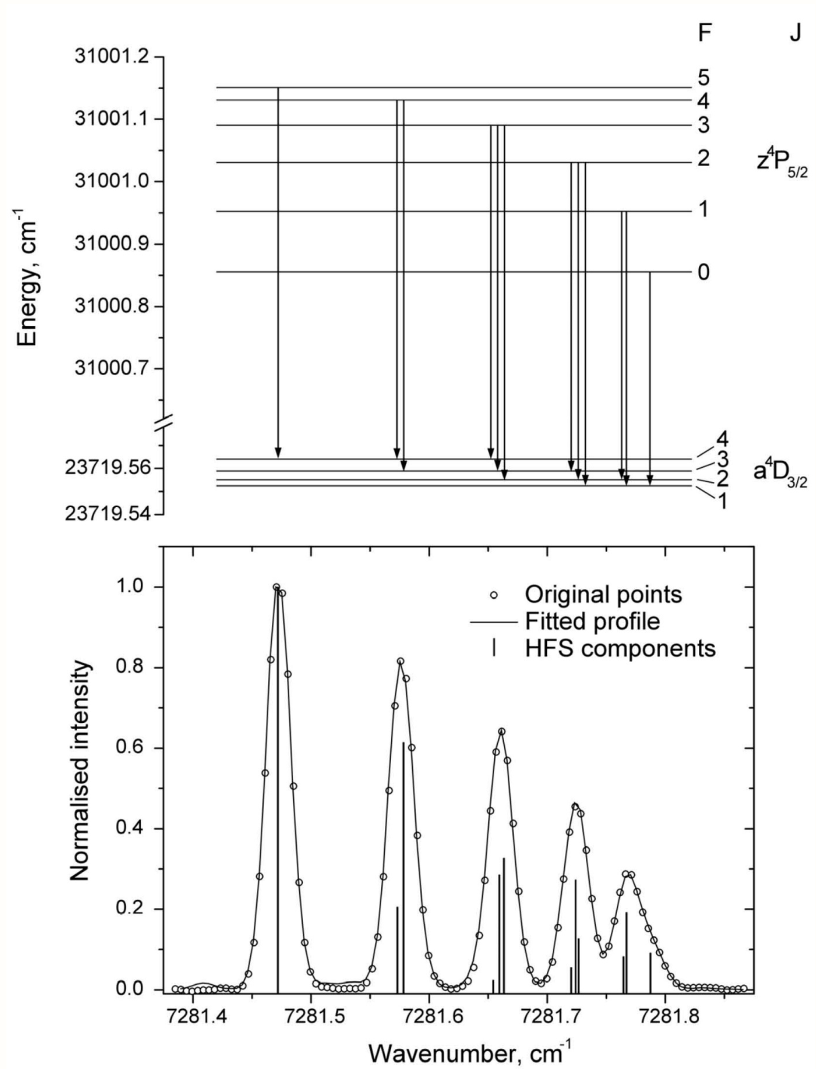
- Relative intensities = intensity calibration
- D_2 from 1650 – 3600A, W at longer
- Many sources of uncertainty:
  - Lifetimes
  - Lamp calibration
  - Alignment
  - Separation of spectral lines
  - Missing lines
  - Self-absorption
- **Typical log(gf) uncertainties 5% - 10%**





Nuclear Effects

- Hyperfine Structure:
  - Orders of magnitude smaller than fine structure
  - Caused by interactions of the nuclear dipole moment (I) with atomic magnetic and electric fields
  - Affects isotopes with odd mass numbers

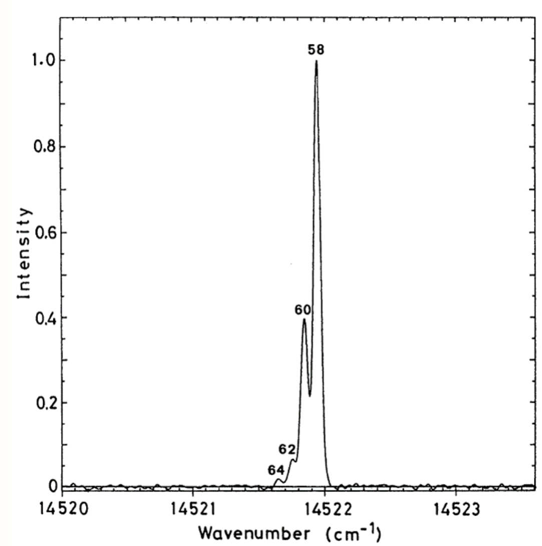


Mn I transition from $3d^6(^5D)4s - 3d^5(^6S)4s4p(^3P)$ [1]

[1] Blackwell-Whitehead, R. J. et al., 2005, ApJS., **157**, 402-409

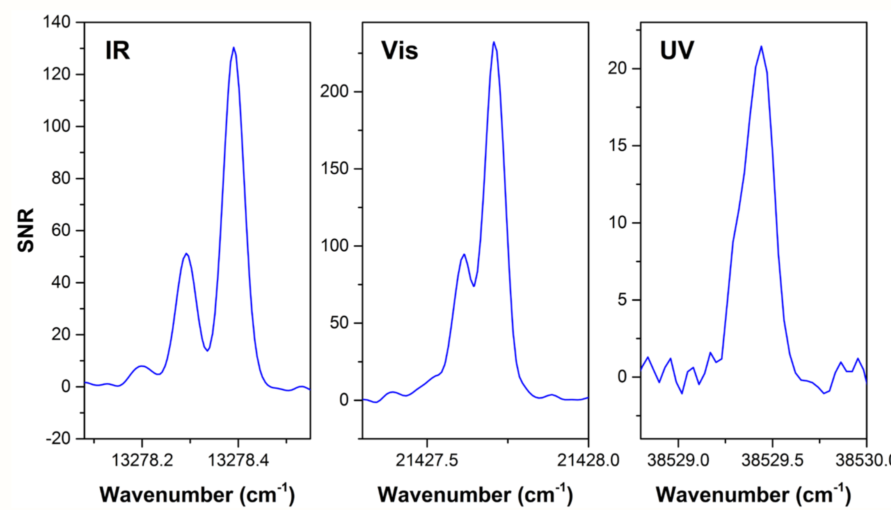
Nuclear Effects

- Hyperfine Structure:
  - Orders of magnitude smaller than fine structure
  - Caused by interactions of the nuclear dipole moment (I) with atomic magnetic and electric fields
  - Affects isotopes with odd mass numbers
- Isotope Structure:
  - Additional neutrons give:
    - Mass effect
    - Volume effect
  - Component intensities are proportional to relative abundance



Isotope structure in Ni II λ6884 Å [1]

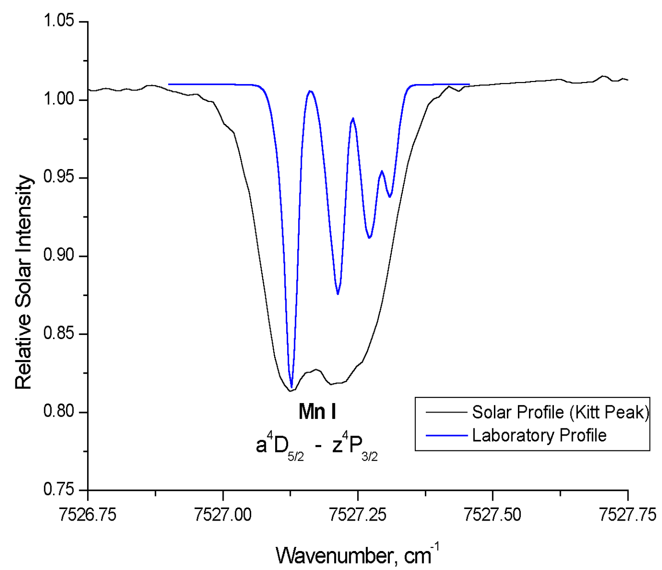
^{x}Ni	%
58	68.1
60	26.2
61	1.14
62	3.63
64	0.93



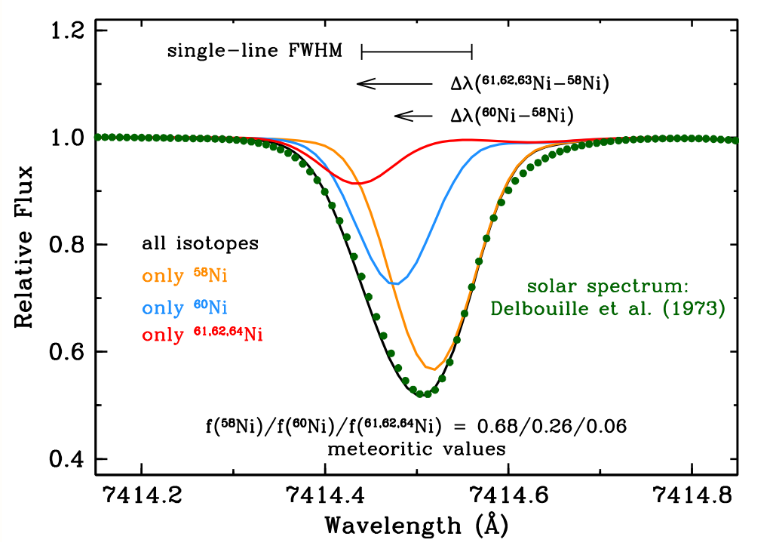
[1] Rosberg, M., et al., 1993, MNRAS, **262**, L1-L5

Nuclear Effects

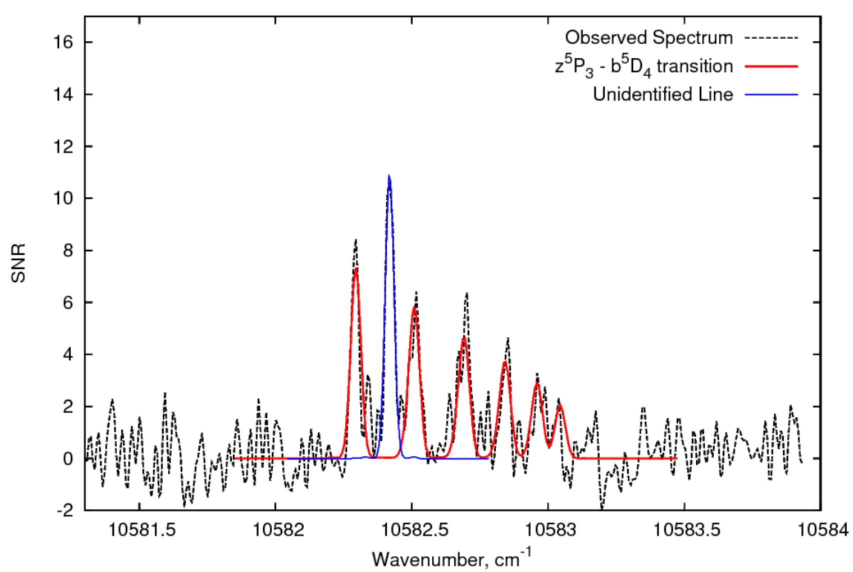
- Well resolved in experiment, but blended in stellar spectra
- Wavelengths shifted
- Systematic errors in width – lead to incorrect abundances
- FTS able to determine HFS A values to **few %**



Solar and laboratory Mn I spectral line comparison



Isotope structure in Ni I [1]



Blending of HFS Mn II and unidentified line [2]

[1] Sneden, C. et al, 2014, PhyS, **89**, 11
[2] Liggins, F. S. et al., 2021, ApJS, **252**, 10-22

Recent Successes

Ni II	**58 new energy levels** identified and **489 energy levels revised** with at least an order of magnitude reduction in uncertainty. Ritz wavelengths of forbidden lines. Theoretical calculations undertaken with Raassen & Uylings. Clear et al., ApJS, 261, 35, (2022)
Fe III	First FTS measurements in the VUV. **Revision of > 300 levels. 456 Ritz wavelengths** to be used as wavelength standards in the UV-VUV (for the calibration of spectra of hot stars). Concepcion F. PhD Thesis, Imperial College London, (2022)
Mn II	New accurate data for **614 energy levels and 6019 lines.** New Ritz wavelengths for 1130 forbidden transitions. Liggins et al., ApJS, 252, 10, (2021) & Liggins et al., ApJ, 907, 69, (2021)
Co II	Magnetic hyperfine interaction constants for **292 energy levels**, only 28 were previously known. Characterises **broadening** of stellar absorption lines, essential for accurate abundance analyses. Ding & Pickering, ApJS, 251, 1, (2020)
Nd III	Fourier transform spectra of Nd-Ar lamps from the VUV to IR **measured over 22,000 lines**. Term analysis of these transitions produced over **240 new energy levels with over 900 transitions identified as Nd III.** Ding et al., *in preparation* (2023)

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DOUBLY-IONISED IRON : NEW ACCURATE WAVELENGTHS AND ENERGY LEVELS

Florence Concepcion

THE SPECTRUM AND ENERGY LEVELS OF DOUBLY IONISED NEODYMIUM

Milan Ding

Summary

- Line identifications and accurate line **wavelengths**
  - accurate to at least **1 part in 10^7** (0.15mÅ at 1500Å, 0.001 cm-1)
- Atomic **energy levels**
  - Typically, **0.001 – 0.006 cm^{-1}** uncertainty
- **Hyperfine and isotope** structure parameters (line broadening)
  - Fitting to a **few %**
- **Oscillator strengths**, transition probabilities, f-values
  - accurate to **<10%**
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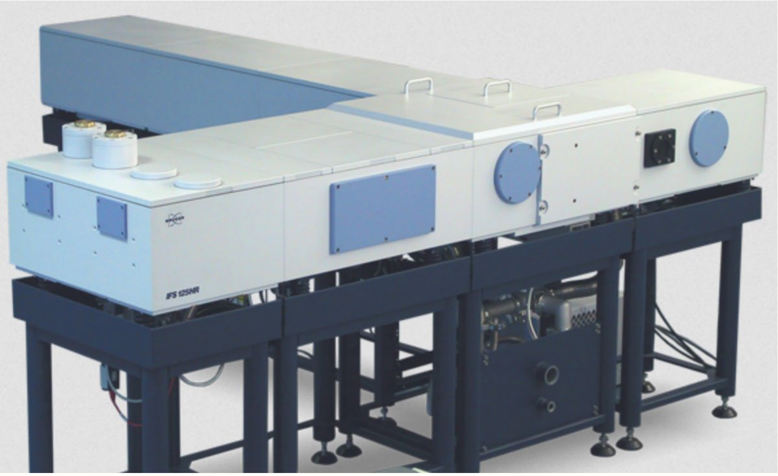
- Conclusion: **Imperial needs an IR FTS!**

New Instrument

Bruker IFS 125HR



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Max. path difference	50 cm
Resolving power	1 x 10^6 at 1000 nm
Maximum resolution	0.018 cm^{-1}
Range	~400 – 1720 nm
Wavenumber accuracy	±0.001 cm^{-1}

Future work

Ni II	**New transition probabilities in the UV.** Lifetimes from experimental laser induced fluorescence (LIF) measurements.
Ni II	**Extension of energy level analysis beyond FTS lower wavelength limit**. Grating plates have been recorded in collaboration with NIST.
Mn I	FT and grating spectra have been recorded across the IR-visible-VUV region. **A full energy level analysis is planned**.
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We are open to data requests and collaborations!

Please come and discuss your atomic data needs with us.