A New Approach to the Analysis of Experimental Atomic Spectra

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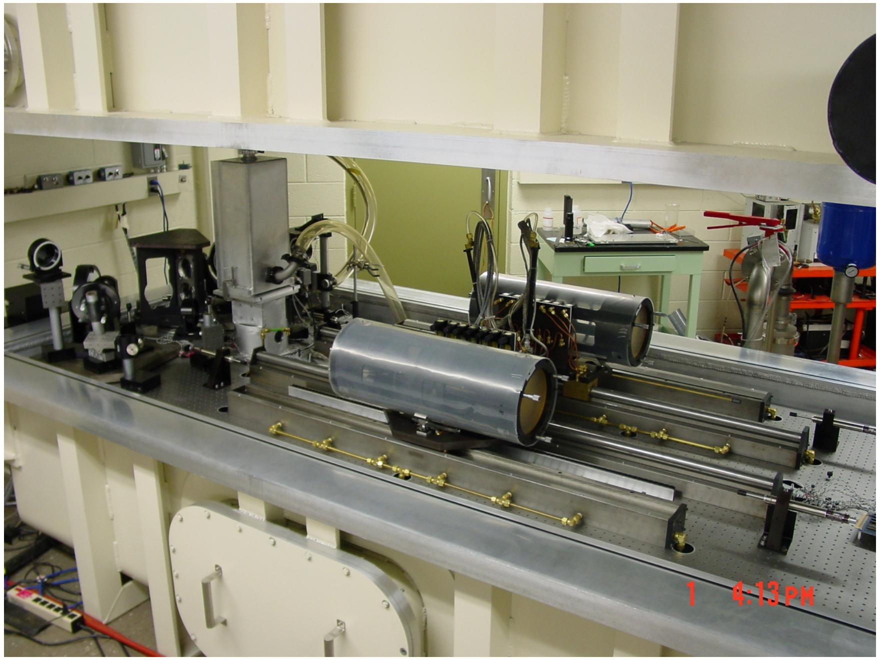
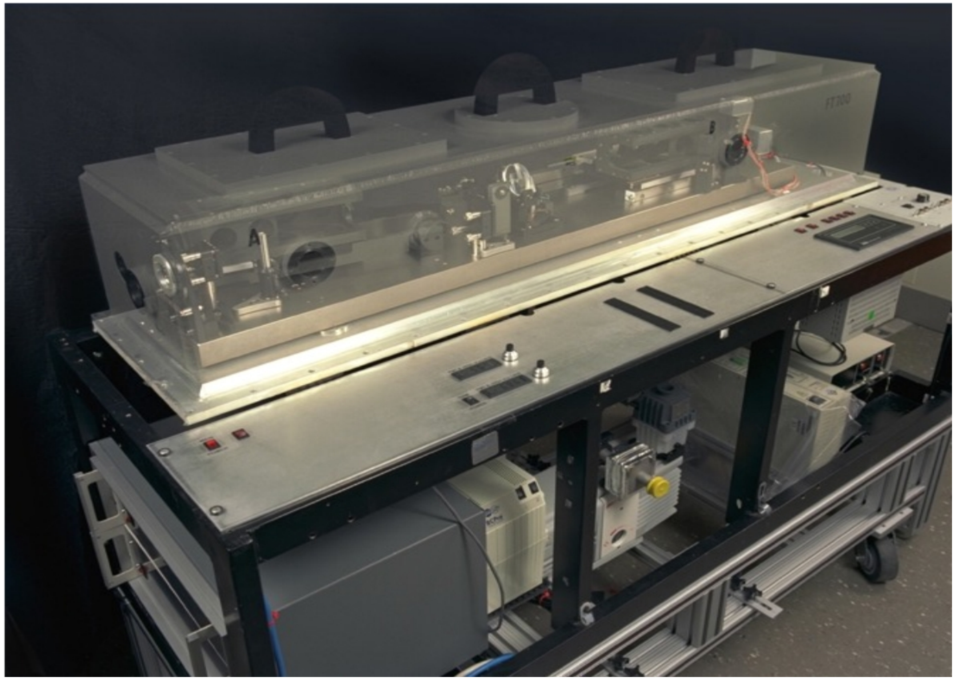
Dedicated to James E. Lawler, 1951 - 2023

29 years of Fourier transform spectroscopy at NIST





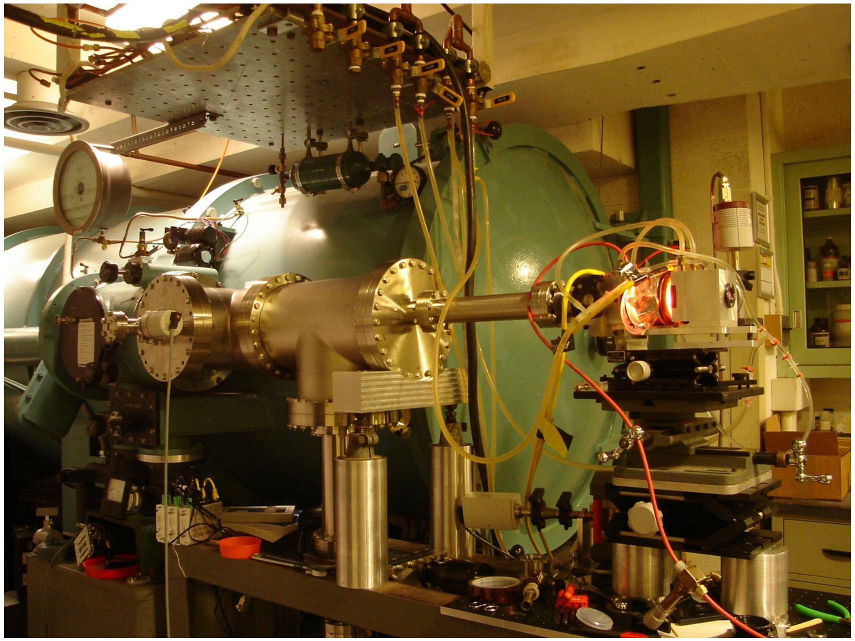
2-m FTS. Wavelength range 2200 Å – 5.5 µm. Resolution 0.0025 cm^{-1} (4 million at 1 µm).

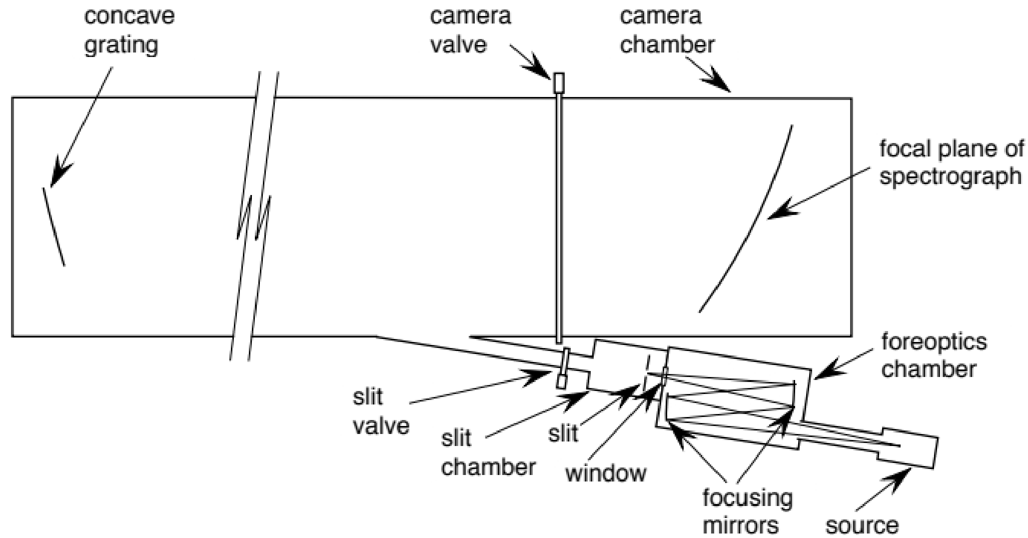
Brought to NIST in 1994 from Los Alamos National Laboratory by Craig Sansonetti and Joseph Reader

Vacuum ultraviolet FTS. Wavelength range 1400 Å– 9000 Å. Resolution 0.025 cm^{-1} (2 million at 2000 Å).

Brought to NIST in 1996 by Ulf Griesmann

Normal Incidence Spectrograph





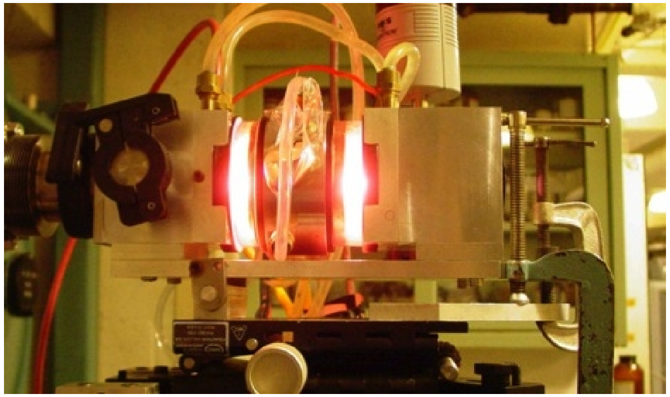
Normal incidence vacuum spectrograph.

Wavelength range: 300 Å - 5000 Å.

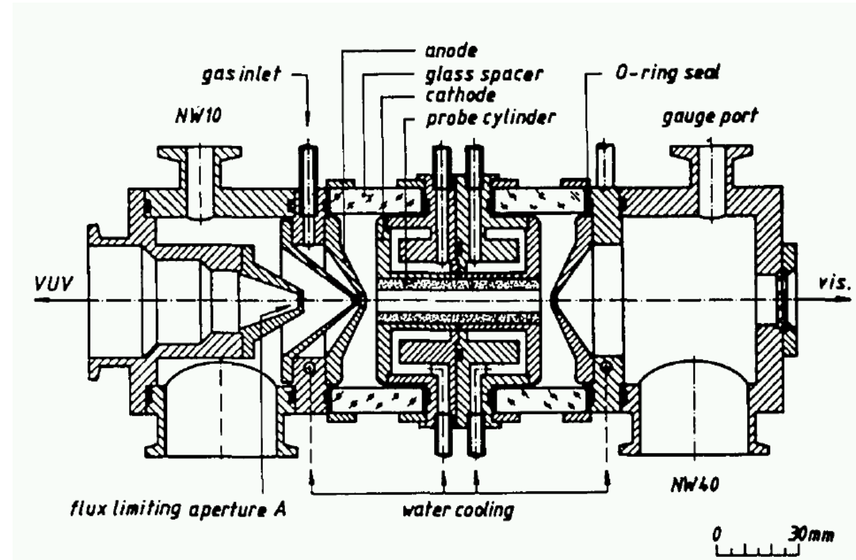
Resolving power: ≈150000 (1st order) with photographic plates.

Also used with image plates at lower resolution

Hollow cathode lamps



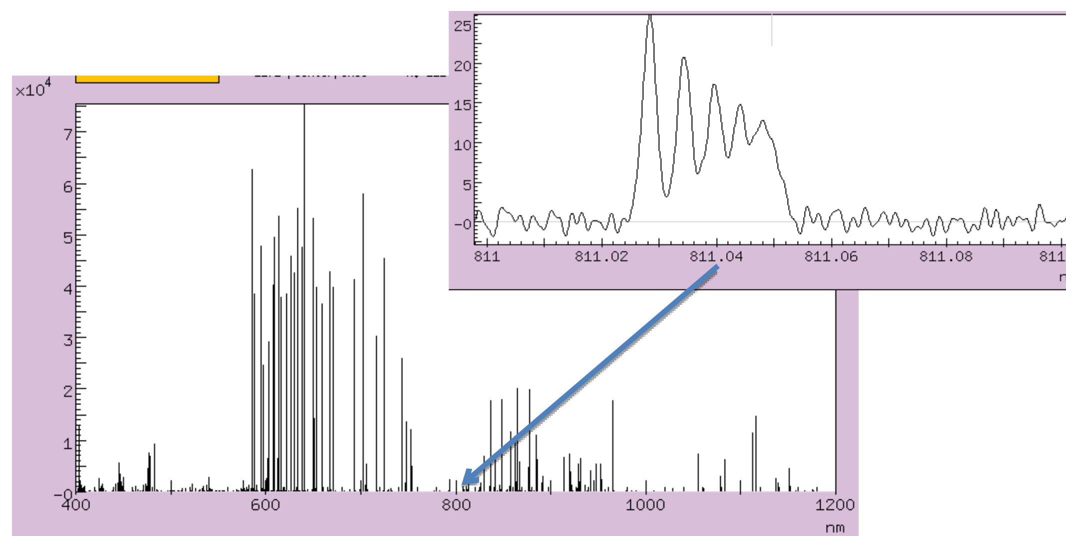
High current (1-2 A) hollow cathode source.



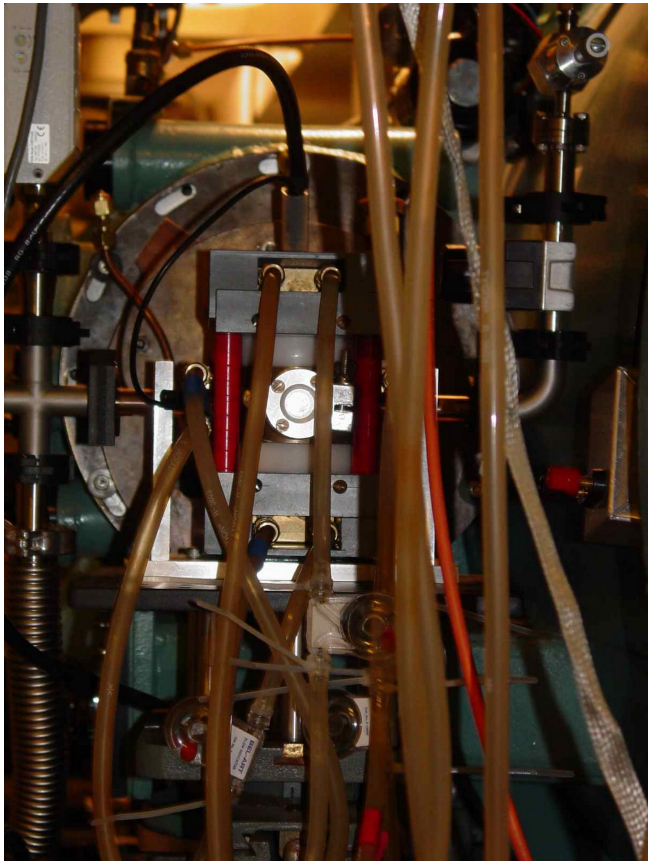
Danzmann, Fischer, Kock, Kühne, Apl Opt. 27, 4947 (1988)

Commercial (10-20 mA) hollow cathode lamp

A typical spectrum of an iron-group element will contain several thousand lines



Sources for higher ionization stages



Penning discharge source. Suitable for singly-ionized and doubly-ionized spectra.

Sliding spark source used to excite doubly-ionized through seven-times ionized spectra.

Rare Earth Elements (1996 - 2003): Measurements for Lighting Industry

- Metal halide lamps were the main sources used in commercial lighting, for street lights, stadiums, large commercial buildings, and more.
- Many had a poor color (e.g. sodium lamps, with a yellow color), and the ones with better color had poor efficiency.
- Both color and efficiency can be improved by adding rare-earth elements – dysprosium, holmium. These have very complex spectra.
- Better wavelengths, energy levels, and transition probabilities required.

M. E. Wickliffe, J. E. Lawler, G. Nave,"Atomic transition probabilities for Dy I and Dy II," Journal of Quantitative Spectroscopy and Radiative Transfer 66, 363 (2000).

G. Nave, U. Griesmann, "New energy levels and classificiations of spectral lines from neutral and singly-ionized dysprosium (Dy I) ," Physica Scripta 62, 463 (2000).

G. Nave, “Atomic transition rates for neutral holmium (Ho I)", J. Opt. Soc. Am. B 20, 2193 (2003).

Measurements for astrophysics: Wavelengths and energy levels for Sc II-Ni II

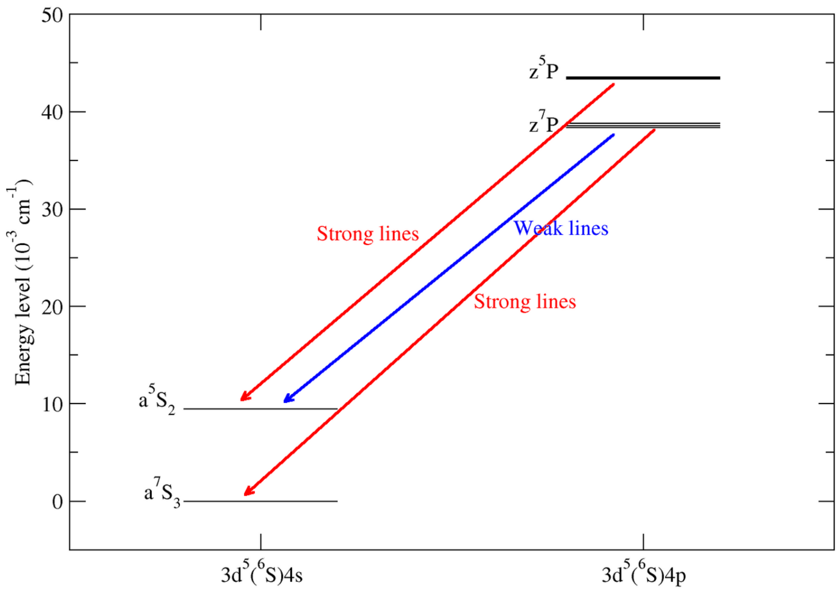
Ion	Previous	Our work	
Fe II	1978	Completed	Nave & Johansson (2011)
Cr II	1951	Completed	Sansonetti & Nave (2014)
Mn II	1964	Completed	Liggins et al. (2021)
Ni II	1970	Publications in progress	Clear, ICL PhD Thesis (2022, 2023)
Sc II	1980	Publication in progress	Hala & Nave (2023)
Co II	1998	Spectra recorded, analysis begun	
V II	1988	Completed	Thorne et al. (2013)
Ti II	1982	Completed	Saloman (2012)
HFS (Mn II, Co II, Sc II)		Completed	Townley-Smith et al. (2016), Lawler et al. (2016), Ding (2020), Hala (accepted)

Complications

- Large number of lines and energy levels.
- Hyperfine or isotope structure
- Self Absorption / Self Reversal
- Mis-identified lines
- Blends
- Incorrect uncertainties
- Inaccurate calculations
- Problems in lines connected to levels

Connecting ground level in Mn II

Liggins et al. 2021, ApJS 252:10



The intercombination lines connecting the quintet system to the septet system are weak.

Care is needed otherwise all of the quintet levels will be wrong!

In our highest current spectra, we have good SNR for the intercombination lines. But the LS-allowed strong lines are too strong to be usable!

Combining several different spectra and paying close attention to the wavelength calibration is necessary to get this right.

Spectra recorded using NIST FT spectrometers

Spectra	Purpose
Lanthanides: Ce, Tb, Dy, Ho	Atomic data for lighting (Wl, TP, En, HFS) astrophysics.
Iron group elements: Sc-Cu, mainly I-II, some III	Atomic data for astrophysics (Wl, TP, En, HFS), Wavelength standards
Noble gases: He-Xe	Atomic data, wavelength and intensity calibration of spectra
Others: F,Na,Al,Si,K,Ge,Ag,Pt	Many of these for wavelength calibration varying to atomic clocks (Ag) to astronomical spectra (Pt)
Actinides: Th, U	Wavelength calibration of spectrographs on ground-based telescopes
Molecules: I_2, S_2, HCN, CO, C_2H_2,	Wavelength calibration of astronomical spectrographs in visible (I_2) & IR (HCN,CO,C_2H_2); atmospheric chemistry (S_2).
Others	Laser-frequency comb for calibration of IR astronomical spectrograph; Fiber Fabry-Perot for calibration of visible astronomical spectrograph

Use of archival spectra for Cr II transition probabilities

Table 1. Table of Spectra

ID	Date	Wavelength Range (nm)	**Wavenumber (cm^{-1})**	Coadds	Resolution (cm^{-1})	Gas	Pressure (Pa)	Current (A)	Detector	Calibration Lamp	Comments
1	2000 Oct 27 #1	**183 to 317**	**31500 to 54600**	64	0.08	Ar	80	0.7	R7154	D_2 # BQ0057	HCL[a]
2	2000 Oct 27 #3	**183 to 317**	**31500 to 54600**	64	0.08	Ar	85	1.5	R7154	D_2 # BQ0057	HCL[a]
3	2000 Nov 06 #1	**249 to 400**	**25000 to 40100**	64	0.033	Ar	85	0.7	R106UH	D_2 # BR0065	HCL[a] 11[b]
4	2000 Nov 06 #3	**183 to 320**	**31200 to 54600**	128	0.09	Ar	85	1.5	R7154	D_2 # BR0065	HCL[a]
5	2000 Nov 07 #1	**183 to 317**	**31500 to 54600**	128	0.06	Ar	85	1.5	R7154	D_2 # BR0065	HCL[a]
6	2000 Nov 07 #2	**183 to 317**	**31500 to 54600**	64	0.06	Ar	85	0.7	R7154	D_2 # BR0065	HCL[a]
7	2000 Dec 08 #1	**183 to 322**	**31000 to 54600**	128	0.15	Ne	0.4	1.4	R7154	None	Penning 17[b]
8	2011 Jun 10 #7	**285 to 1207**	**8280 to 35000**	107	0.02	Ne	400	2	diode	W lamp IR456	HCL[a] 18[b]
9	2016 Apr 24 #5	**190 to 704**	**14200 to 52500**	259	0.1	Ne	-[c]	0.02	R106UH & R636-10	D_2 #V0236 & W #IR456	HCL

[a] HCL: High current hollow cathode lamp

[b] Number of spectrum in Table 2 of Lawler et al. (2017b)

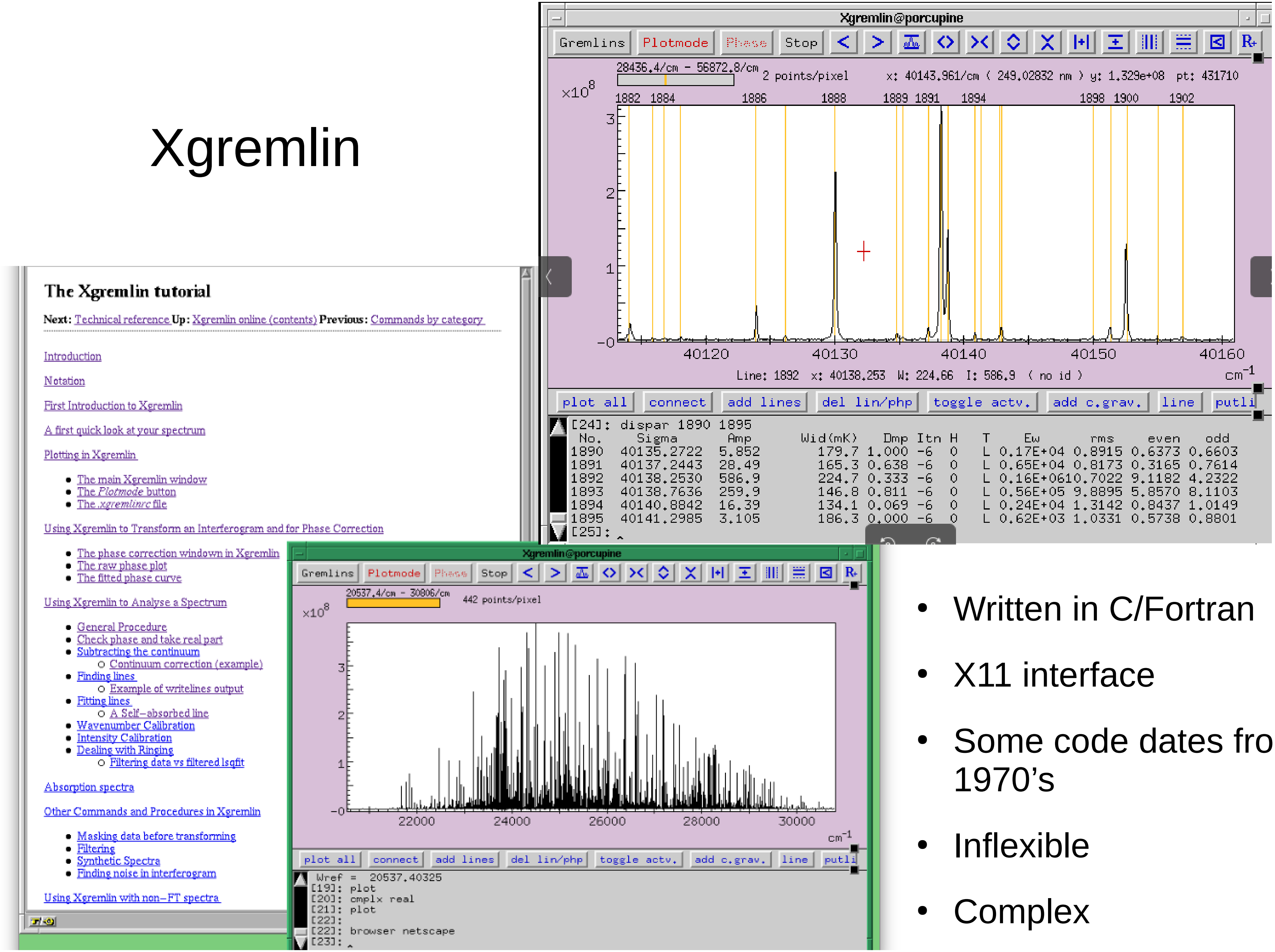
[c] Spectrum 9 was of a commercial Cr/Ne hollow cathode lamp and the gas pressure is unknown.

Spectra 1-7: Recorded in 2000 for TP work but never analyzed
Spectrum 7: Radiometric calibration file was damaged
Spectrum 8: Recorded for wavelengts/energy level work
Spectrum 9: Low current lamp recorded to validate calibration of other files

Analysis challenges

- Too few people for analysis.
- Analysis of complex spectra (tens of thousands of lines, several hundred energy levels) has a steep learning curve and takes a long time to learn.
- Reliance on short-term students (both PhD and summer students).
- No continuity.
- Steep learning curve for current software.
- Different conventions for coding and matching atomic parameters (experiment and theory).

Xgremlin



- Written in C/Fortran
- X11 interface
- Some code dates from 1970's
- Inflexible
- Complex

Analysis software

- Old code written in languages rarely taught (C, Fortran), but preserves key knowledge from experts. Many written for computers with small amounts of memory.
- Interfaces are platform specific (X11, Windows), and often not portable.
- Solution is every new person (student, intern) writes their own ‘wrapper’ specific to their platform and needs, that is often not easily understood by others and takes time out of a short summer project.
- Software does not preserve the analysis history of data, so the next student/intern cannot understand what has been done.

Solutions

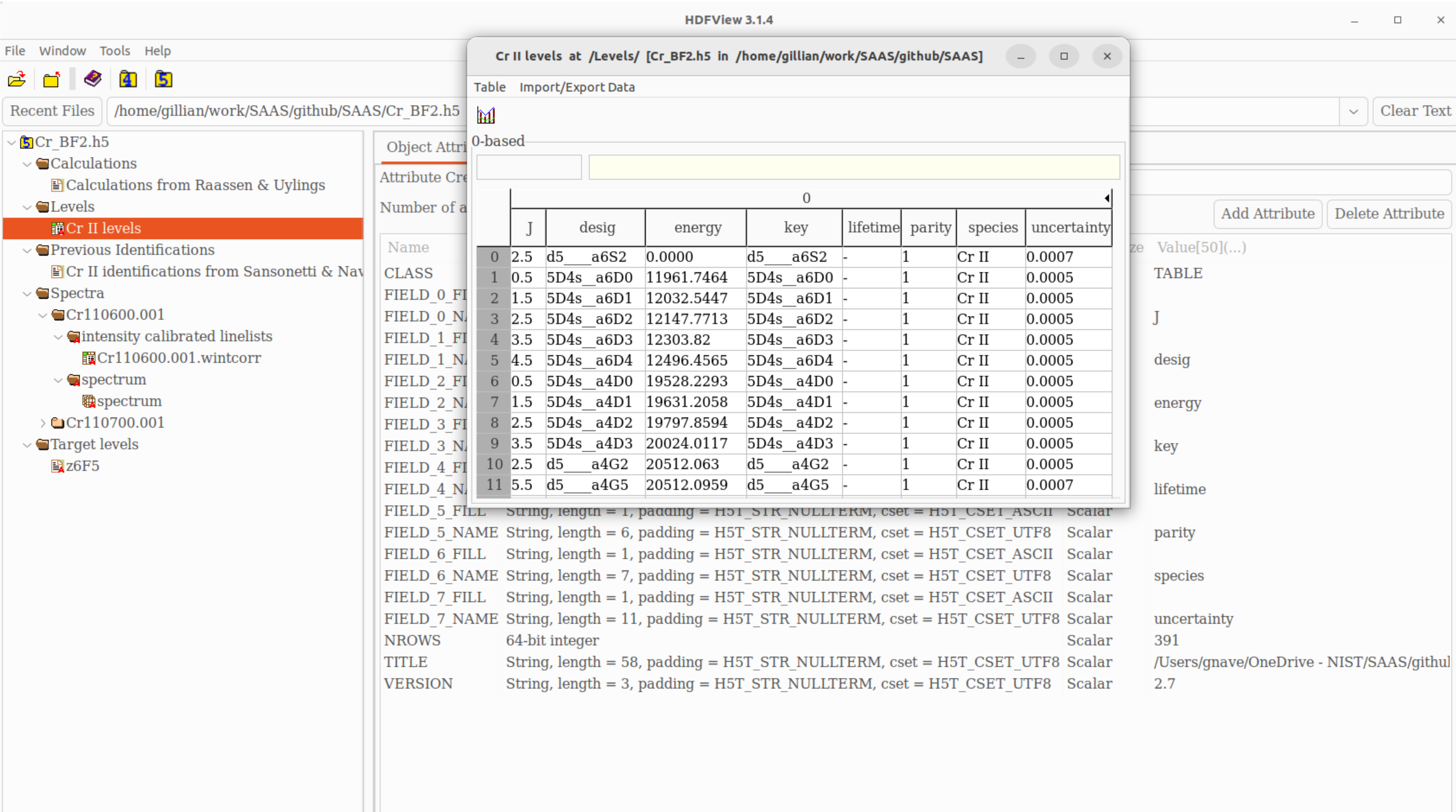
- Data needs to be accompanied by code
- Version history of data and its processing needs to be conserved and easily accessible
- Needs to be common interface that is platform-independent and easily understood by new people
- Structure that is flexible enough that new analysis programs can easily be added to existing software

Heirarchical Data Format

- HF5 format consists of two structures:
  - Datasets (analogy – a data file)
  - Groups (analogy – a directory)

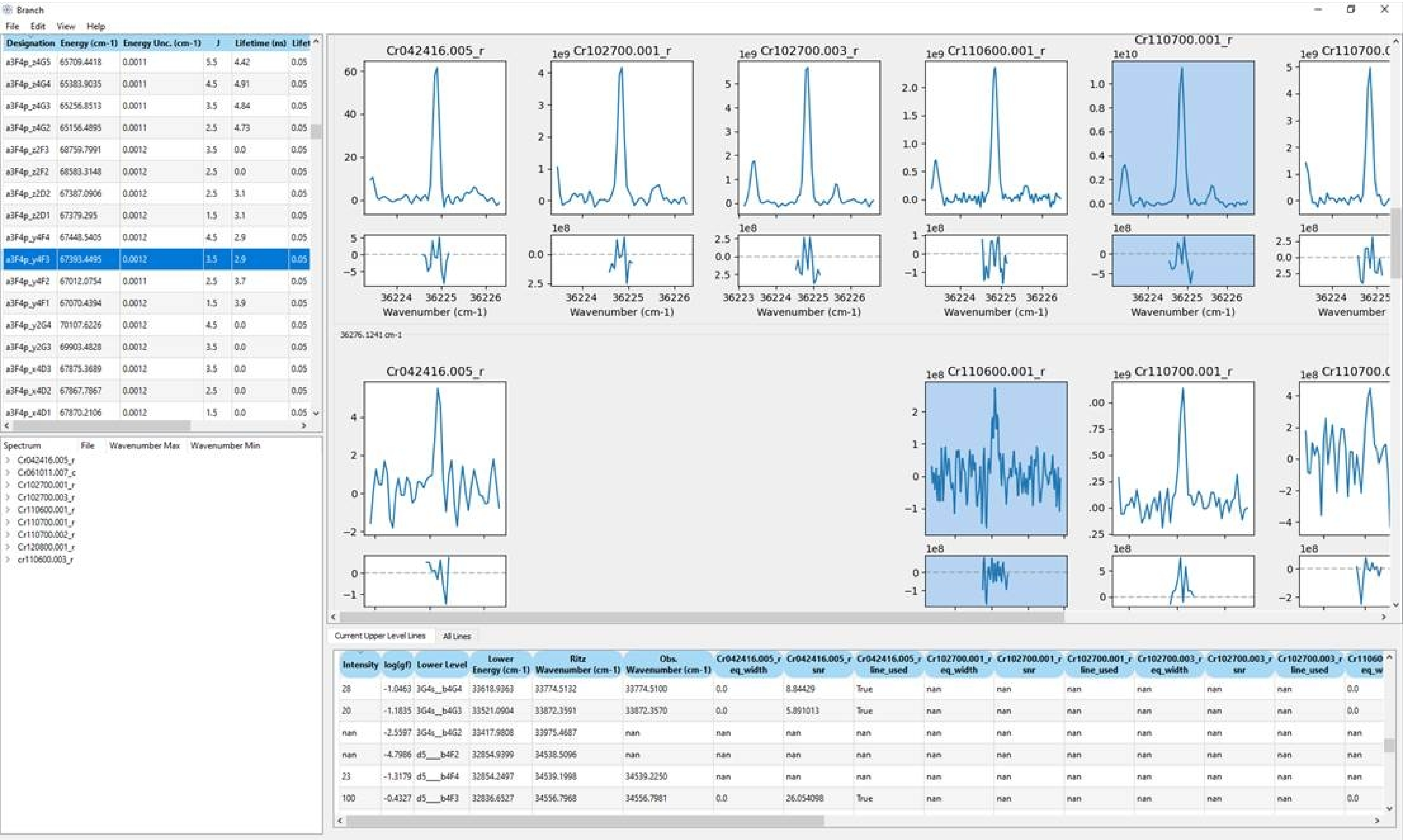
- Data are accompanied by metadata.
- More than one version of an analysis can be kept, so history of file processing can be preserved and easily accessed.

Example HDF5 file structure



	J	desig	energy	key	lifetime	parity	species	uncertainty
0	2.5	d5___a6S2	0.0000	d5___a6S2	-	1	Cr II	0.0007
1	0.5	5D4s_a6D0	11961.7464	5D4s_a6D0	-	1	Cr II	0.0005
2	1.5	5D4s_a6D1	12032.5447	5D4s_a6D1	-	1	Cr II	0.0005
3	2.5	5D4s_a6D2	12147.7713	5D4s_a6D2	-	1	Cr II	0.0005
4	3.5	5D4s_a6D3	12303.82	5D4s_a6D3	-	1	Cr II	0.0005
5	4.5	5D4s_a6D4	12496.4565	5D4s_a6D4	-	1	Cr II	0.0005
6	0.5	5D4s_a4D0	19528.2293	5D4s_a4D0	-	1	Cr II	0.0005
7	1.5	5D4s_a4D1	19631.2058	5D4s_a4D1	-	1	Cr II	0.0005
8	2.5	5D4s_a4D2	19797.8594	5D4s_a4D2	-	1	Cr II	0.0005
9	3.5	5D4s_a4D3	20024.0117	5D4s_a4D3	-	1	Cr II	0.0005
10	2.5	d5___a4G2	20512.063	d5___a4G2	-	1	Cr II	0.0005
11	5.5	d5___a4G5	20512.0959	d5___a4G5	-	1	Cr II	0.0007

Very preliminary UI for BFs



Potential methods

- Wavelength/Intensity calibration of spectra
- Optimization of energy levels using LOPT
- Energy level searches
- Measurement of branching fractions and transition probabilities
- Hyperfine/Isotope structure analysis
- ???

Conclusions

We have too few people in atomic spectroscopy to maintain the field – we need new people, a more efficient way of training them, and better tools to archive, distribute, and analyze our data.

Combination of a ‘storage container’ like hdf5 with better user-friendly software offers promise for increasing our efficiency.

This is a multi-year project and cannot be achieved with a few people working on their own.

Come and join our team!