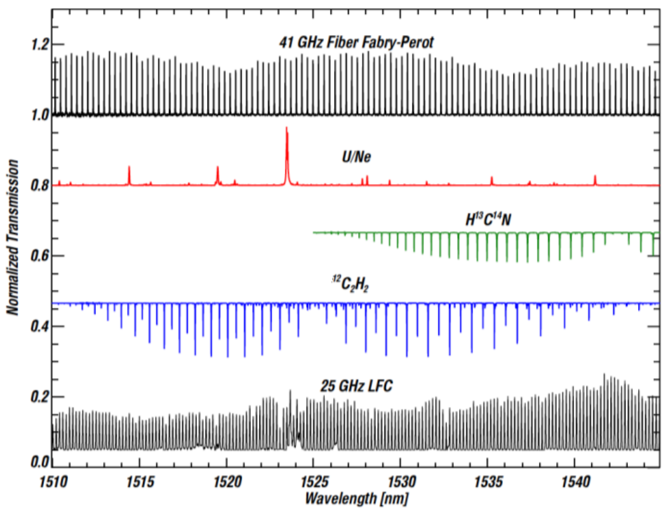
PHYSICAL MEASUREMENT LABORATORY

Wavelength references for the calibration of astronomical telescopes



Gillian Nave

Stephen Redman
NRC Postdoc

Craig Sansonetti
(now retired)

Florian Kerber

Physical Reference Data

Elemental Data Index

Provides access to the holdings of NIST Physical Measurement Laboratory online data organized by element.

Periodic Table: Atomic Properties of the Elements

Contains NIST critically-evaluated data on atomic properties of the elements.
Suitable for high-resolution color printing for desk or wall-chart display.

Physical Constants

Contains values of the fundamental physical constants and a related bibliographic database.

Atomic Spectroscopy Data

Contains databases for energy levels, wavelengths, and transition probabilities for atoms and ions and related bibliographic databases.

Molecular Spectroscopic Data

Includes databases containing spectroscopic data for small molecules, hydrocarbons, and interstellar molecules. In addition, there are two publications containing equations and the underpinning theory for molecular spectroscopy.

Atomic and Molecular Data

Contains databases on thermophysical properties of gases, electron-impact cross sections (of atoms & molecules), potential energy surfaces of group II dimers, and atomic weights and isotopic compositions.

X-Ray and Gamma-Ray Data

Contains databases on the interaction of x-rays and gamma-rays with elements and compounds.

Radiation Dosimetry Data

This database calculates stopping-power and range tables for electrons, protons, or helium ions.

Nuclear Physics Data

Contains a table of the half lives of 65 radionuclides and a database of the isotopic compositions, atomic weights and relative atomic masses of the elements.

Condensed Matter Physics Data

This database consists of evaluated data for use in total-energy calculations of electronic structure by density-functional theory. It contains total energies and orbital energy eigenvalues for all atoms from hydrogen to uranium.

Other NIST Data

PHYSICAL MEASUREMENT LABORATORY

Atomic Spectroscopy Databases

- Atomic Spectra Database
- Handbook of Basic Atomic Spectroscopic Data
- Energy Levels of Hydrogen and Deuterium
- Ground Levels and Ionization Energies
- NLTE Databases and Codes
  - FLYCHK Collisional-Radiative Code
  - SAHA Plasma Population Kinetics Database
  - NLTE4 Plasma Population Kinetics Database
- Spectrum of Platinum Lamp for Ultraviolet Spectrograph Calibration
- Spectrum of Th-Ar Hollow Cathode Lamps
- X-ray Transition Energies
- Atomic Spectra Bibliographic Databases
  - Bibliographic Database on Atomic Transition Probabilities
  - Bibliographic Database on Atomic Spectral Line Broadening and Shifts
  - Bibliographic Database on Atomic Energy Levels and Spectra

NIST
PHYSICAL MEASUREMENT LABORATORY

omic Spectra Database Lines Form

Best viewed with the latest versions of Web browsers and JavaScript enabled

Spectrum Fe I e.g., Fe I or Na;Mg; Al or mg i-iii

Lower Wavelength: 370 or Upper Wavenumber (in cm^{-1})

Upper Wavelength: 375 or Lower Wavenumber (in cm^{-1})

Units: nm

Reset input | Retrieve Data

Dynamic Plots

Line Identification Plot:

Saha-LTE Spectrum:

Electron Temperature T_e(eV): | Doppler-broadened spectrum

Electron Density N_e(cm^{-3}): | Ion Temperature T_i(eV): (if $T_i \neq T_e$)

Grotrian Diagram

Java subwindow size:
640 x 640 | 800 x 640 | 1024 x 768 | 1280 x 1024

Group by configurations | Term multiplicity
Show only radiatively linked levels

Make Grotrian Diagram (requires Java2)
Java Security Level should be Medium. For Java 8 Update 20, add http://physics.nist.gov to the Java Control Panel exception site list.

Output Options

Format output: HTML (formatted)

No JavaScript

Energy Level Units: cm-1

Display output: in its entirety

Page size: 15

Output ordering: Wavelength / Multiplet

Optional Search Criteria

Maximum lower level energy: 5000 (e.g., 100000)

Maximum upper level energy: (e.g., 400000)

Transition strength bounds will apply to: Aki

Minimum transition strength: (e.g., 1.2e+05)

Maximum transition strength: (e.g., 2.5e+12)

Accuracy minimum: (e.g., C+)

Additional Criteria

Lines:
- All
- Only with transition probabilities
- Only with energy level classifications
- Only with observed wavelengths
- Only with diagnostics

Include diagnostics data

Bibliographic Information: TP references, Line references

Wavelength Data:
- Observed
- Ritz
- Observed - Ritz (difference)
- Wavenumber (in cm^{-1})

Wavelengths in:
- Vacuum (< 200 nm) Air (200 - 1,000 nm) Wavenumber (> 1,000 nm)
- Vacuum (< 1,000 nm) Wavenumber (> 1,000 nm)
- Vacuum (< 200 nm) Air (200 - 2,000 nm) Vacuum (> 2,000 nm)
- Vacuum (all wavelengths)
- Vacuum (< 185 nm) Air (> 185 nm)
- Wavenumber (all wavelengths)

Transition strength: A_{ki} | g_kA_{ki} | in units of 10^8 s^{-1}

f_{ik} | S_{ik} | log(gf)

Relative Intensity

Transition Type: Allowed (E1) | Forbidden (M1,E2,...)

NIST Atomic Spectra Database Lines Data

Fe I: 9 Lines of Data Found

Z = 26, Fe isoelectronic sequence

Example of how to reference these results:
Kramida, A., Ralchenko, Yu., Reader, J., and NIST ASD Team (2015). *NIST Atomic Spectra Database* (ver. 5.3), [Online]. Available: http://physics.nist.gov/asd [2017, January 10]. National Institute of Standards and Technology, Gaithersburg, MD.
BibTex Citation (new window)

Wavelength range: 370 - 375 nm
Wavelength in: vacuum below 200 nm, air between 200 and 2000 nm, vacuum above 2000 nm
Lower State Energy limit: 5000 cm^{-1}

Highest relative intensity: 2510000
Some data for neutral and singly-charged ions are available in the Handbook of Basic Atomic Spectroscopic Data

		Primary data sources	Query NIST Bibliographic Databases for Fe I (new window)
Energy Levels:	Nave et al. 1994	The wavenumber measurements in Nave et al 1994 were calibrated with respect to Ar II lines measured by Norlén 1973 , which were re-measured later by Whaling et al. 1995 and found to be systematically too small. To account for this calibration error, the original measured wavenumbers and energy level values from Nave et al. 1994 have been increased here by 6.7 parts in 10^8. The ionization energy is from Schoenfeld et al. 1995 , adjusted by the same scaling factor.	Fe I Energy Levels
Lines:	Nave et al. 1994	Observed wavenumbers have been increased by 6.7 parts in 10^8, similar to the energy levels.	Fe I Line Wavelengths and Classification
Transition Probabilities:	Fuhr and Wiese 2006		Fe I Transition Probabilities

Observed Wavelength Air (nm)	Ritz Wavelength Air (nm)	Rel. Int. (?)	A_{ki} (s^{-1})	Acc.	E_i (cm^{-1})		E_k (cm^{-1})	Lower Level Conf., Term, J			Upper Level Conf., Term, J			Type	TP Ref.	Line Ref.
370.55658	370.556548	1290000	3.21e+06	A	415.933	-	27 394.691	$3d^6 4s^2$	$a\ ^5D$	3	$3d^6(^5D)4s4p(^3P°)$	$z\ ^5F°$	3		T3547	L11631
370.78218	370.782181	81000	6.33e+05	B	704.007	-	27 666.348	$3d^6 4s^2$	$a\ ^5D$	2	$3d^6(^5D)4s4p(^3P°)$	$z\ ^5F°$	1		T5720	L11631
371.99345	371.993444	r	1.62e+07	A	0.000	-	26 874.550	$3d^6 4s^2$	$a\ ^5D$	4	$3d^6(^5D)4s4p(^3P°)$	$z\ ^5F°$	5		T5720,T3957,T6116	L11631
372.25627	372.256272	1290000	4.97e+06	A	704.007	-	27 559.583	$3d^6 4s^2$	$a\ ^5D$	2	$3d^6(^5D)4s4p(^3P°)$	$z\ ^5F°$	2		T3547	L11631
373.33173	373.331716	1000000	6.48e+06	B+	888.132	-	27 666.348	$3d^6 4s^2$	$a\ ^5D$	1	$3d^6(^5D)4s4p(^3P°)$	$z\ ^5F°$	1		T5720	L11631
373.71313	373.713125	r	1.41e+07	A	415.933	-	27 166.820	$3d^6 4s^2$	$a\ ^5D$	3	$3d^6(^5D)4s4p(^3P°)$	$z\ ^5F°$	4		T3547	L11631
374.55610	374.556086	2510000	1.15e+07	A	704.007	-	27 394.691	$3d^6 4s^2$	$a\ ^5D$	2	$3d^6(^5D)4s4p(^3P°)$	$z\ ^5F°$	3		T3547	L11631
374.58993	374.589910	1100000	7.32e+06	A	978.074	-	27 666.348	$3d^6 4s^2$	$a\ ^5D$	0	$3d^6(^5D)4s4p(^3P°)$	$z\ ^5F°$	1		T3547	L11631
374.82619	374.826189	1910000	9.15e+06	A	888.132	-	27 559.583	$3d^6 4s^2$	$a\ ^5D$	1	$3d^6(^5D)4s4p(^3P°)$	$z\ ^5F°$	2		T3547	L11631

Query time: 0.4 sec

If you did not find the data you need, please inform the ASD Team.

NIST Atomic Spectra Bibliographic Databases

Welcome to the NIST Atomic Spectra Bibliographic Databases. References to publications may be selected and displayed after choosing one of the following three databases.

Atomic Transition Probability Bibliographic Database This interactive database contains references on atomic transition probabilities (oscillator strengths, line strengths, and radiative lifetimes). Both theoretical and experimental papers are listed.

Atomic Spectral Line Broadening Bibliographic Database This interactive database contains references on atomic spectral line broadening (line shapes and shifts). Both theoretical and experimental papers are listed.

Atomic Energy Levels and Spectra Bibliographic Database This interactive database contains references on atomic energy levels and wavelengths. Preference is given to experimental papers.

These databases provide access and search capability for NIST bibliography databases on atomic energy levels, wavelengths, transition probabilities, and line broadening and shapes. The Atomic Energy Levels Data Center and Data Center on Atomic Transition Probabilities and Line Shapes have implemented these databases, which are the main bibliography source for the NIST critical compilations. Both Data Centers are located in the Physical Measurement Laboratory at the National Institute of Standards and Technology (NIST).

These databases were funded [in part] by NIST's Standard Reference Data Program (SRDP) and by NIST's Systems Integration for Manufacturing Applications (SIMA) Program.

Spectroscopy

Atomic Spectroscopy Databases

- Atomic Spectra Database
- Handbook of Basic Atomic Spectroscopic Data
- Energy Levels of Hydrogen and Deuterium
- Ground Levels and Ionization Energies
- NLTE Databases and Codes
  - FLYCHK Collisional-Radiative Code
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  - Bibliographic Database on Atomic Energy Levels and Spectra

The Spectrum of the Th Ar Hollow Cathode Lamp

NIST
National Institute of Standards and Technology
Physical Meas. Laboratory

Custom Dataset

To get a specific dataset, Please choose your output preference and range of interest.

Choose the output format: **HTML or ASCII**	Chose your range: ◉ Range by Wavenumber 1700 - 14500 cm^{-1} ○ Range by Vacuum Wavelength 691 - 5804 nm
◉ HTML table ○ ASCII format	Minimum: [ ] Maximum: [ ] Submit
	Any field left blank will be set to its default value.

The Complete Dataset is available in 3 formats

HTML table without images (508 Compliant Version)	ASCII text file without images	PDF with images(6.2 MB)

Images are available in 100 cm^{-1} segments in either pdf or gif format

PDF images	gif images

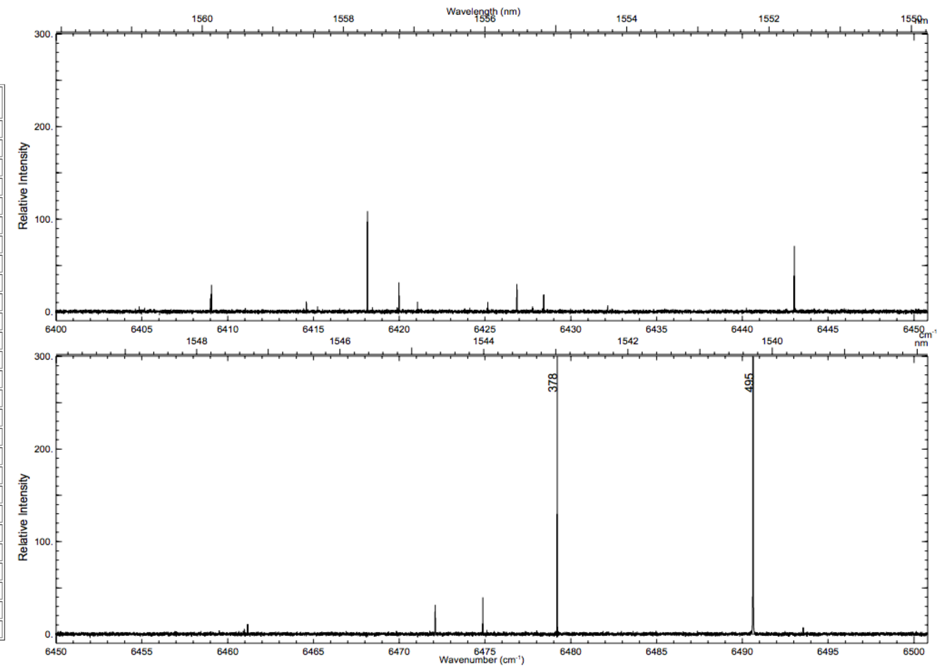
Spectrum of Th-Ar Hollow Cathode Lamps

Th-Ar Lamp Spectrum 6400 - 6500 Range

Custom Dataset input variable is Wavenumber
Requested output format is html
Requested range is 6400-6500 cm^{-1}

Make a new request for a custom dataset

Wavenumber	(unc) le-3	SNR	FWHM le-3	Intensity	Species	Lower Level	Lower J	Upper Level	Upper J	Vacuum Wavelength	(unc) le-3
6404.8394	0.9	6	9	83	Th I	20566	4	26971	4	1561.3194	0.2
6405.1612	1.3	4	9	52	Th I	23609	5	30014	4	1561.2410	0.3
6408.9893	0.4	14	9	196	Th I	7795	4	14204	5	1560.30842	0.09
6409.0503	0.2	29	8	350	Th I	15493	4	21902	4	1560.29357	0.05
6414.5824	0.5	11	8	136	Th I	13088	3	19503	3	1558.94794	0.11
6415.2370	1.0	5	9	74	Th I	17354	1	23769	1	1558.7889	0.2
6418.14278	0.13	121	8	1500	Th I	16783	4	23201	3	1558.08313	0.03
6418.4359	0.9	5	7	53	Th I	21077	5	27495	4	1558.0120	0.2
6419.8805	1.3	4	9	68	Th I	19503	3	25923	4	1557.6614	0.3
6419.98159	0.20	33	8	400	Th I	16217	2	22637	3	1557.63687	0.05
6421.0602	0.5	11	9	150	Th I	22141	3	28562	4	1557.37521	0.12
6425.1186	1.0	4	5	30						1556.3915	0.2
6425.1623	0.5	10	7	123						1556.38092	0.12
6426.8541	0.3	29	21	920	Ar I	107290	2	113717	3	1555.97122	0.07
6427.7722	0.8	6	7	59	Th I	15166	3	21594	3	1555.74896	0.18
6428.4191	0.3	19	8	221	Th I	13088	3	19516	2	1555.59241	0.07
6432.1471	0.6	7	6	74	Th I	19948	4	26380	5	1554.69081	0.15
6440.2312	1.6	3	8	45	Th I	21902	4	28342	5	1552.7393	0.4
6443.01968	0.14	78	8	920	Th I	7502	3	13945	3	1552.06728	0.03
6460.9752	1.0	5	8	69	Th I	13962	1	20423	1	1547.7540	0.2
6461.1631	0.5	11	8	142	Th I	27260	3	33721	2	1547.70897	0.11
6472.0924	0.3	31	22	1070	Ar I	113717	3	120189	2	1545.09538	0.07 *
6474.86889	0.18	41	8	500	Th I	18930	3	25405	4	1544.43282	0.04
6475.1049	1.2	4	8	78	Th I	15863	2	22338	3	1544.3765	0.3
6479.20330	0.13	378	8	4600	Th I	15618	3	22098	4	1543.39963	0.03
6490.61823	0.13	495	22	17300	Ar I	113717	3	120207	4	1540.68529	0.03 *
6493.5409	0.7	7	9	100	Th I	16783	4	23277	5	1539.99185	0.17

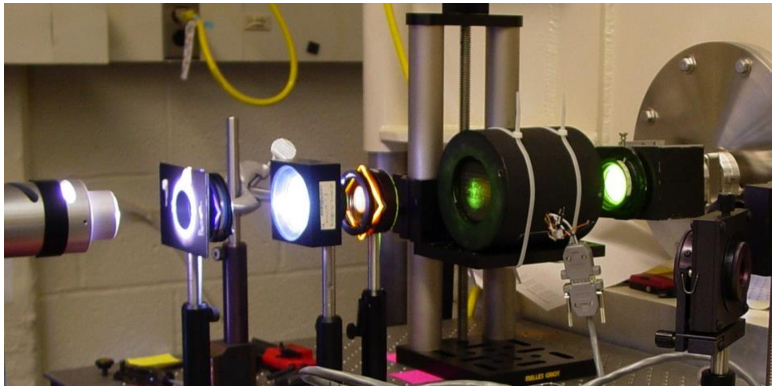


Th/Ar hollow cathode lamp, 20 mA, sapphire window. NIST 2m FTS

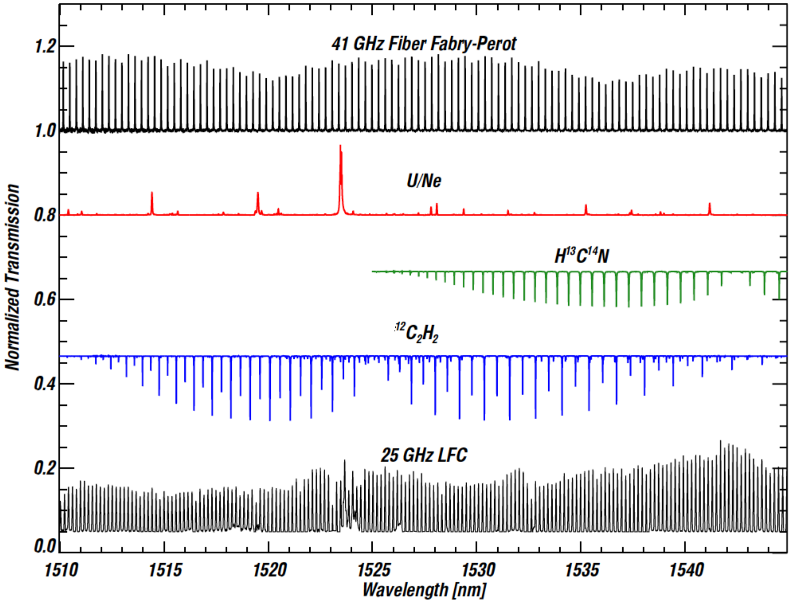
NIST is re-evaluating its databases and would welcome input. Would you like to see this database kept? Expanded? Improved? How useful are atlases? Would you like to see more of them?

NIST work on wavelength calibration standards for ground-based telescopes

- Hollow cathode lamps (Pt/Ne, Pt/Cr/Ne (HST); Th/Ar; U/Ne
- Gas cells (CO, HCN, C_2H_2, I_2)
- Fiber Fabry-Perot
- Frequency combs

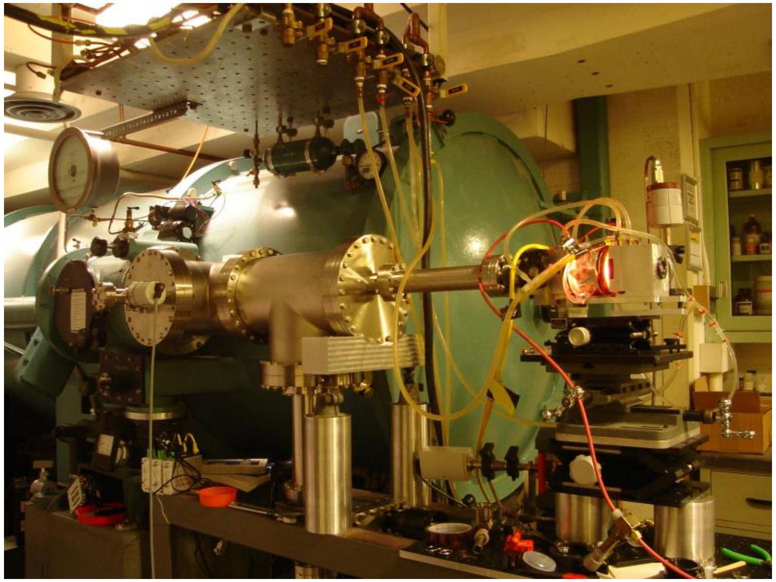


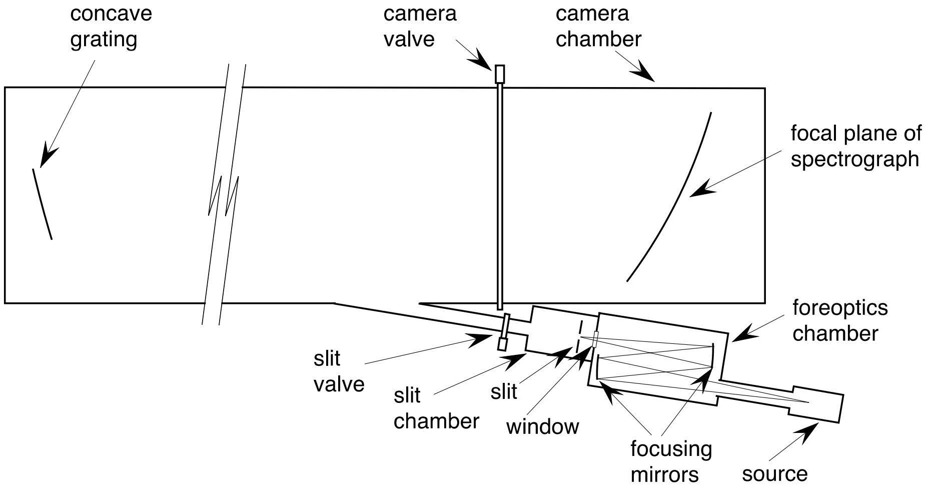
Keck HIRES I_2 cell being measured on the NIST 2-m FTS



Calibration sources for H-band using the NIST 2-m FTS

Normal Incidence Spectrograph





Normal incidence vacuum spectrograph.

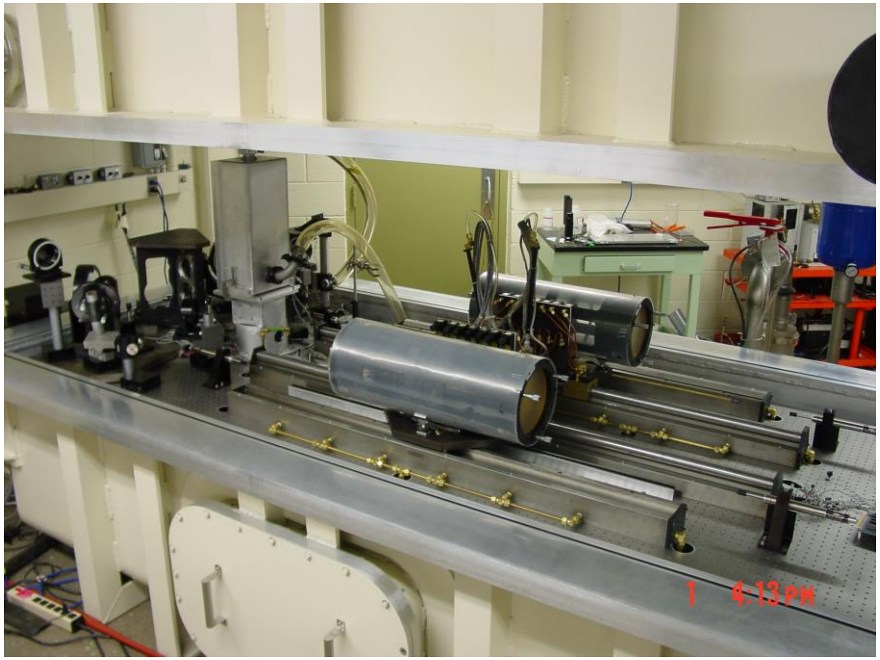
Wavelength range: 300 Å - 5000 Å.

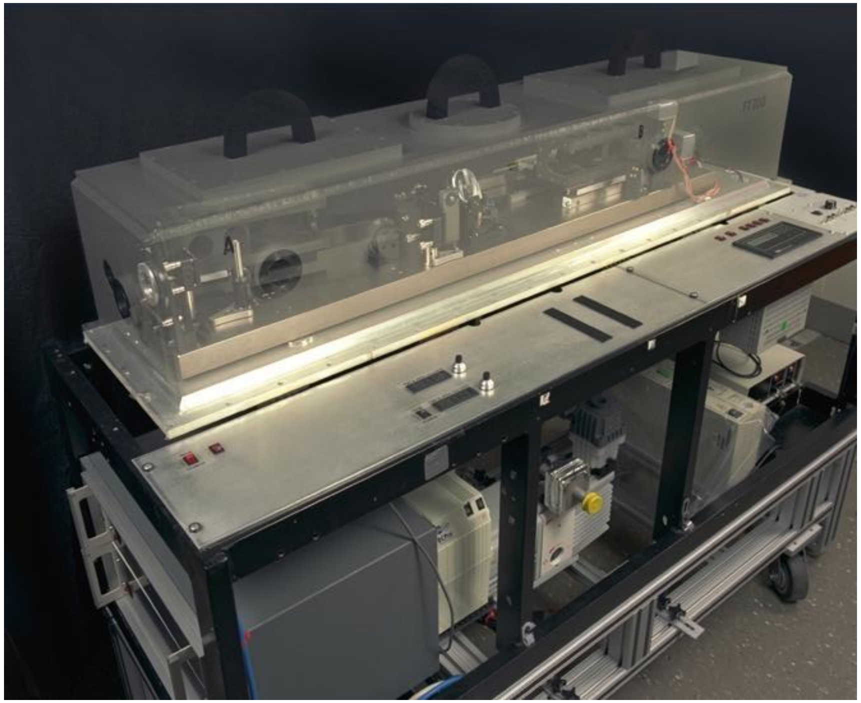
Resolving power: ≈150000 (1st order) with photographic plates. Less with phosphor image plates.

Projects:
Pt/Ne hollow cathode lamps on GHRS/COS
Pt/Cr/Ne hcls on STIS
(Pt atlas on NIST website)

Currently used for spectra of neutral through singly-ionized elements Sc-Cu

Fourier transform spectrometers





2-m FTS. Wavelength range 300 nm – 5.5 µm.

Resolution 0.0025 cm^{-1}

(4 million at 1 µm).

Vacuum ultraviolet FTS.

Wavelength range ~~140 nm~~133 nm – 900 nm.

Resolution 0.025 cm^{-1}

(2 million at 200 nm).

Advantages of FTS for wavelength calibration:

- Linear wavenumber scale –
  absolute wavenumber calibration to $1:10^8$ with only one standard
- Very high resolution – can resolve Doppler width of most laboratory sources
- large spectral range observed simultaneously
  (e.g. 300 nm – 1200 nm; 600 nm – 5500 nm)

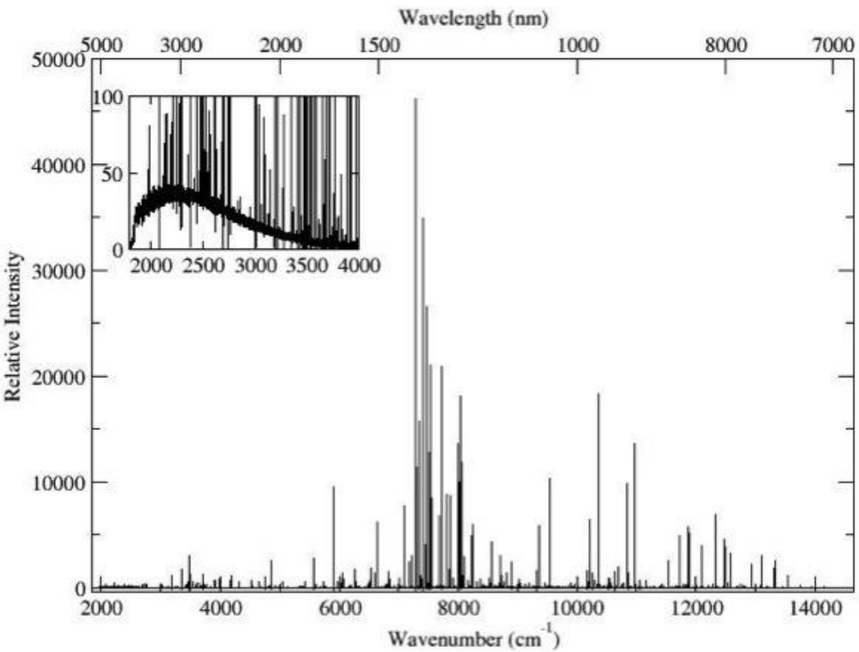
Disadvantages of FTS:

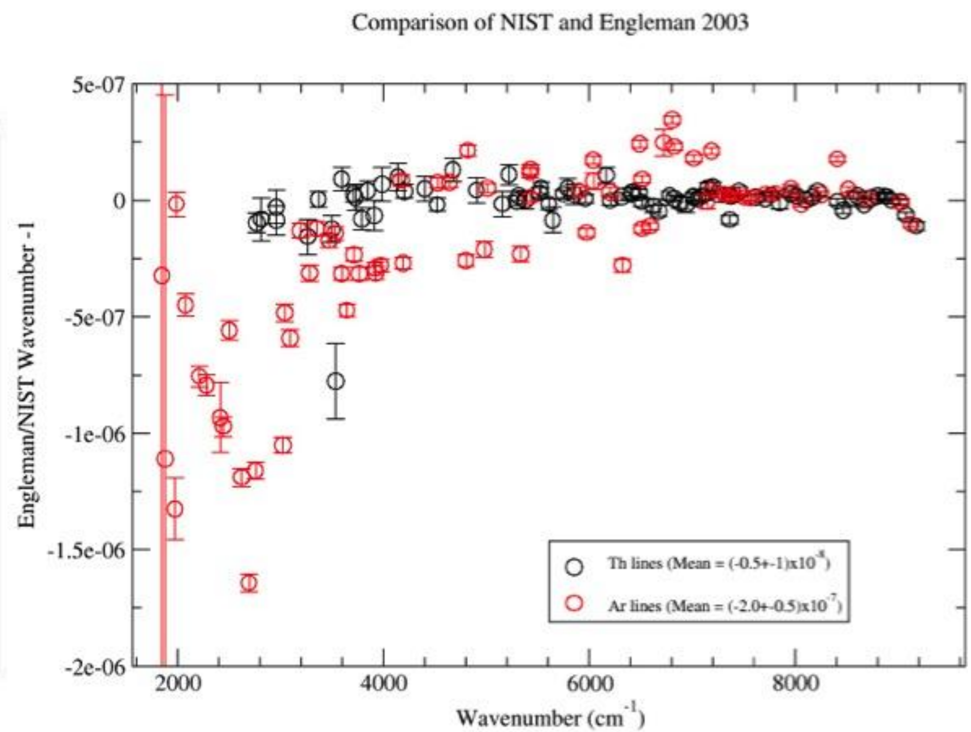
- Requires stable sources (CW)
- Low sensitivity compared to Echelle instrument with array detector.

Th/Ar linelists and atlases

- **B. A. Palmer, R. Engleman**, “Atlas of the Thorium Spectrum”: Los Alamos report LA-9615 (1983) (**75 mA**).
  - FTS wavenumbers for about 12800 lines to ± 0.002 cm^{-1}.
  - Covers 7400 – 36000 cm^{-1} (**1350 - 277 nm**).
  - Atlas used to derive 624 Th I levels, 464 Th II levels.
- **C. Lovis & F. Pepe,** “A new list of thorium and argon spectral lines in the visible,” Astron. Astrophys. **48**, 1115 (2007).
  - HARPS measurement of Th/Ar hollow cathode lamp at **9 mA**.
  - Claim improved precision over Los Alamos atlas, but absolute accuracy no better than atlas (worse?).
  - Claim global calibration which is precise at the 20 cm s^{-1} level (6.7 parts in 10^{10})
- **F. Kerber, G. Nave, and C. J. Sansonetti**, “The Spectrum of Th-Ar Hollow Cathode Lamps in the **691-5804 nm** Region: Establishing Wavelength Standards Calibration of Infrared Spectrographs,” Astrophys. J., Suppl. Ser. **178**, 374 (2008).
  - FTS wavenumbers for about 2400 lines in infrared. Th/Ar lamp at **25 mA**. Uncertainties of 2:10^8 to 6:10^7.
- **R. Engleman, K. H. Hinkle, L. Wallace**, “The near-infrared spectrum of a Th/Ar hollow cathode lamp,” J. Quant. Spectr. Radiat. Transfer 78, 1-30 (2003)
  - FTS wavenumbers for about 5988 lines in IR from hollow cathode lamp run at **320 mA**.
  - Ar lines as wavenumber standards
- **S. Redman, G. Nave, C. J. Sansonetti**, “The spectrum of thorium from **250 nm to 5500 nm** Ritz wavelengths and optimized energy levels,” ApJSS 211:4 (2014)
  - **20 0000 Ritz wavelengths** based on 787 energy levels of Th I, 516 levels of Th II, and 65 levels of Th III.

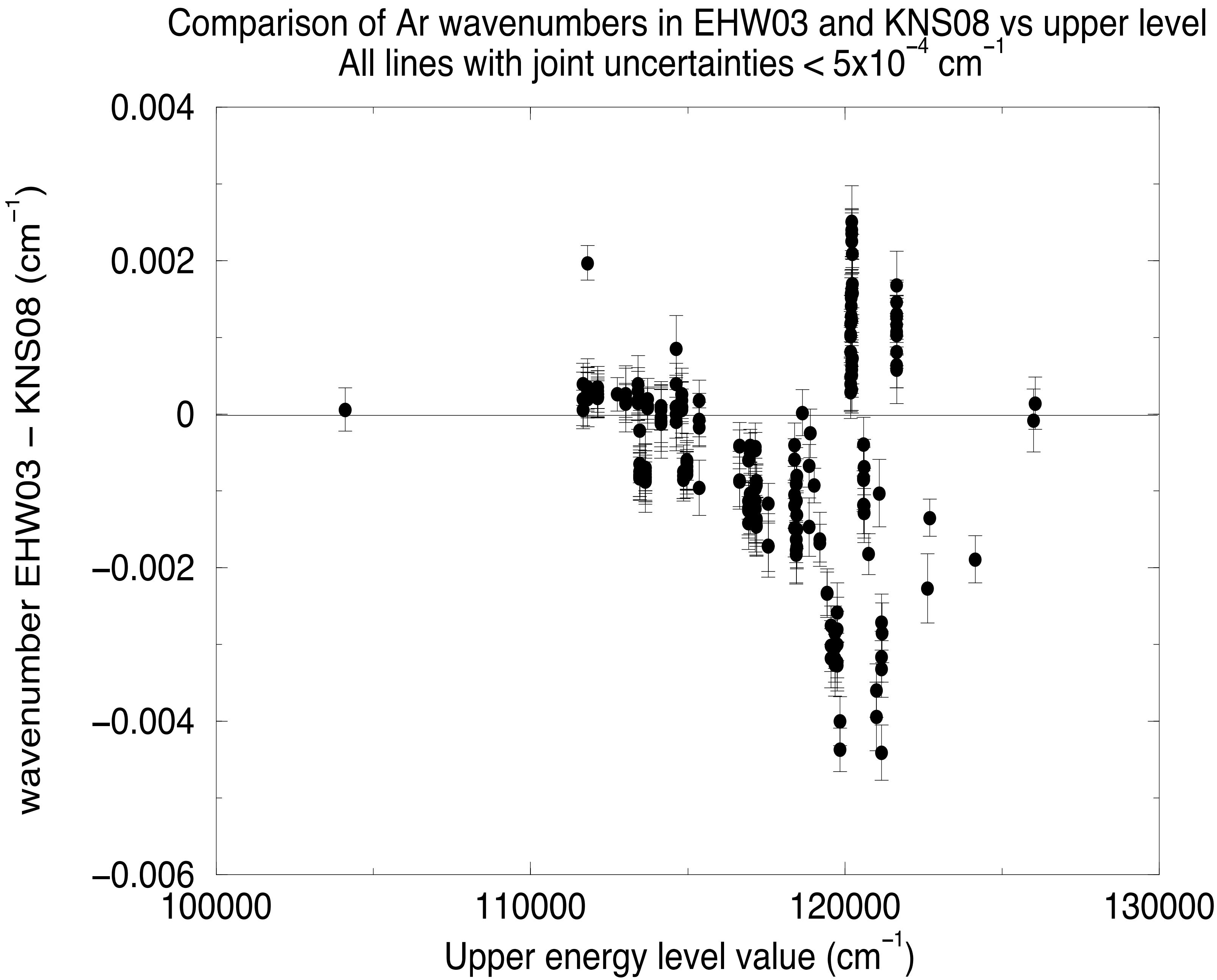
Comparison of NIST wavenumbers with Engleman, Hinkle & Wallace, 2003





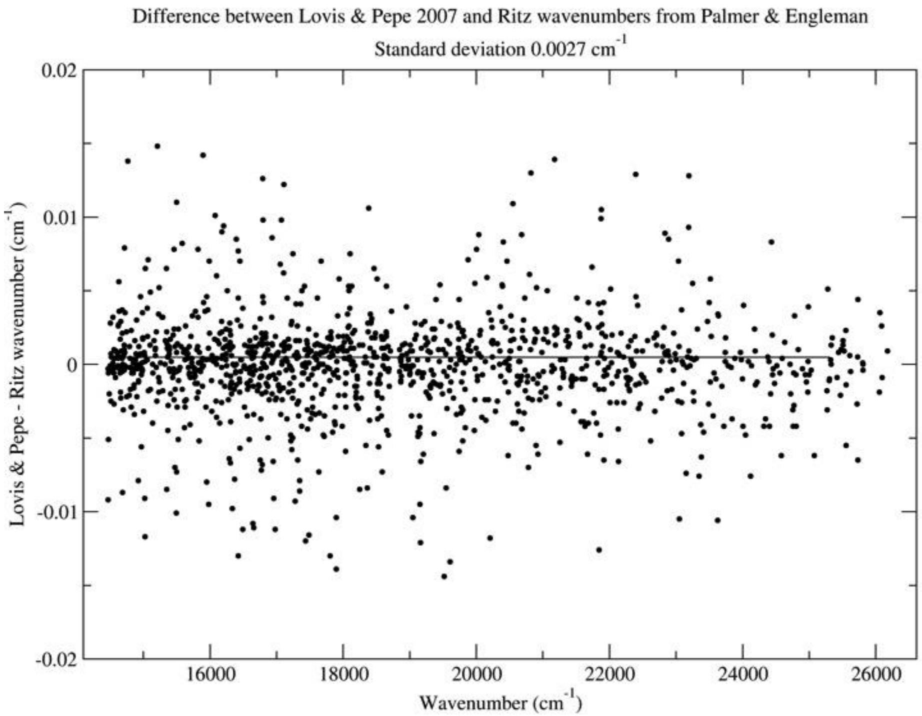
Roughly 2000 Th lines available for calibration of CRIRES.

Th lines agree well with 320 mA lamp of Engleman et al., but Ar lines do not.

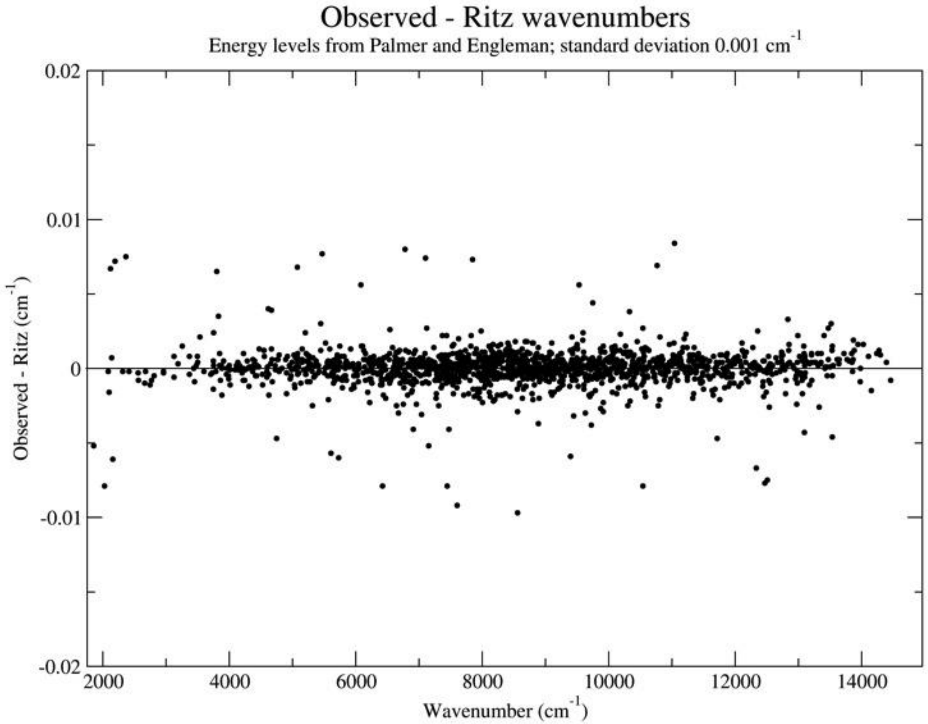


Comparison of Ar wavenumbers in EHW03 and KNS08 vs upper level
All lines with joint uncertainties < 5x10^-4 cm^-1
wavenumber EHW03 – KNS08 (cm^-1)
0.004
0.002
0
–0.002
–0.004
–0.006
100000
110000
120000
130000
Upper energy level value (cm^-1)

Comparisons with Ritz wavenumbers



Visible-region measurements using HARPS
C. Lovis & F. Pepe, A&A **48**, 1115 (2007).



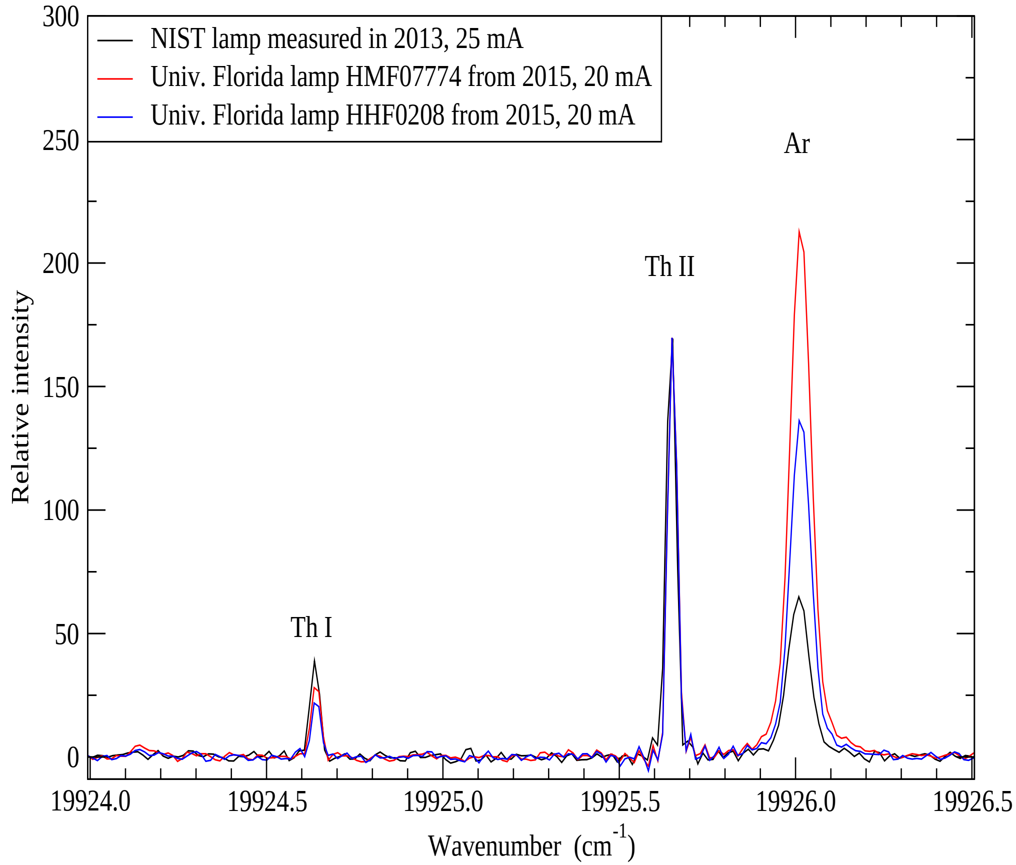
Infrared measurements from Kerber et al.
ApJ, Suppl. Ser. **178**, 374 (2008).

Primary reason: detector inhomogeneity folded into linelist

Other reasons? Can we expect the wavelengths to change over the life of the lamp?

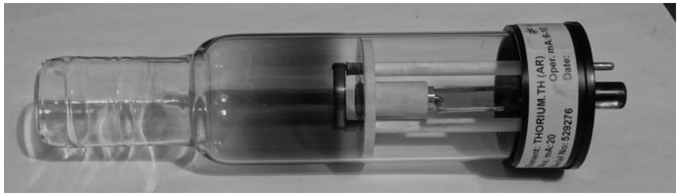
New measurements of current dependence of lamps

Jian Ge, Univ. Florida purchased 3 lamps in Oct, 2015, but could not match spectra up to previous linelists. Asked NIST to measure them.



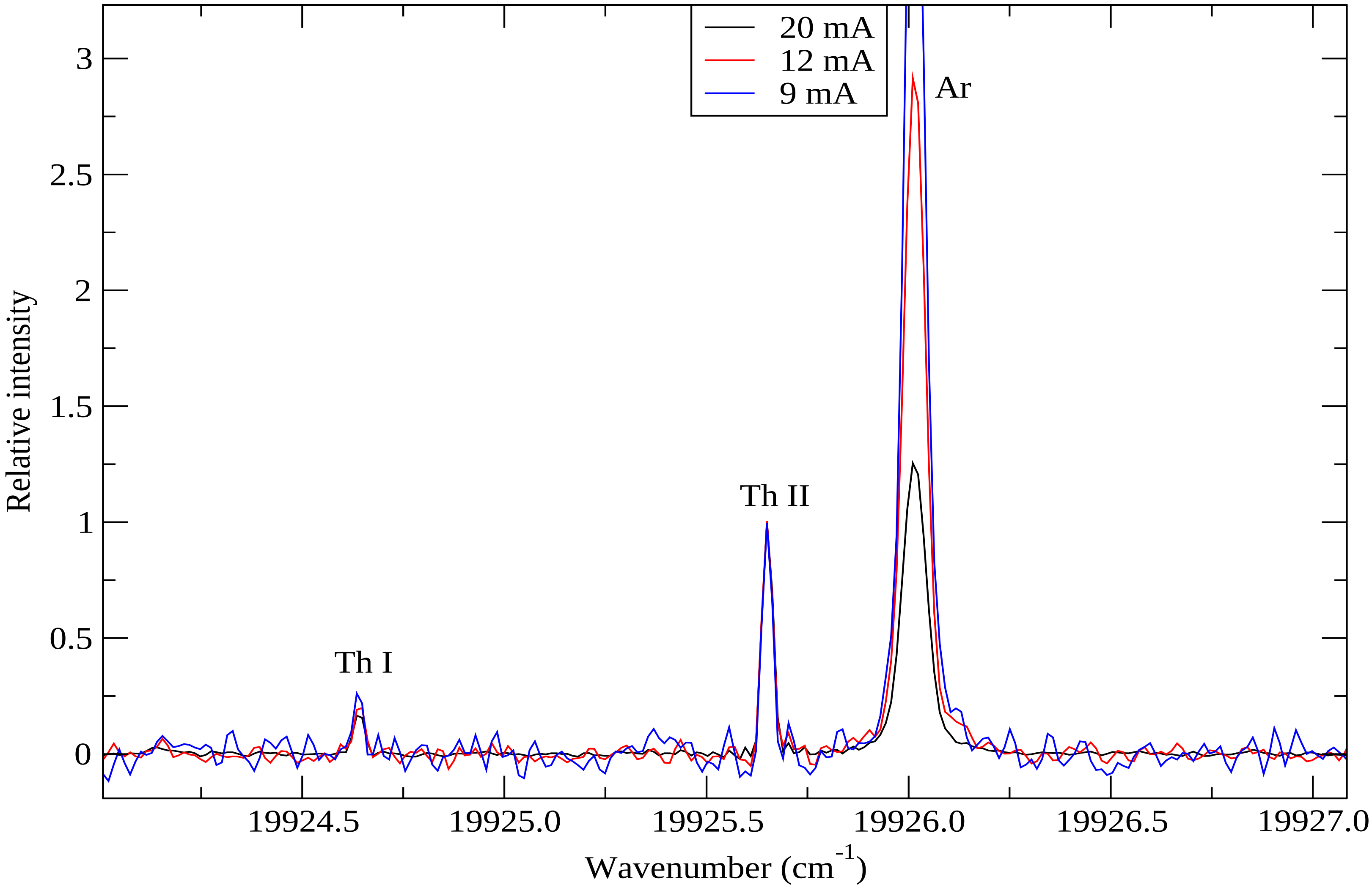
HHF0208 (Photron)

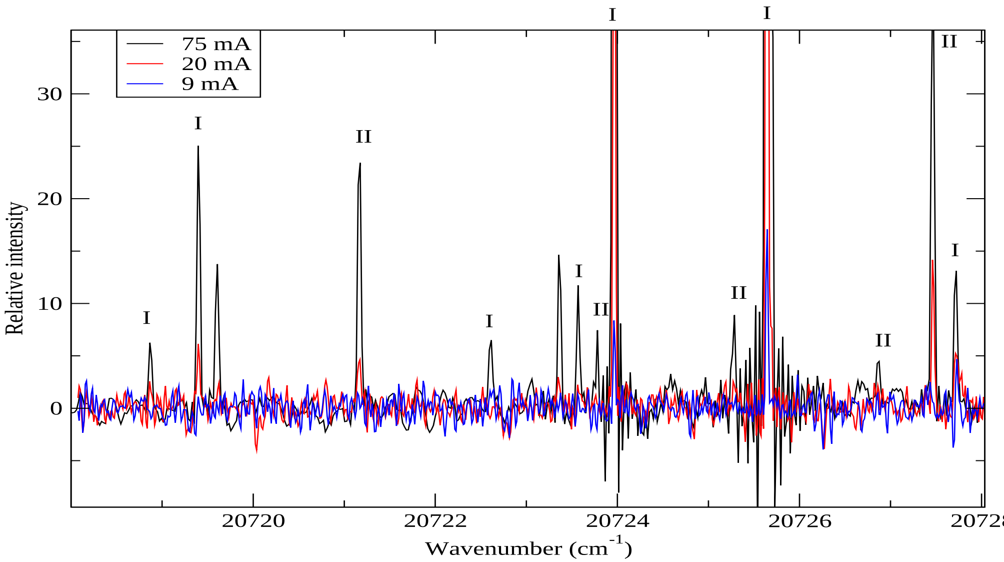
HMF0774 (Photron)



NIST lamp (S.J. Juniper)

Current dependence of Th and Ar lines in a hollow cathode lamp.





Black: Palmer & Engleman
Blue/Red: NIST

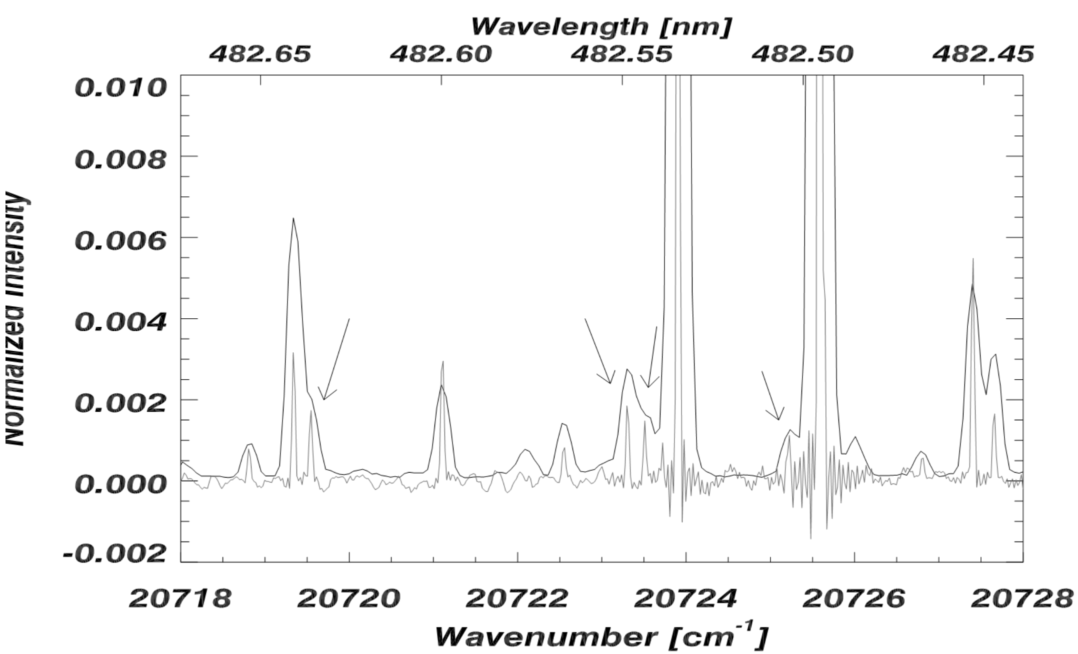
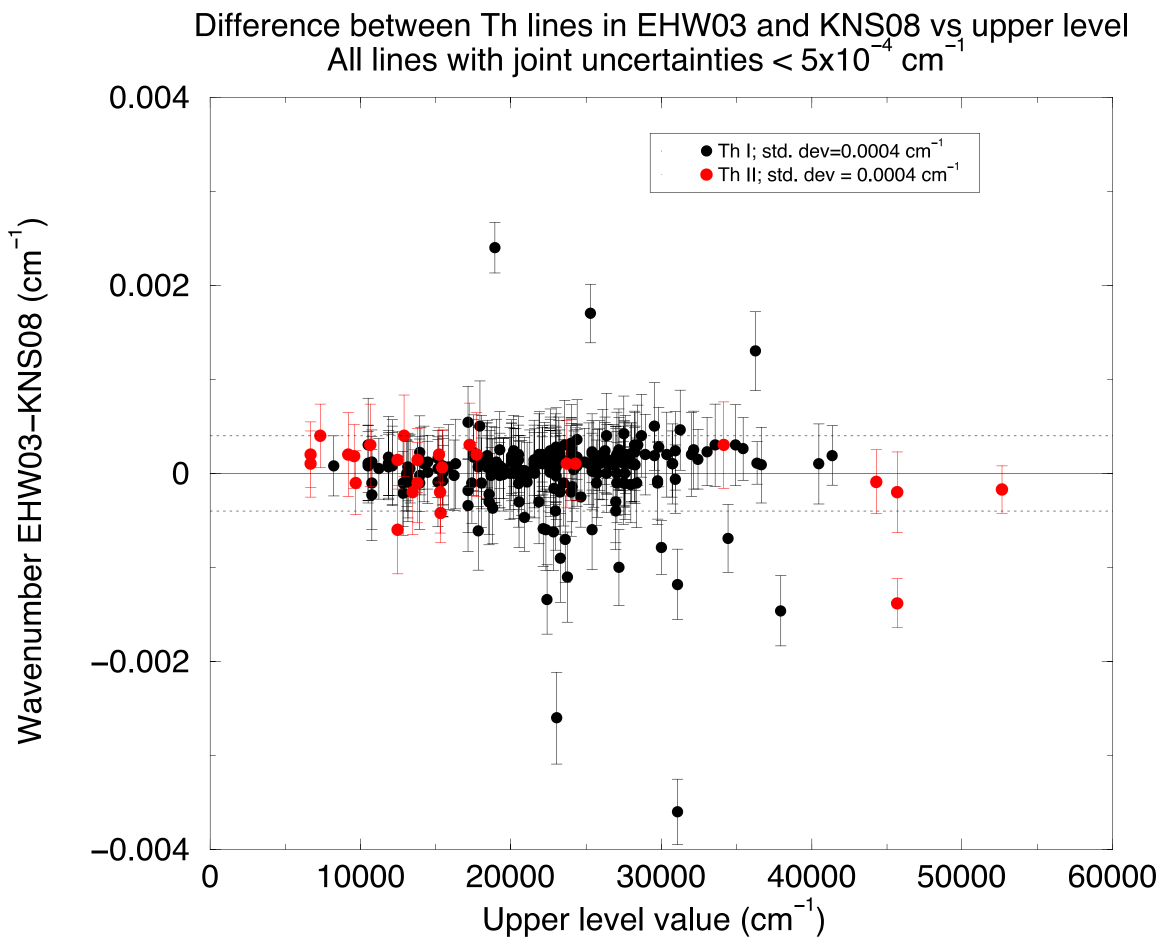


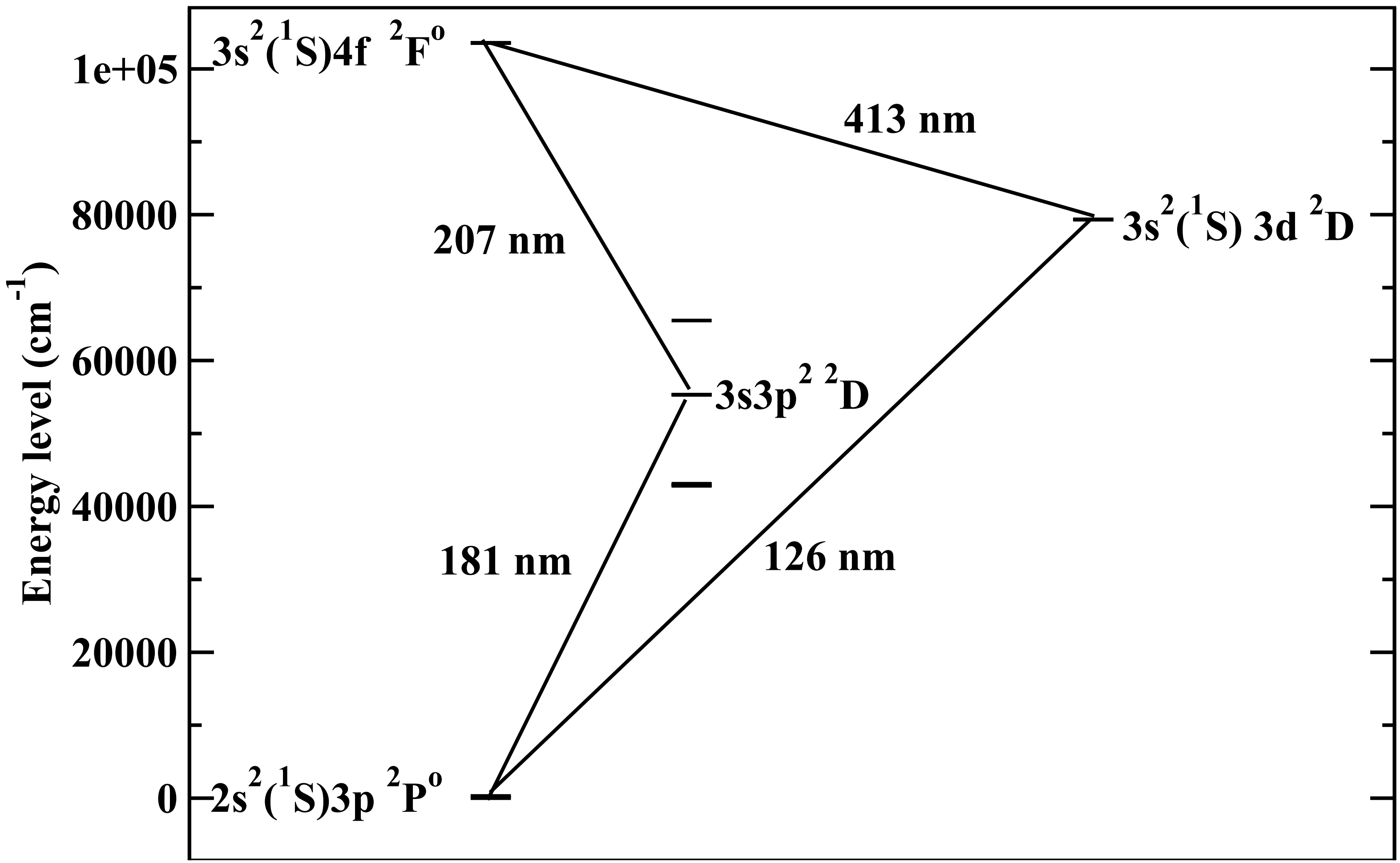
Fig. 6 from Redman Nave & Sansonetti (2014)

Lower resolution is HARPS data
Higher resolution is Palmer & Engleman (75 mA lamp)



EHW03: Engleman Hinkle & Wallace, 2003: Th/Ar hcl, 2.2 Torr, 320 mA
KNS08: Kerber, Nave & Sansonetti, 2008: Th/Ar hcl, 5 Torr, 25 mA

Ritz wavelengths: example of Si II



Ritz wavelengths in thorium

Table 3
Classification Match Summary by Source

Source	Search Window (cm^{-1})	Classifiable Lines	Contribution to Final List
GBCZ74	0.01	2715	133
ZC74 $\leqslant$ 10000	0.012	396	6
ZC74 > 10000	0.042	4784	2166
Z76 $\leqslant$ 10800	0.012	1789	55
Z76 > 10800	0.05	6585	2533
PE83	0.01	9850	8644
EHW03	0.003	3689	3606
LP07	0.1	1622	1433
KNS08	0.005	1685	496
RNS13	0.003	3785	1035

GBCZ74: Giacchetti, A., Blaise, J., Corliss, C., & Zalubas, R. 1974, JRNBS, 78A, 247
ZC74: Zalubas, R., & Corliss, C. 1974, JRNBS, 78A, 163
Z76: Zalubas, R. 1976, JRNBS, 80A, 221
PE83: Palmer,B.A.,& Engleman,R. 1983, Atlas of the Thorium Spectrum (LLNL)
EHW03: Engleman, R., Jr., Hinkle, K. H., & Wallace, L. 2003, JQSRT, 78, 1
LP07: Lovis, C., & Pepe, F. 2007, A&A, 468, 1115
KNS08: Kerber, F., Nave, G., & Sansonetti, C. J. 2008, ApJS, 178, 374
RNS13: Redman, S., Nave, G., & Sansonetti, C.J., 2014, ApJS,211:4

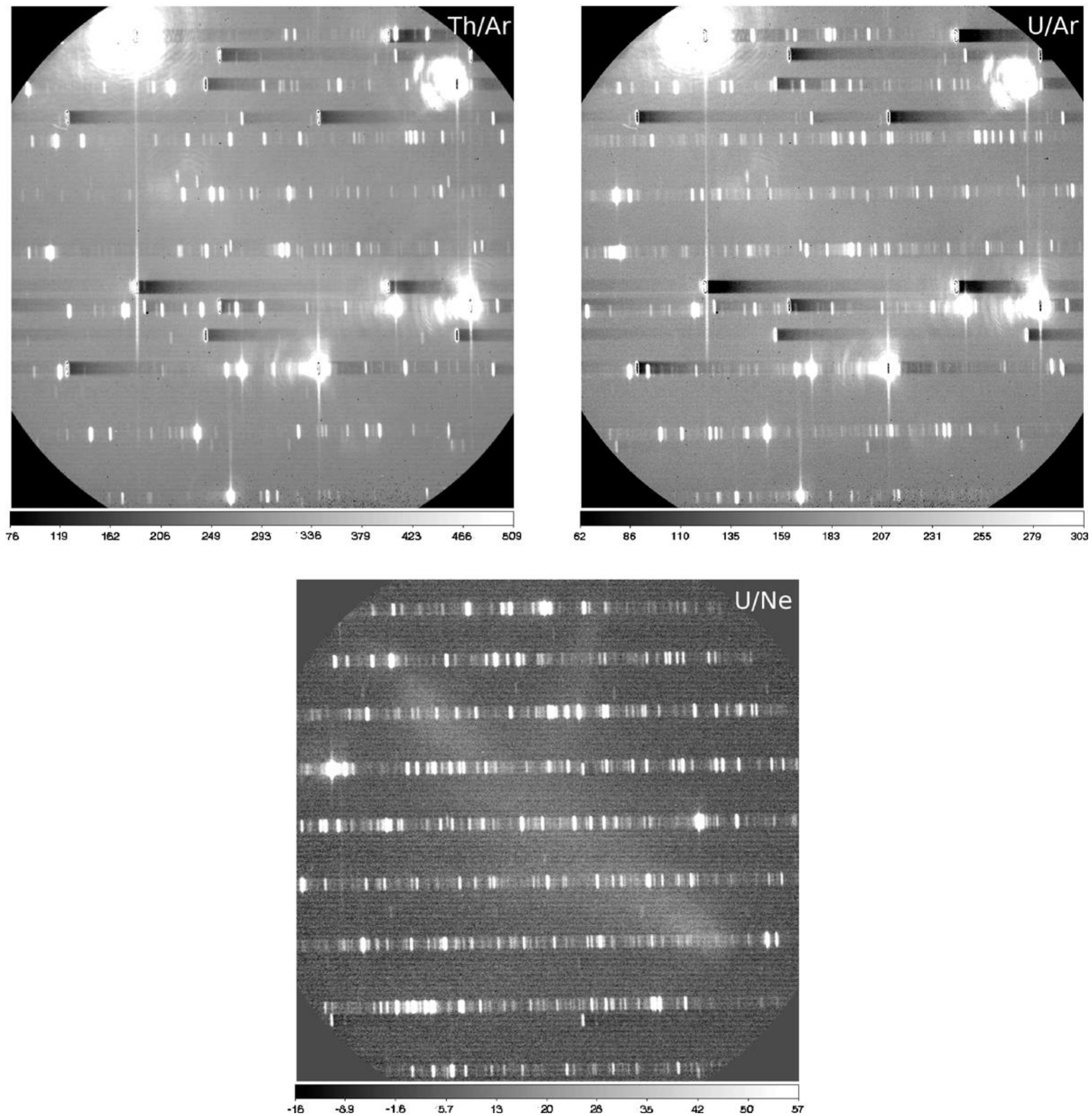
19874 Spectral lines in thorium.
Ritz wavelengths based on
- 787 energy levels of Th I,
- 516 levels of Th II,
- 65 levels of Th III.

Lines only contribute to linelist if they appear in one of the 8 studies, some of which are lower resolution grating measurements.

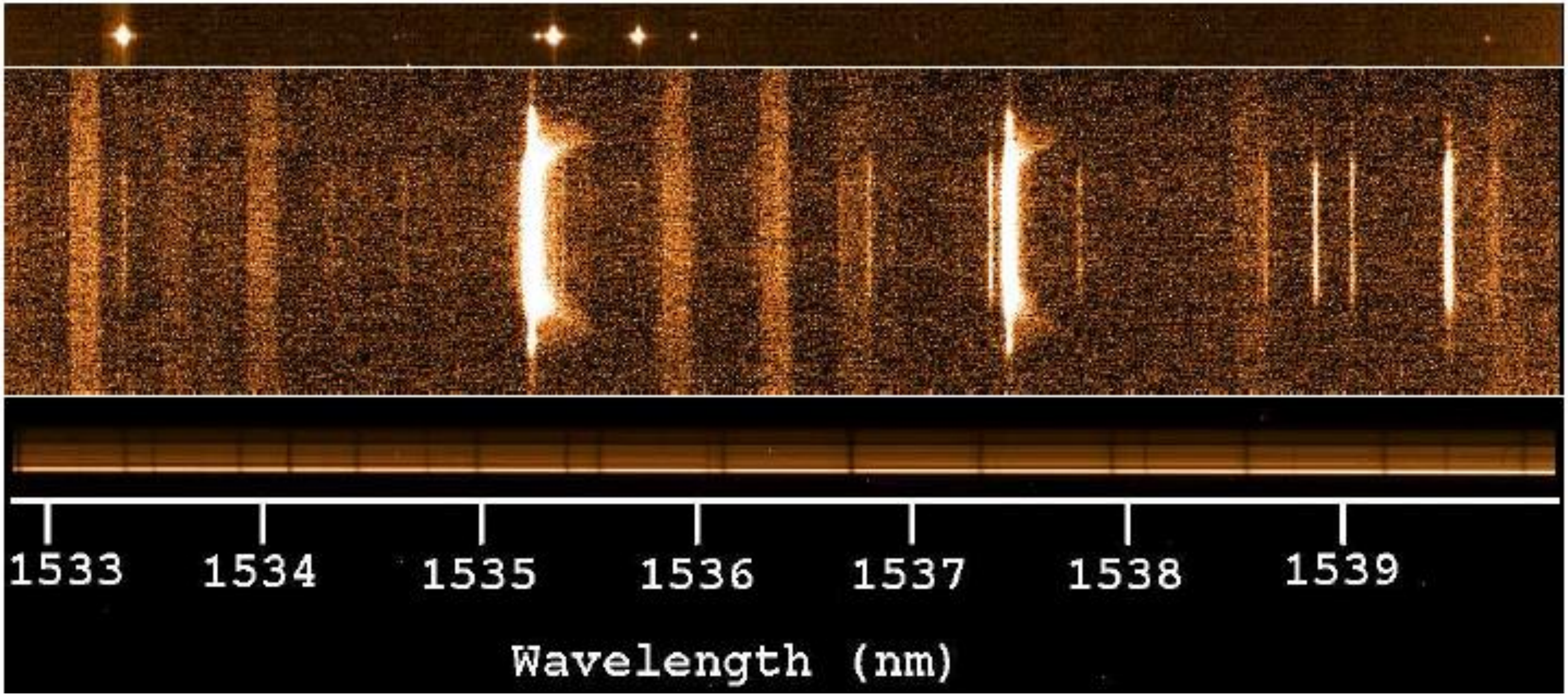
However, accuracy of Ritz wavelengths is determined by high-accuracy FTS measurements.

Hence the Ritz wavelengths for weak lines can be determined as well as those for strong lines.

Comparison of hollow cathode sources in near-IR (1 – 1.6μm)
25 s exposures of 14 mA lamp using Pathfinder spectrograph
(Redman et al. ApJSS 195, 2011).

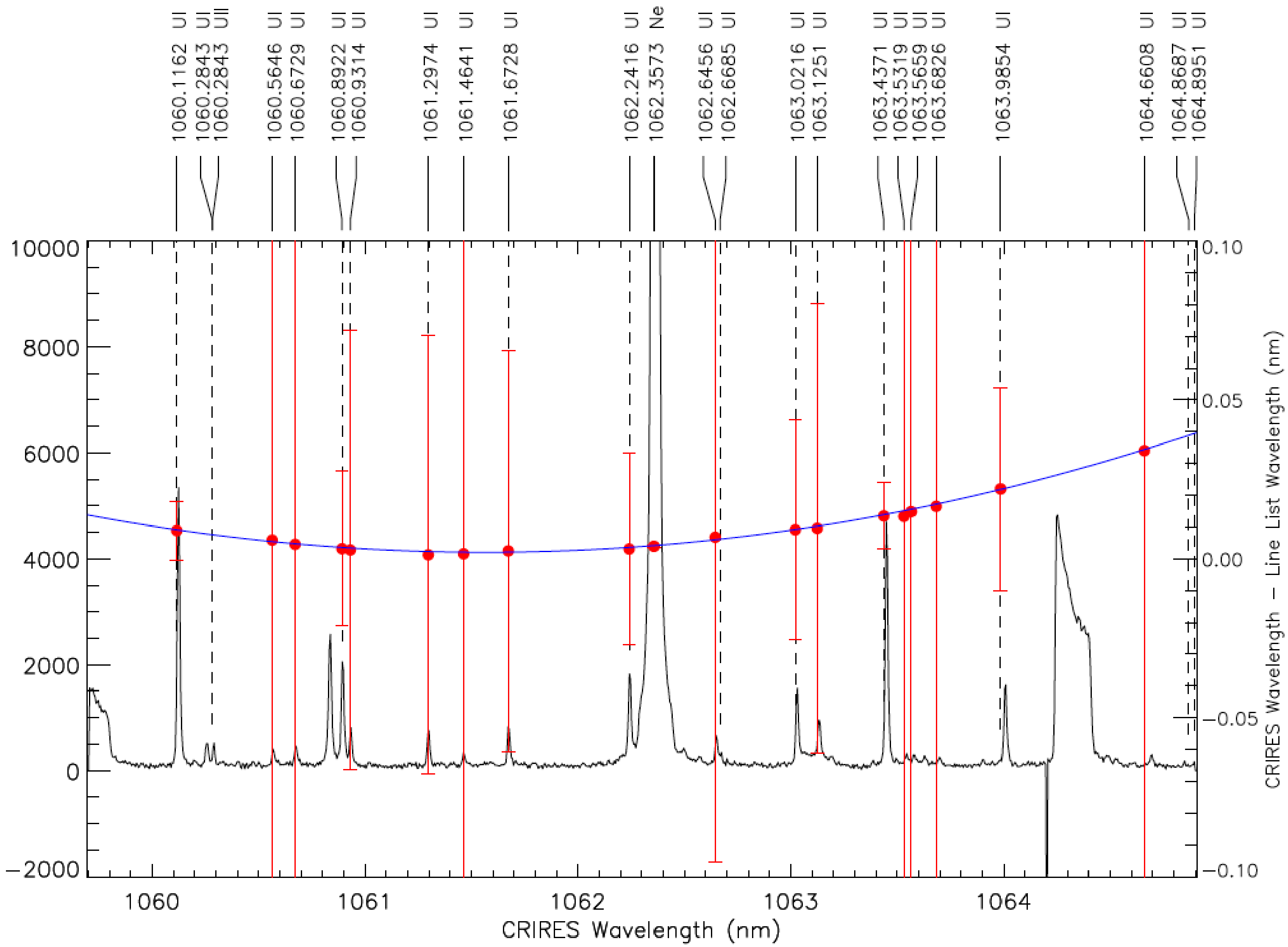


Atlases for CRIRES

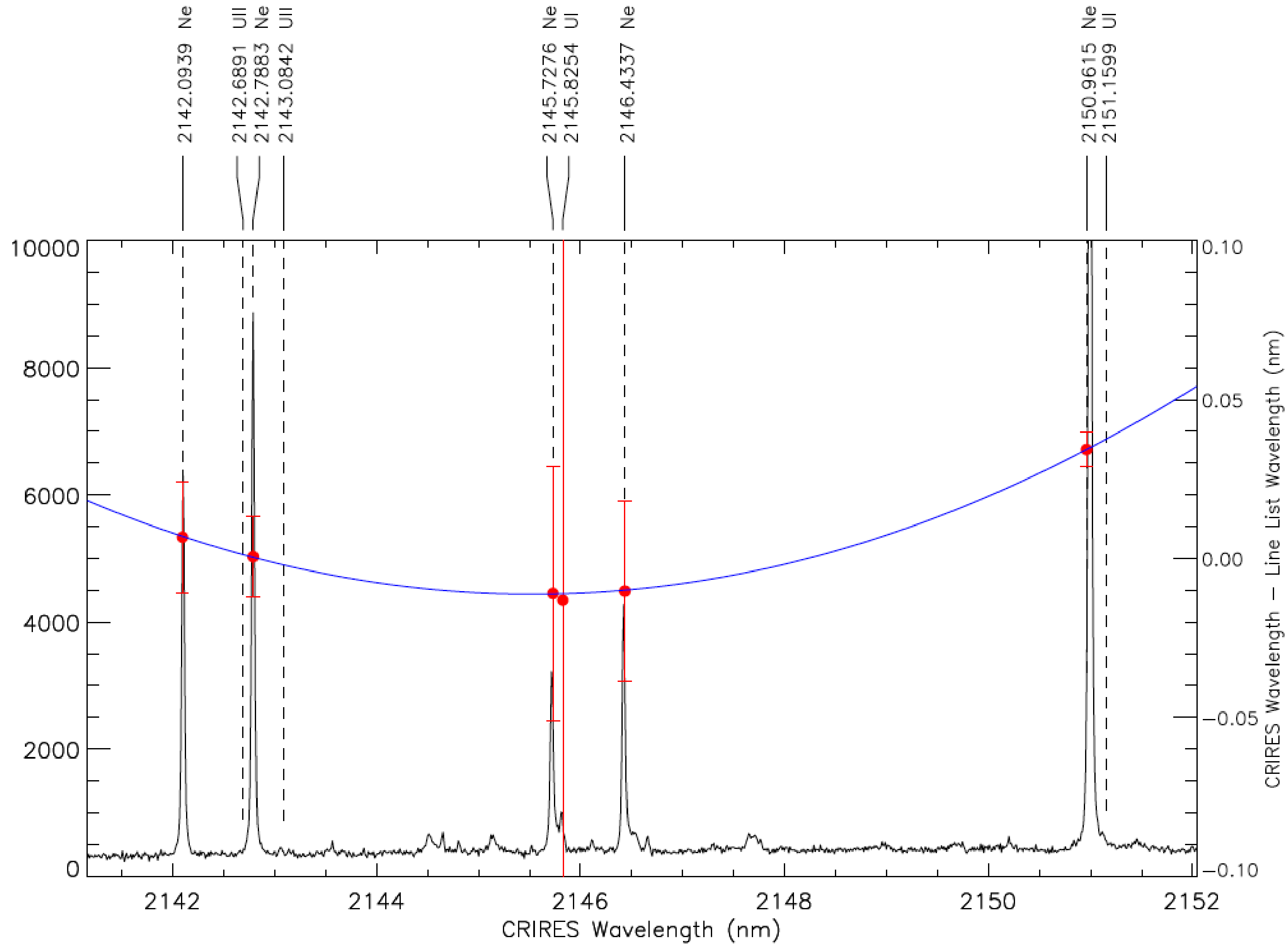


Comparison between three different calibration sources over a region of the H-band.
Top: Th/Ar spectrum Middle: U/Ne spectrum Bottom: Gas cell spectrum

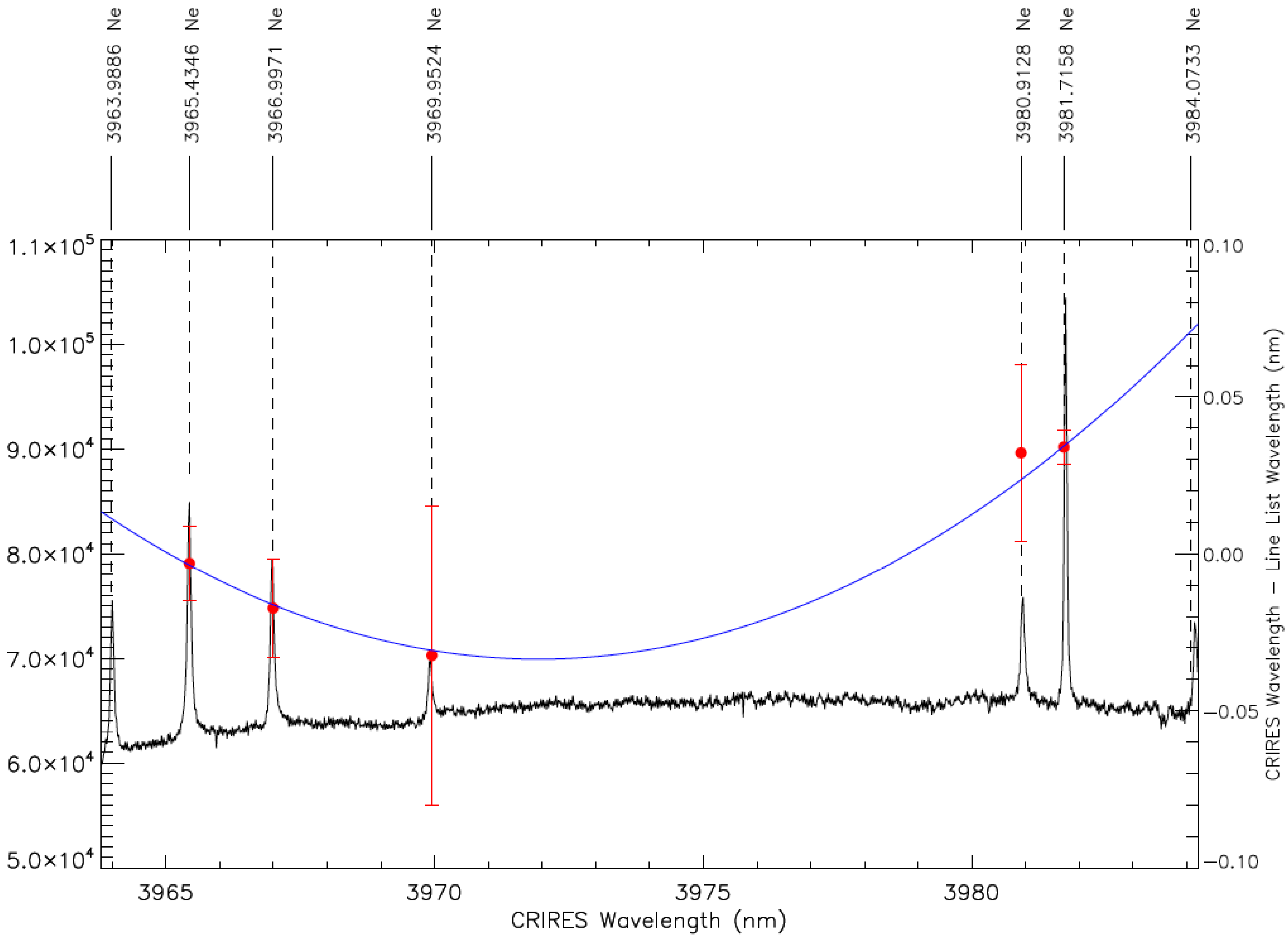
Example dispersion solution around 1050 nm using U lamp on CRIRES.



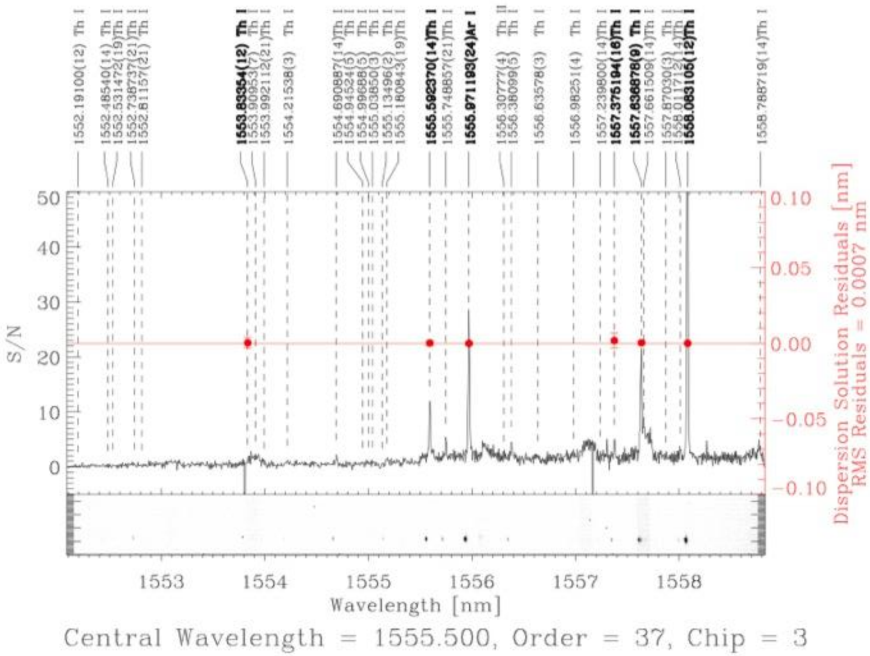
Example dispersion solution around 2150 nm using U lamp on CRIRES

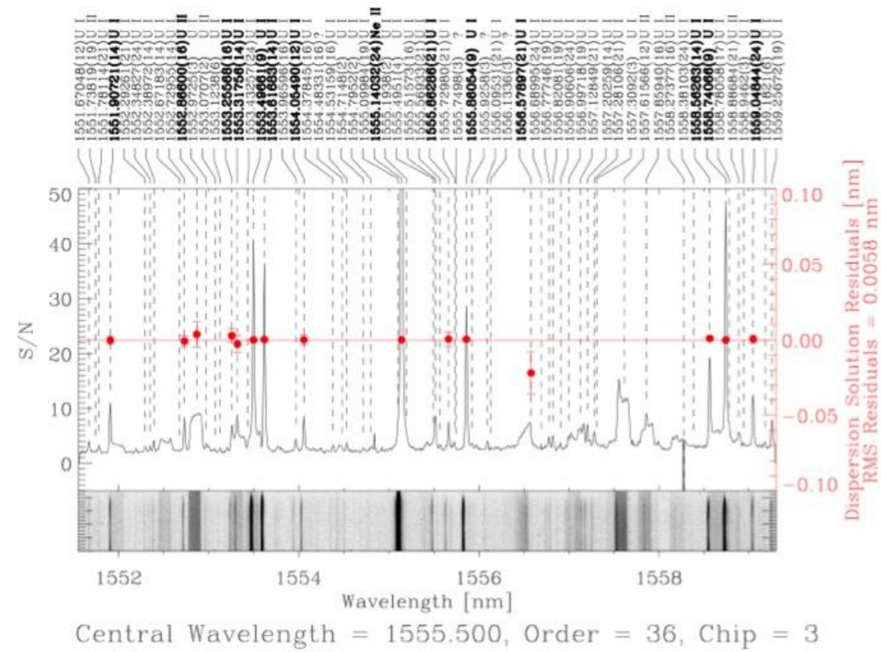


Example dispersion solution around 3975 nm using U lamp on CRIRES.
No U lines seen about 2600 nm.



CRIRES atlas





In some regions, U/Ne lamps much better for calibration.

Summary

NIST Atomic spectroscopy group’s activities on wavelength standards include:

- Th/Ar hollow cathode lamps
- U/Ne hollow cathode lamps
- Iodine cells
- Gas cells
- Fiber Fabry-Perot
- Laser frequency combs

High-resolution Fourier transform spectroscopy underpins all these activities