Atomic Data from the UV to the IR: Application to NASA missions

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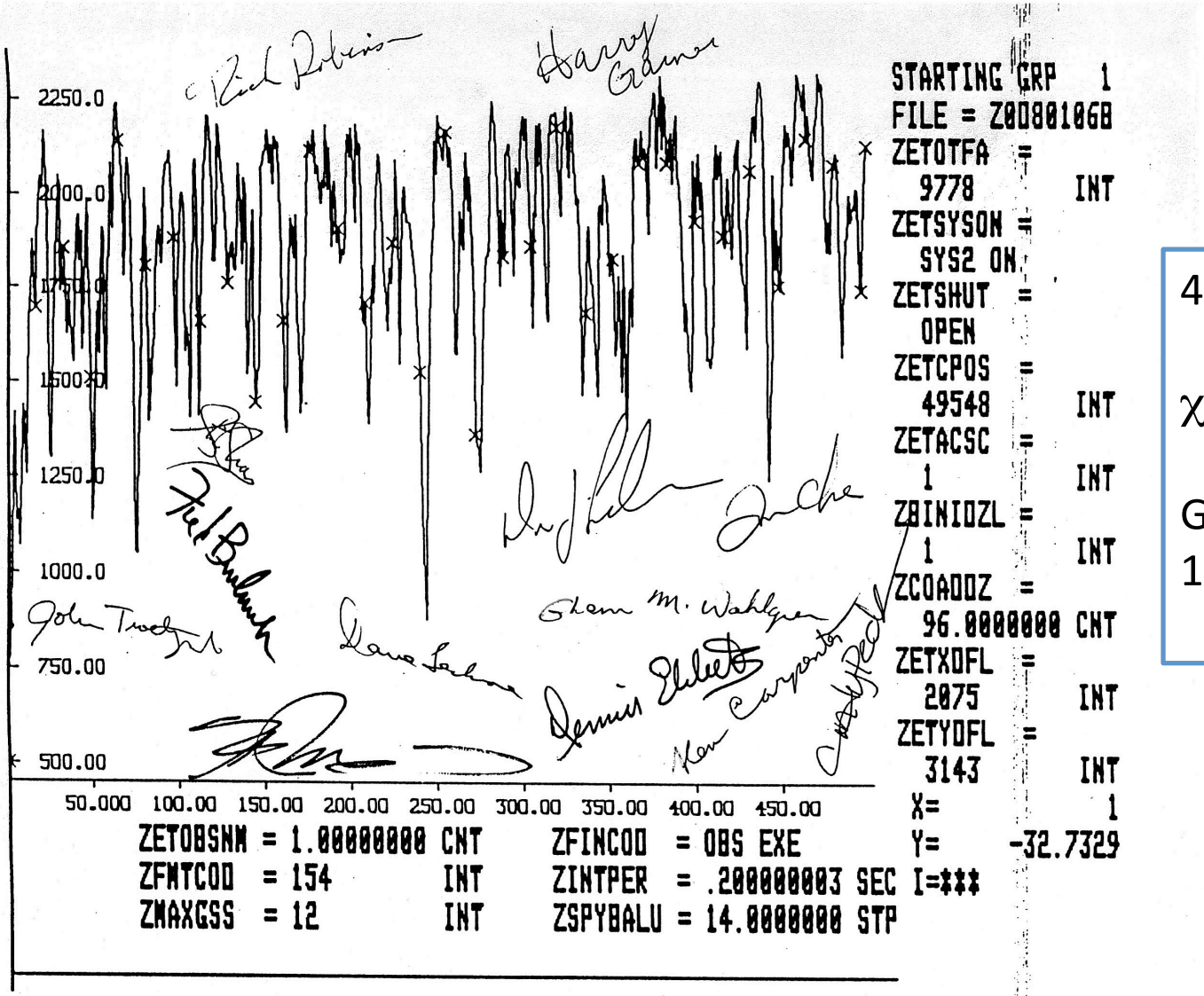


4 October 1990

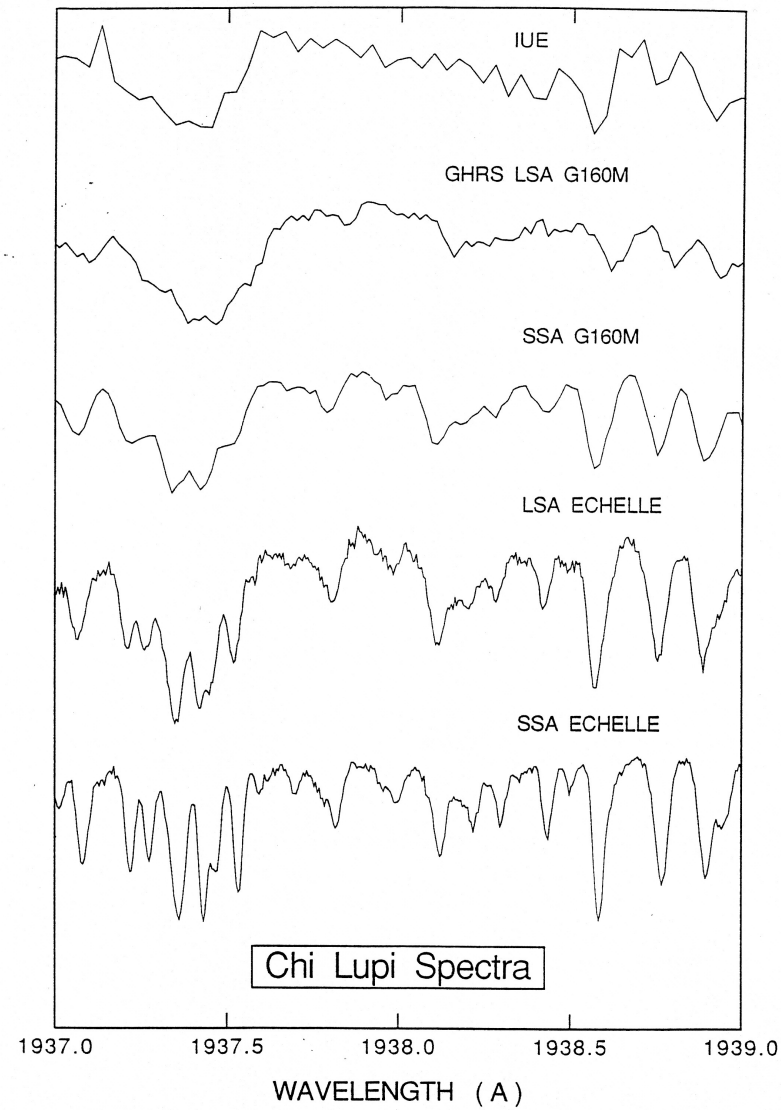
χ Lupi

GHRS, G160M, LSA
1925 – 1960 A

"The spectrum that launched a hundred studies"

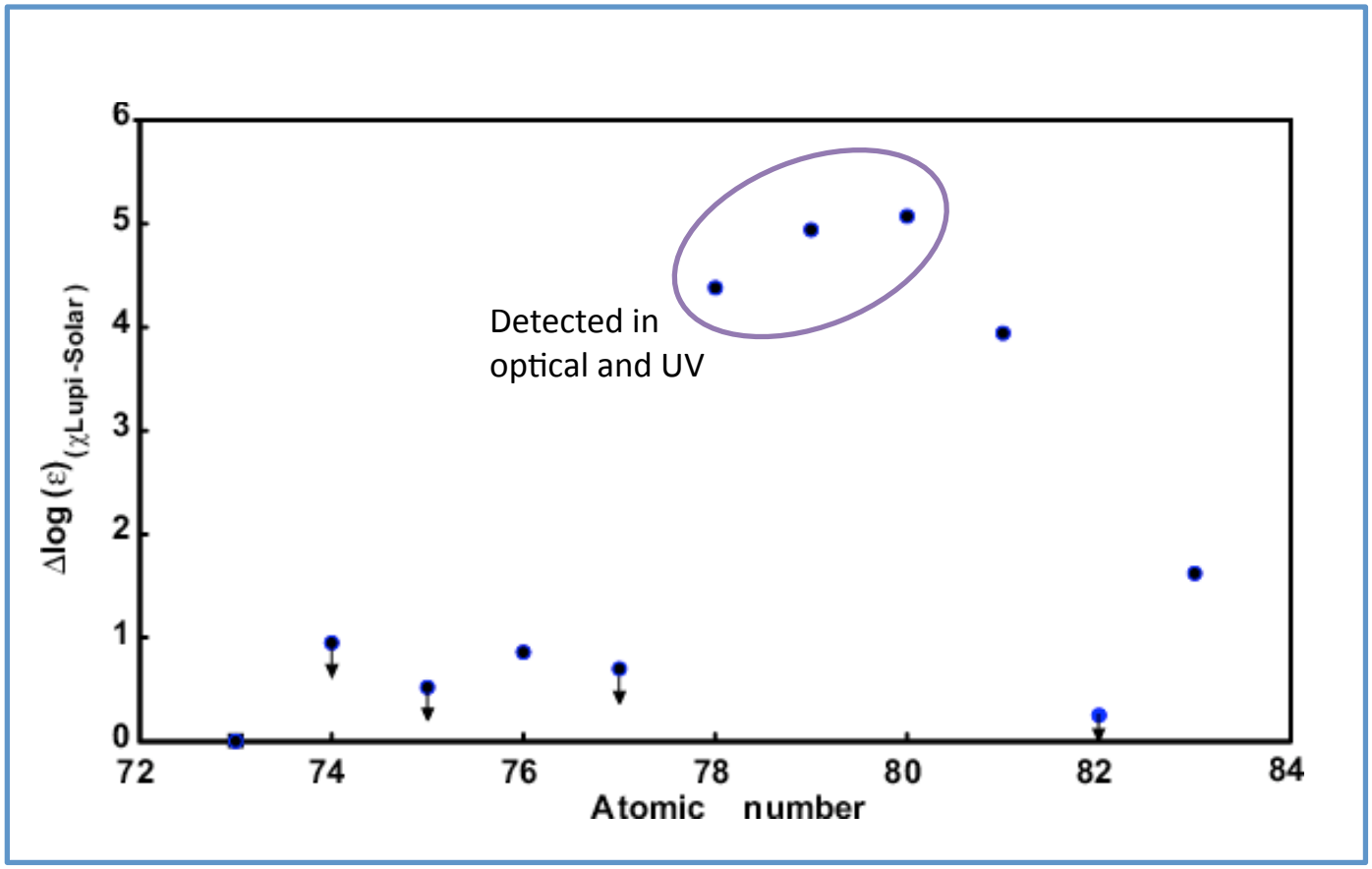
A giant leap for UV astronomy

	R
	12 000
STIS G#M	15 000
COS G#M	28 000
STIS E#M	45 000
STIS E#H	87 000



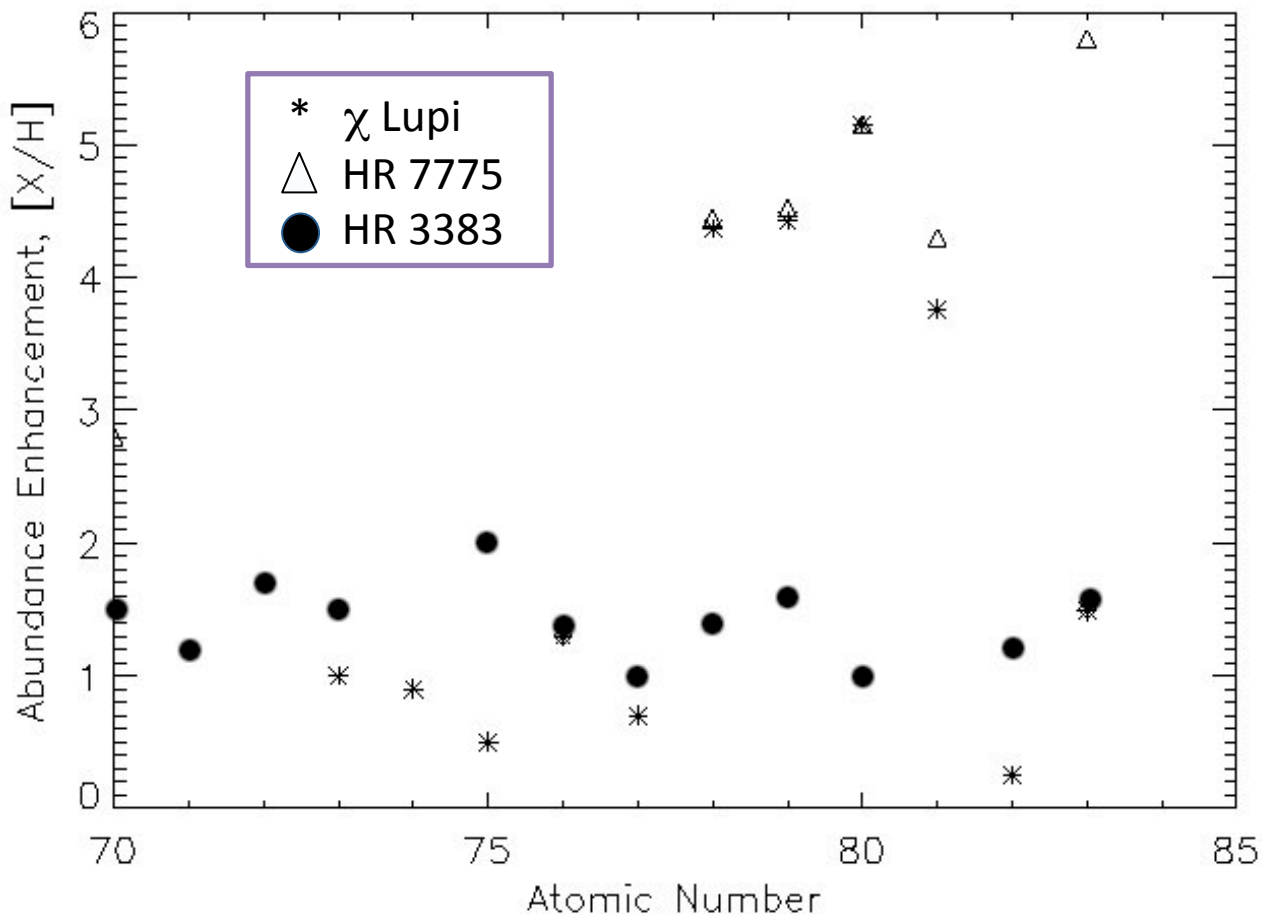
Pre-costar observations

Heavy element abundances in χ Lupi A (B9.5p HgMn)
A decade of atomic spectroscopy



Ivarsson et al. 2004, A&A 425, 353

The application of a decade's work



T_{eff}: χ Lupi (10650K), HR 3383 (9750K)

Atomic Data Themes

I. Availability

II. Needs

III. Resources

Atomic Data

Observables: position (σ, ν, λ), lifetime (τ), intensity (I), profile

Determined: *E*, *IP, J, g, BF, A, f*, *Lande-g*
Related: partition functions, u(T)
Other: line broadening parameters (γ), HFS constants, IS

Non-LTE: collision strengths for excitation and ionization,
photo-ionization cross-sections

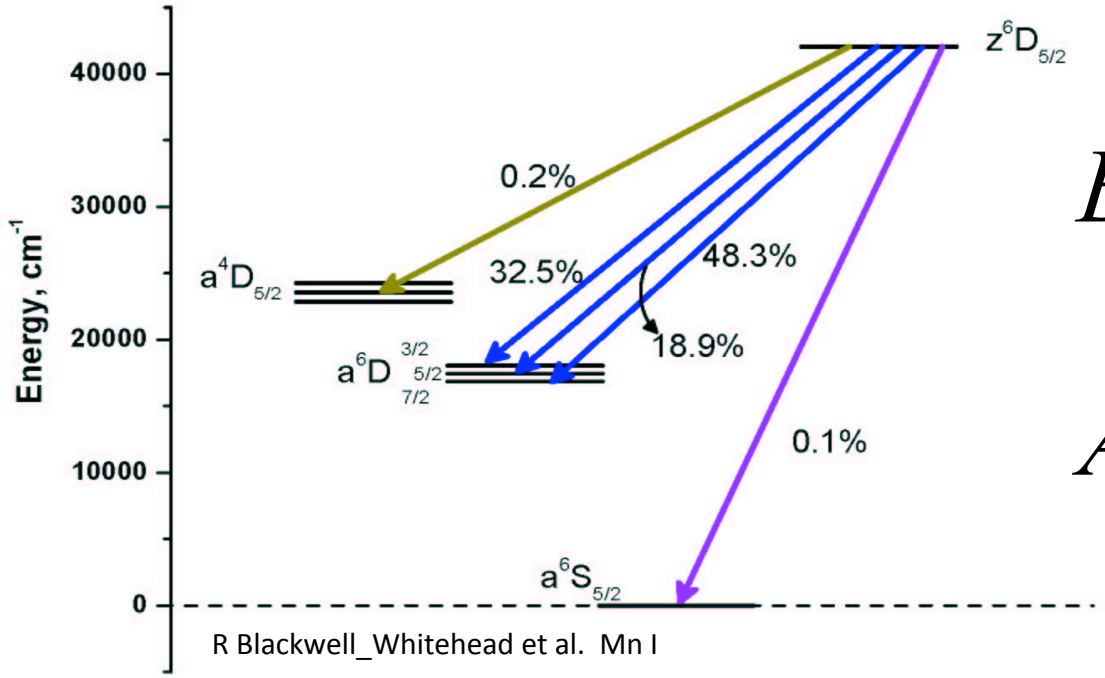
Equation for line absorption coefficient, ℓ :

$$\ell_{ij}(\lambda) \sim \lambda^2 \, f_{ij} \, (N_i/N_{total}) \, V$$

g_{ij}, E_i, IP, u(T) $\quad$ γ, λ

The uncertainty in a derived element abundance depends on the uncertainties in all of these parameters, among other things.

Large uncertainties for unobserved lab lines



R Blackwell_Whitehead et al. Mn I

$$BF_{ul} = I_{ul} / \Sigma I_u$$

$$A_{ul} = BF_{ul} / \tau_u$$

Wide spectral range (UV – optical – IR) is required for accurate intensity calibration and energy level determination.

I. Data Availability

Database Resources: UV to IR

- NIST spectral database and bibliographic sites
  - large compilations of Corliss, Bozman, Meggers, Scribner (~1960)
  - new compilations and large data sets under current evaluation:
    H, He, Li, Be, B, F, Ne, Ar, Cl, Ti, Cr, Fe, Ni, Ba, Sr, W
- Cambridge (R. Kurucz) extensive calculations + compilation of exp. results
- DREAM and DESIRE (Mons University) rare-earth and sixth-row elements

- VALD (Vienna Atomic Line Database)
- The Atomic Line List v2.04 (Univ. Kentucky): Ritz wavelengths from *E* levels in NIST database
- Weizmann Institute of Science – Databases for Atomic and Plasma Physics

New publications in atomic data reported in IAU triennial reports of Commission 14 – Atomic and Molecular Data (100s of new papers compiled)

Completeness vs. accuracy ➔ opacities and abundances

See posters 17,19

A chronicle of NASA UV spectroscopy missions

- *Copernicus* (90 – 315 nm, years 1972 – 1981)
- *IUE* (120 – 335 nm, years 1978 – 1996)
- small missions (STS): ASTRO (1990, 1995) and ORPHEUS (1993, 1996)
- *HST*/STIS, COS, GHRS, FOS (115 – 320 nm, years 1990 - present)
- *FUSE* (90 – 118 nm, years 1999 - 2007)

No new missions planned for UV spectroscopy by NASA or ESA

(*World Space Observatory – UV* 1.7 m telescope, launch in 2014, R ~ 50 000)
(conference *UV Universe-2010*, showed continued interest in UV astronomy)

The legacy of these missions is their open-access archives.

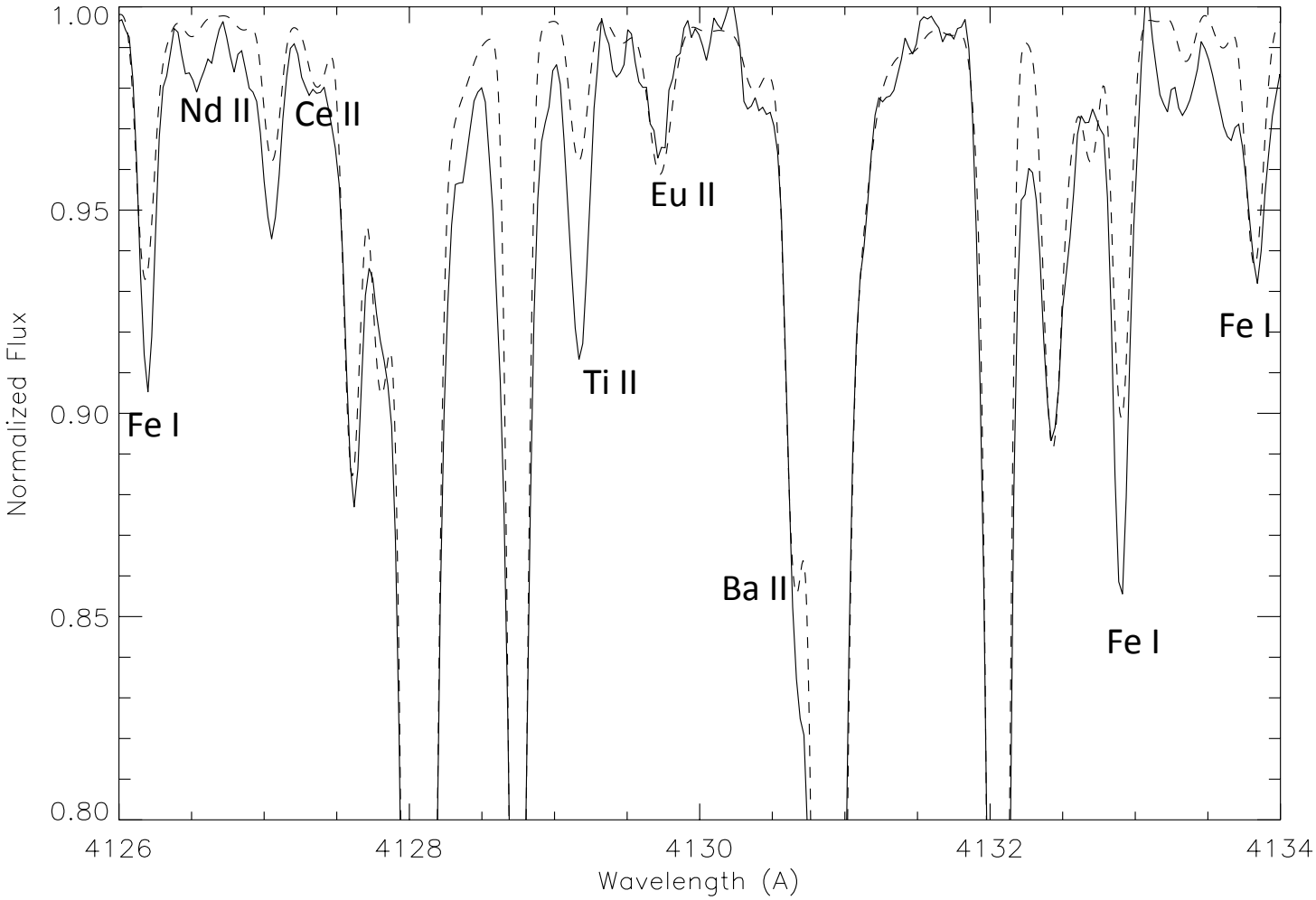
The optical region from space

Relevant space instruments:
HST/STIS 300 - 1115 nm, R ~ 10 000 , $\Delta v > 30$ km/s
HST/NICMOS 800 - 2500 nm, 3 grisms, R ~ 200

Residence to lines of most elements (neutrals, single-ions),
dominated by iron-group elements, but
heavier elements are well represented.

In general, progress in detectors has:
- improved data quality (resolution, signal-to-noise)
- extended the ground-based wavelength regime to be 310 – 1100 nm
- driven the need for more accurate and complete atomic data and will serve, to some extent, to replace the need for UV observations.

Can optical spectroscopy mitigate the loss of the UV?



HR 3383 spectra: observed (solid) and synthetic (dashed)

Wahlgren & Nielsen, in prep.

A Renaissance for the IR

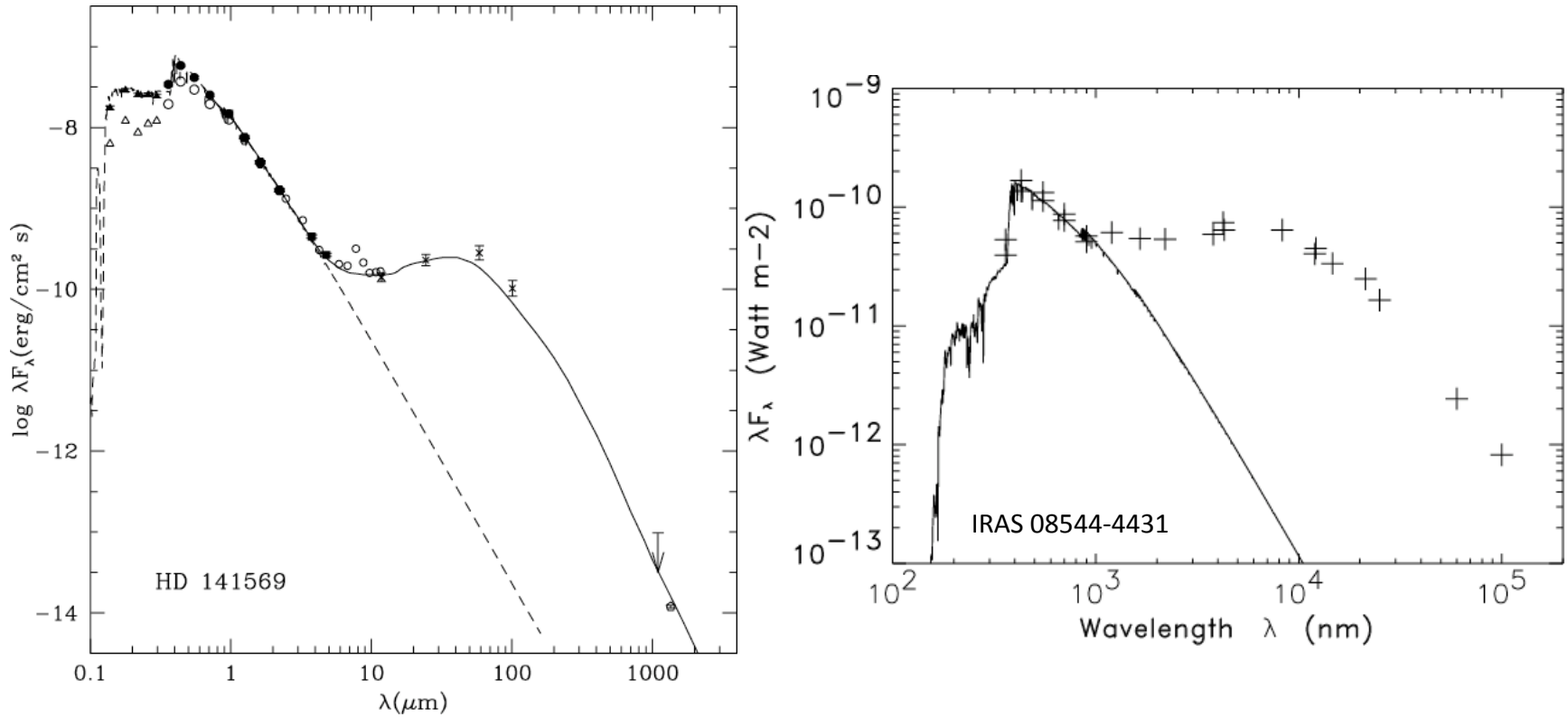
For decades the IR has been used to study cool stars, mostly at low spectral resolution, but included high resolution observations.

The new reality of common operation of high resolution, ground-based instrumentation is increasing the demand for atomic and molecular data.

Importance of IR to astrophysics
- Cool stars have majority of flux in IR
- CS material (dust, gas, disks)
- Exo-planet atmospheres
- Magnetic field measurement (Zeeman broadening proportional to λ^2)
- Accurate velocity measurements
- Presence of certain molecules (CO, SiO) and atomic features (C,N,O)

Problems in the IR
- Terrestrial spectrum needs to be fully characterized (for SOFIA)
- Atomic and molecular data are desperately needed.

Spectral energy distributions (SEDs): veiling the IR (and UV) line spectrum



Merin, B., et al. 2004, A&A 419, 301 - SED for Herbig AeBe star HD 141569

Maas, T. et al. 2003, A&A 405, 271 - SED for the F-type post-AGB star IRAS 08544-4431

IR atomic data available (oscillator strengths)

Few laboratory studies: 118 lines with laboratory measured *f*-values for $\lambda > 1\ \mu$m,
all neutral species Ti (45), V (7), Mn (11), Fe (51), Ni (4), Zn (1)

- Also now for Mn I (Blackwell-Whitehead et al. 2010), Eu II, Sm II, Y I (in progress)

Calculations and compilations (R. Kurucz)

Astrophysical *gf*-values:

- J. Melendez and B. Barbuy (1999) atomic lines in the *J* and *H* bands
- J.M. Borrero et al. (2003) atomic parameters for near-IR lines
- L. Bigot and F. Thevenin (2006) atomic lines in the *Gaia* region (848 – 875 nm)

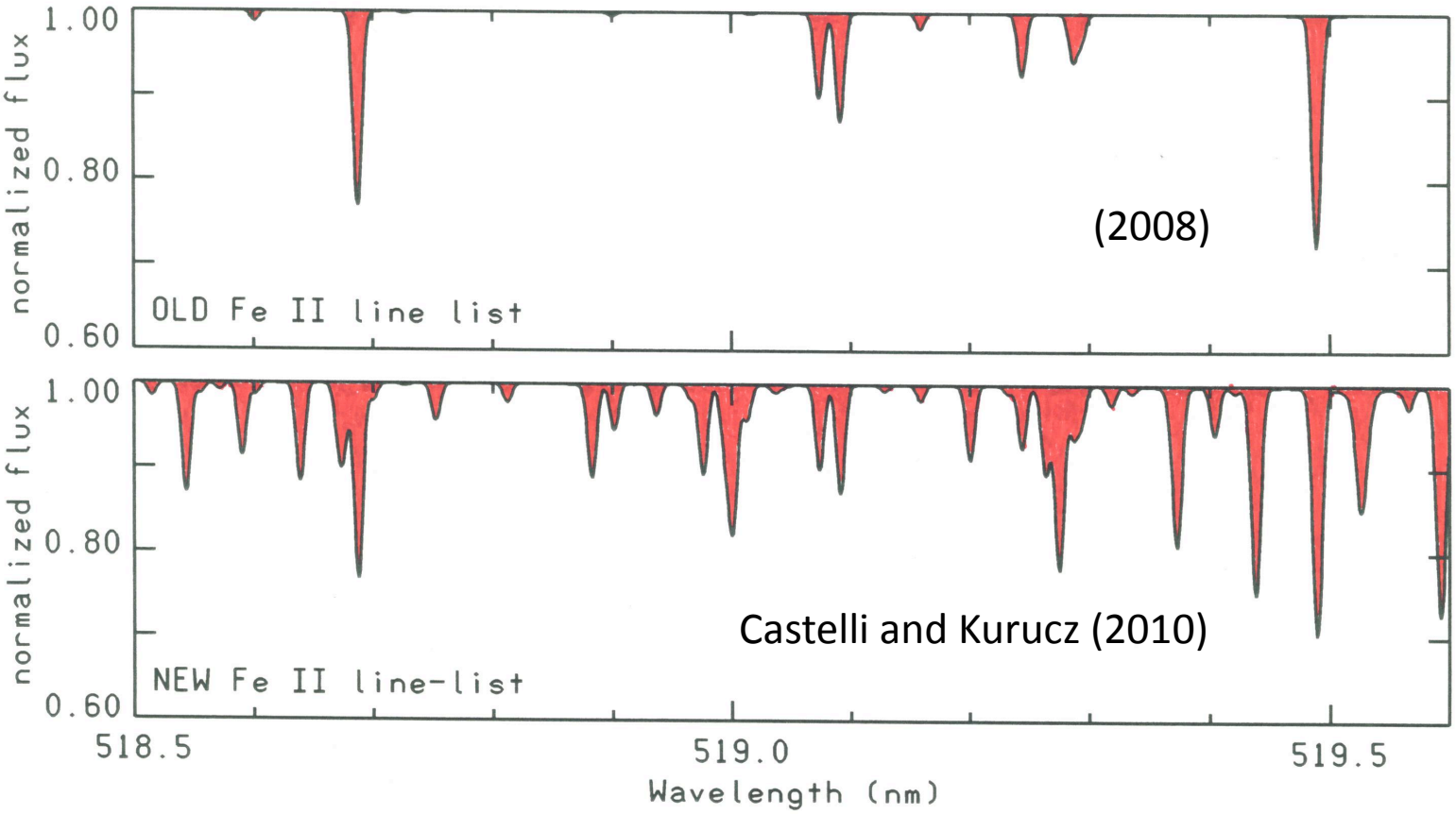
Sample recent calculations

config	levels		-------- E1 lines				
	even	odd	even	odd	good wl	total	old
Cu I	61	61	920	1260	5720	28112	
Cu II	61	61	4303	5758	14959	622985	
Cu IV	55	50	9563	17365	9563	11857712	
Cu X	85	86	508	3002	159	2910966	
Y I	61	61	1634	2141	5393	59226	

TOTAL: new / old = 216 million / 26 million ratio = 8

from R. Kurucz, ASOS10

Computed Fe II spectrum for HR 6000



from R. Kurucz, ASOS10; also, see Poster 19 (Nave) on Fe II

IR line identifications

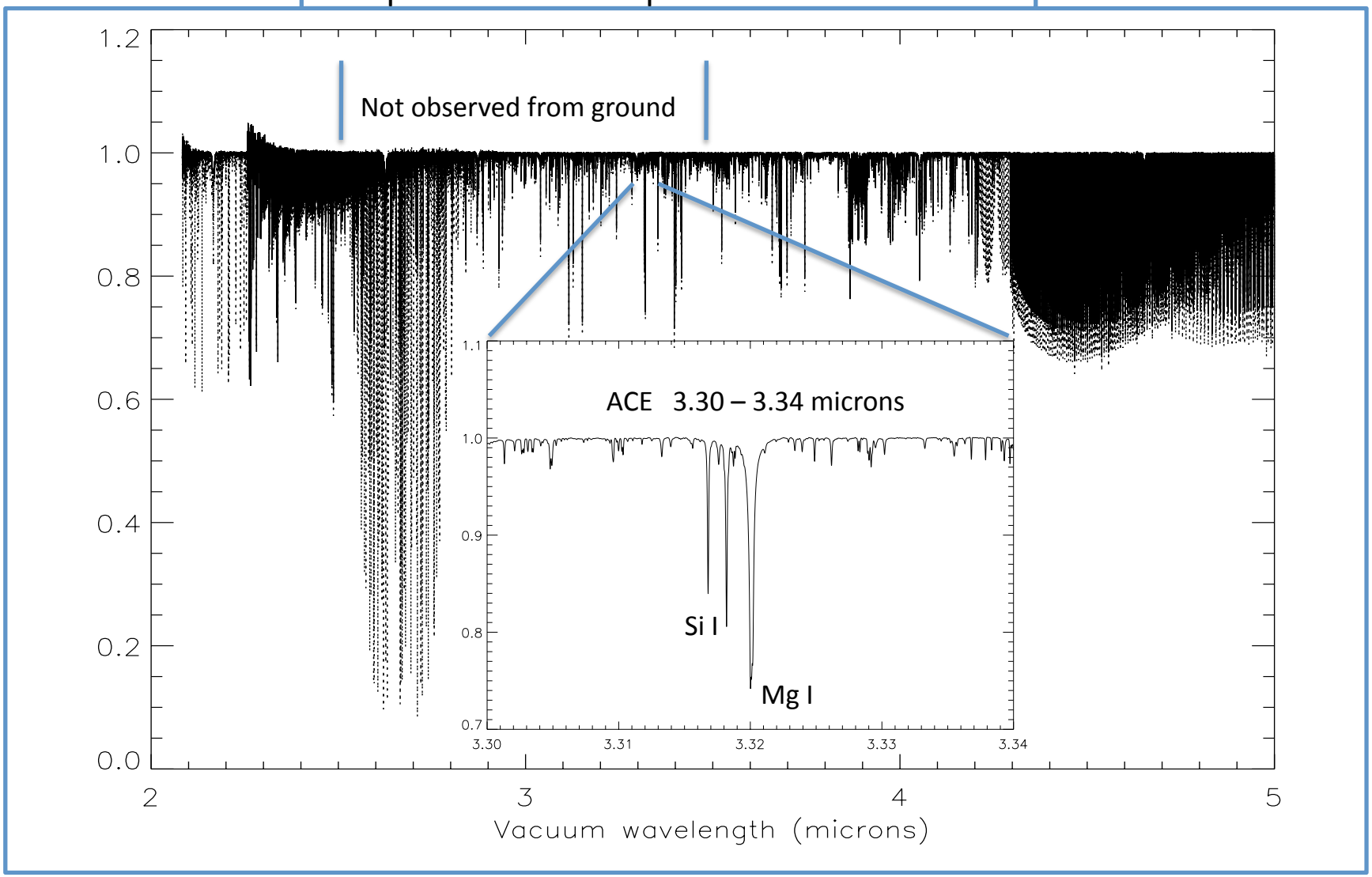
- M. Geller (1992) ATMOS solar spectrum
- L. Wallace (2008) ACE solar spectrum (atomic and molecular)
- F. Hase et al. (2010) ACE-FTS atlas of the infrared solar spectrum
- K. Hinkle, et al. (1995), Arcturus (K2 Iab) atlas 0.9 – 5.3 μm

Laboratory data exist in the literature for:

- Atomic lifetimes for many elements, but
  *BF*s are needed for creating *A*-values

- HFS *A* and *B* constants from optical region studies

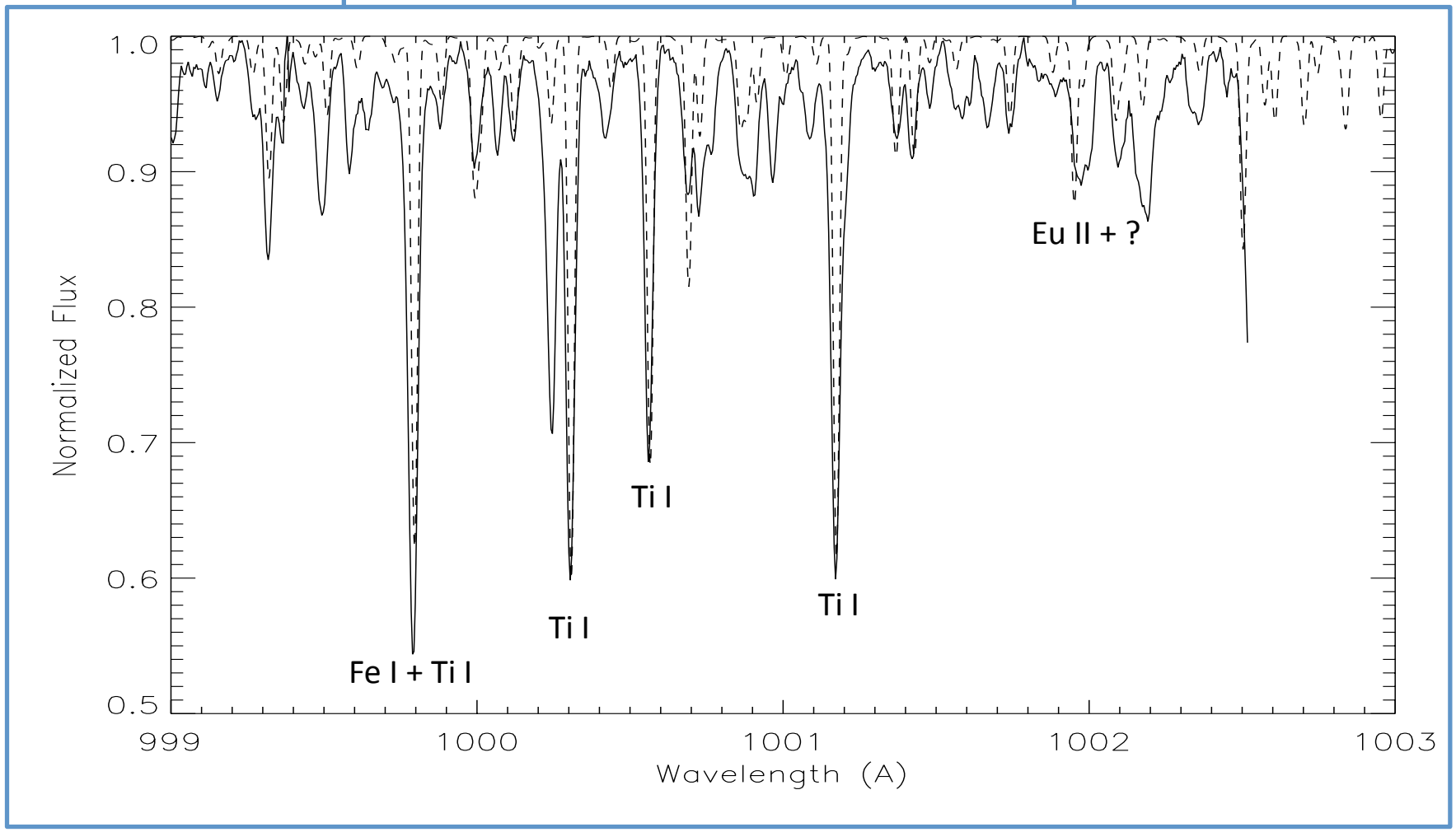
Comparison of solar spectra: ATMOS and ACE



KPNO and ATMOS solar atlases available at kurucz.harvard.edu

ACE (Advanced Chemistry Experiment) solar atlas available at www.ace.uwaterloo.ca

CRIRES-POP: The cool star YY Psc (M3 III)



The mid-IR spectral region (5 – 40 μm)

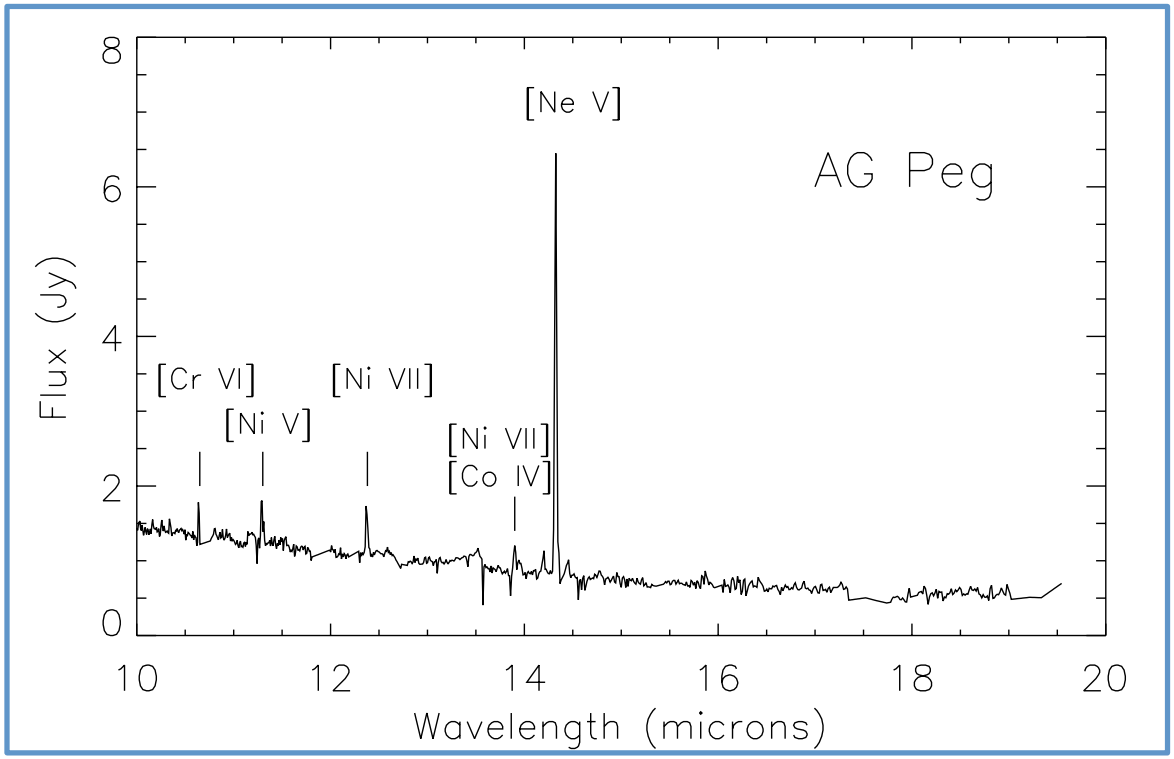
Ground-based facilities:
- ESO/VISIR (N band 8 – 13 μm, Q band 16.5 – 24.5 μm, R = 150 - 30000)

Satellite observatories:
- ISO – Infrared Space Observatory (2.5 – 240 μm, R < 2000)
- Spitzer Infrared Space Telescope (5 – 40 μm, R < 1000)
- AKARI (ASTRO-F) Infrared Astronomical Satellite (50 – 200 μm, R = 500)

Atomic data available: fine-structure lines, (E_{low} < 5000 cm^{-1})
- NIST Atomic Spectra Database: 120 lines (calculated *A* values)
- Univ. Kentucky, The Atomic Line List v2.04: 264 lines (includes low charge states, [Fe II], …)

- Feuchtgruber, H. et al., (1997, 2001) – use of ISO-SWS to identify fine structure lines in AGN and QSO spectra

The mid-IR: The realm of fine-structure lines



Spitzer IR Space Telescope – spectrum of symbiotic star AG Peg

Bruhweiler, Wahlgren, McCollum, Norris, Verner, Eriksson (work in progress)

Status on acquiring laboratory atomic data

UV (priority: Fe-group)
- Work is continuing slowly, both in the lab and with calculations
- FUV-VUV region is very difficult to work in (astro and lab)

Optical (priority: lines that may help us forget the UV)
- Progress over the past decade has been driven by:
  Projects: solar abundances, metal-deficient halo stars, η Carinae, CP stars.
  Individuals in LA community

IR (priorities: Fe-group, post-iron-group elements)
- Few laboratory analyses exist for wavelengths beyond 1 μm
- Data sharing with UV and Opt studies possible to a certain extent
- Data needed for line identification and *f*-values

General needs (encouragement):
- *f*-values for high-excitation transitions of low-charge states (Fe-group, lighter)
- Line data for moderate charge states (IV, V, VI): REE for opacities, heavies for atmospheric modeling

II. Data need – the realities

How can data *need* be characterized?

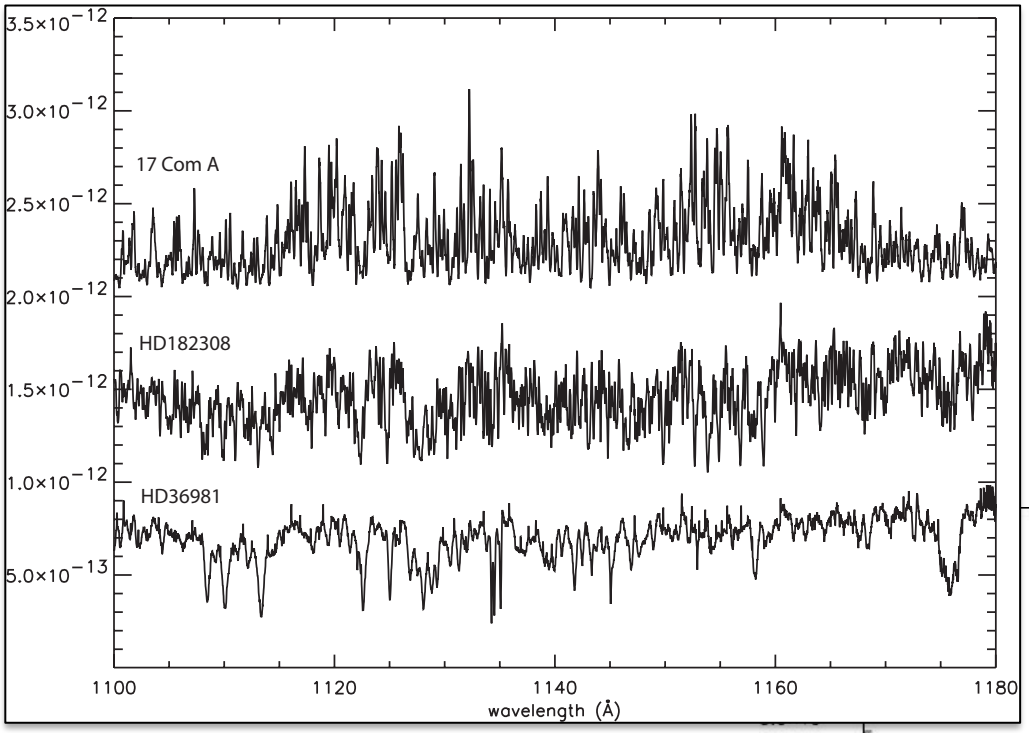
- missing lines

- archived observations (past)

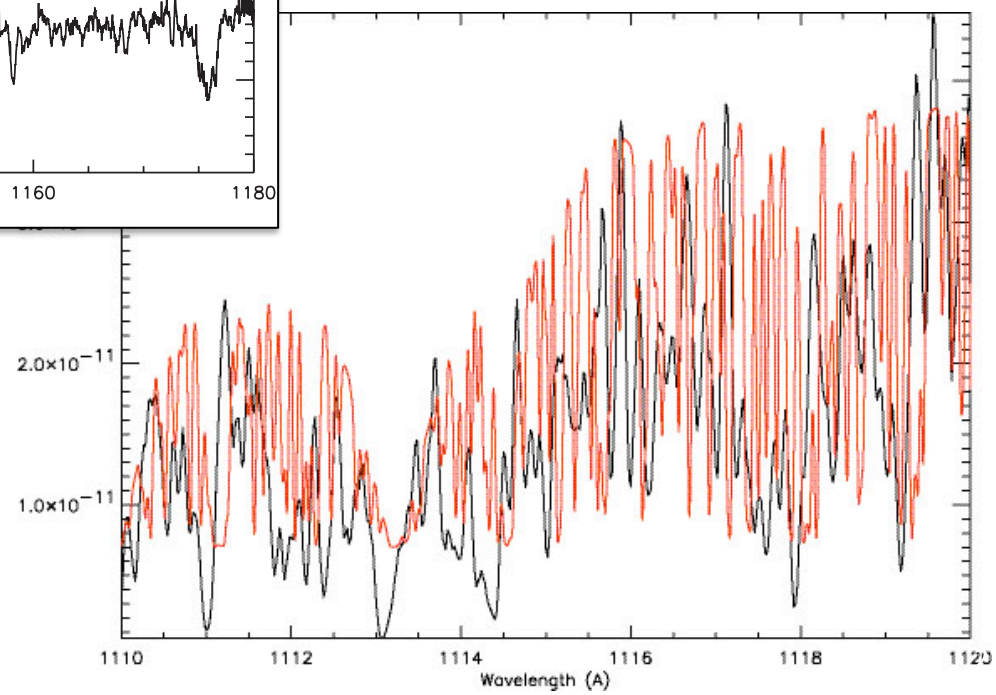
- newly accepted programs (present)

- future directions (future)

Line absorption in the FUV – The Fe group

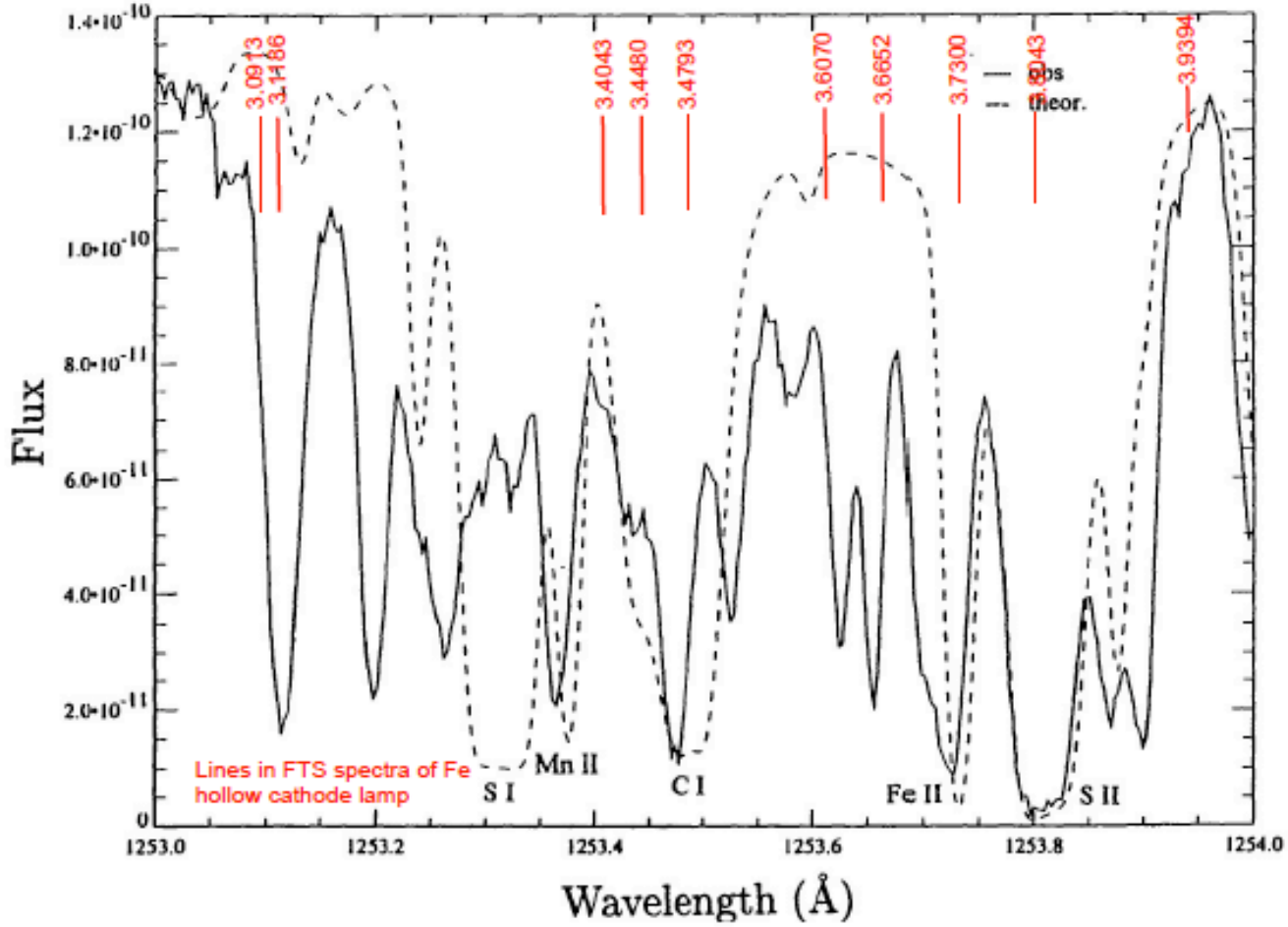


Left: The absorption line spectrum of three B type stars of decreasing metallicity (top to bottom).



Right: Observed spectrum (black) of 17 Com A compared with synthetic spectrum (red). Missing absorption in the calculation is expected to arise from Fe-group elements.

Missing UV lines - Not uncommon for λ < 2000 A
Shifted to the optical-IR region for z > 1.5



The HST spectrum of χ Lupi A (solid) and synthetic spectrum (dashed). The locations of Fe II lines identified from lab spectra have been labeled in red by G.Nave.

Studies highly dependent on atomic data:

1) Modeling of cool chemically peculiar pulsating stars (roAp)

Shulyak, D., Ryabchikova, T., Kildiyarova, R., Kochukhov, O., arXiv: 1004.0246v1, 1 April 2010

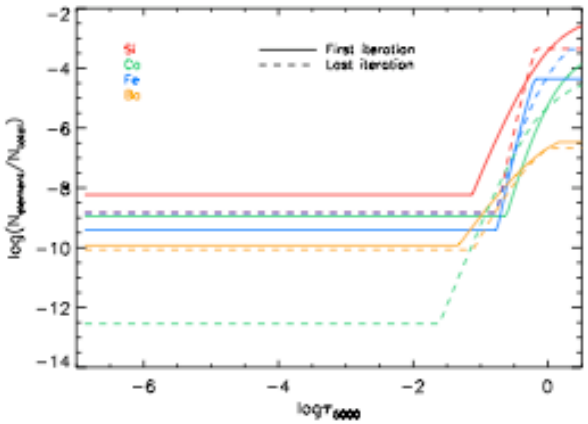


Fig. 3. Stratification of four elements in the atmosphere of HD 101065 derived at the first and last iteration of the abundance analysis.

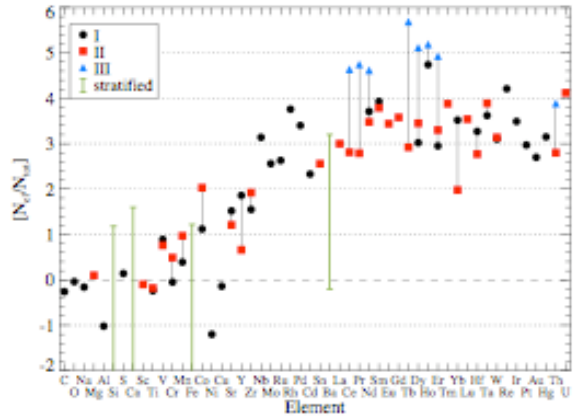


Fig. 2. Chemical composition of the atmosphere of HD 101065. Different symbols correspond to ions from I to III. Bars show abundance ranges for stratified elements.

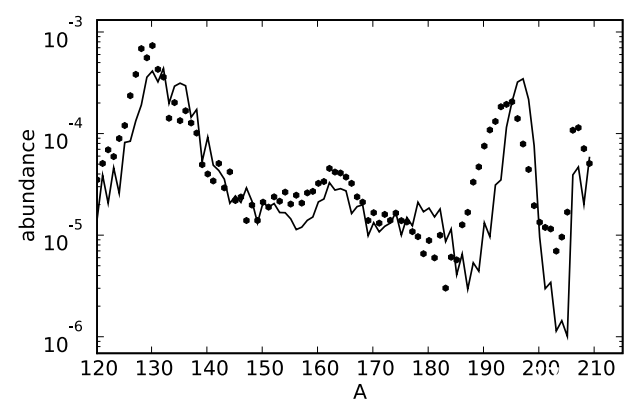
2) ISM: C abundance discrepancies, factor of 2, line dependent, UV C II lines (U.J. Sofia)

3) Missing opacity in UV (2000 – 2500A) in AGN spectra – probably Fe II/III (E. Verner)

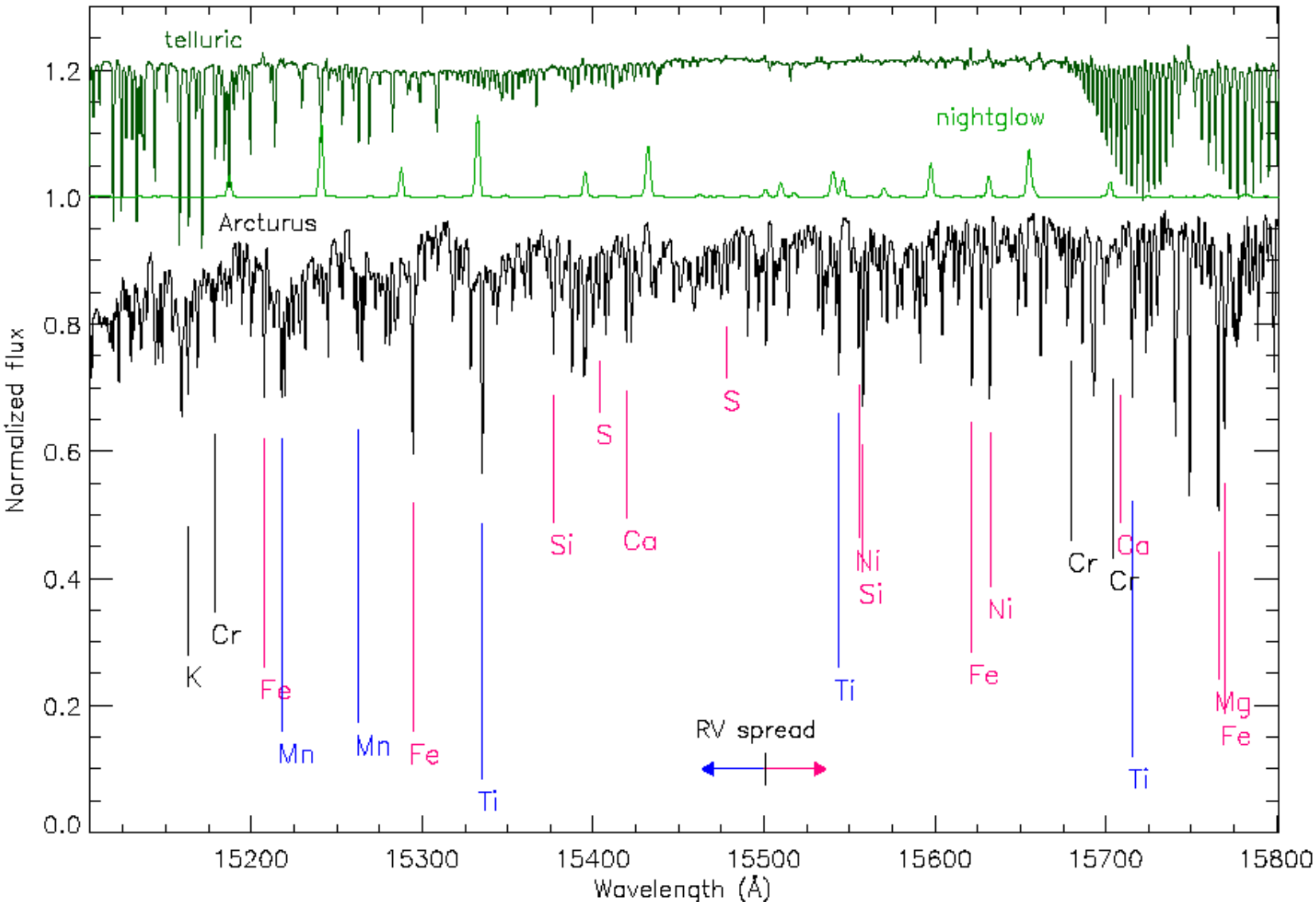
4) Ejecta of neutron star mergers – the creation of *r*-process material after short burst GRBs. (B.Metzger, E. Quataert, et al.)

- UV data for heavy elements (REE & row 6) for opacity, currently using Fe to replicate REE opacity
- Optical data for accurate λ, *f*-values

(Fig.: dots = solar abundances; solid = merger model) →



partial H band spectrum (from J. Pickering, ASOS10)



Allende Prieto et al, Astron.Nach. 329 (9-10) 1018-1021 (2008)

Archived observations

- NASA mission archives are a (buried) treasure trove of potential discovery

- Many data sets have never been part of a publication

- Many spectra have only been used for a single purpose

- Many spectra have never been fully exploited due to the lack of atomic data

New directions – *HST* data needs

A few statistics on *HST* cycle 18 accepted proposals
(from abstracts, Phase I exposure catalogue, and personal inquiry)

155 proposals accepted for acquiring new data
41 proposals accepted for archival studies

75 (of 155) GO proposals include spectroscopy
35 COS: 35 FUV, 8 NUV
37 STIS: 19 FUV, 18 NUV, 1 SC-UV, 9 SC-Opt, 9 SC-IR
10 WFC3: 10 near-IR
2 ACS: 1 WFC/G800L, 1 SBC/PR130L
(51 proposals request only one spectroscopic category above)

7 (of 41) Archive proposals will utilize *HST* spectroscopy
2 will address new atomic data

Cycle 18 GO proposal areas for *HST* spectroscopy

#	Subject	Moderate and High-res modes			
		#E-H	#E-M	#G-M	#COS-M
1	STIS calibration lamp	1	1	-	-
4	Solar system:	-	-	2	-
4	ISM	4	-	-	2
32	Stars:	1	5	7	9
5	Novae and SNe	-	1	1	1
1	Star clusters	-	-	-	1
9	Galaxies	-	-	1	3
1	Galaxy clusters	-	-	-	-
2	Lyα systems	-	-	-	1
2	AGNs	-	-	1	2
13	QSOs	-	-	-	5
1	GRBs	-	-	-	-
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75		6	7	12	24

few proposals (2 or 3) will address new atomic data

Cycle 18 program areas for *HST* stellar spectroscopy

Atmospheres of Cepheid variables
Boron in F stars
Classical novae
ε Aur
Exo-planets
Metal-poor stars
Solar type stars: chromospheres and transition regions
Stellar winds
T dwarfs and brown dwarfs
White dwarfs: element abundances and as light bulb

Advanced spectral library: cool stars (PI: T. Ayres)

β Cassiopeia	(F2 IV)	α Canis Minoris	(F5 IV-V)
α Aquarii	(G2 Ib)	β Draconis	(G2 Iab)
β Geminorum	(K0 IIIb)	γ Draconis	(K5 III)
α Orionis	(M2 Iab)	γ Crucis	(M3.5 III)

Atomic data needs in the future

- *Preparations for JWST* → emission lines (fine-structure lines)

instrumentation	MIR	5 – 28 μm, R ~ 2000
	NIRSPEC	1 – 5 μm, R ~ 1000 & 3000

- *Preparations for SOFIA* → emission lines + ???

instrumentation	FLITECAM	1 – 5.5 μm, R ~ 2000
	EXES	5 – 28 μm, R ~ 3000, 10^4, 10^5
	FIFI LS	42 – 210 μm, R ~ 1700
	GREAT	60 – 200 μm, R ~ 10^4 - 10^8

- *The Decadal Survey* - nice words, but …

Galaxies across time → high-res UV spectroscopy, 4m class
Stars and stellar evolution → needs of precision abund., opacities
Galactic neighborhood → UV/opt spectroscopy, abundances
(circumgalactic medium, metal-poor stars)

III. Resources (talking points)

- Data

- Laboratory facilities

- People

- Funding

Data resources for the spectroscopist

- Astronomical spectra
  - UV spectra for many targets, lacking in wavelength coverage
  - recommendation: a library of high resolution *HST* spectra

  (CRIRES-POP: a high-resolution near-IR spectrum library)

- Laboratory spectra
  - limited number of spectra
  - recommendation: a UV – IR library of high resolution spectra

- Atomic structure calculations
  - much data exists, but needs to be evaluated

Laboratory facilities (UV – IR): working on atomic data

US facilities:
- NIST, Toledo , Univ. Wisconsin
- Sitting on the sidelines: many colleges and universities
- recommendation: more involvement

Foreign facilities:
- China, ESO, Hannover, ICL, Japan, LaPlata, Liege, Lund, Meudon, Moscow, Orsay, Stockholm, UWO, …

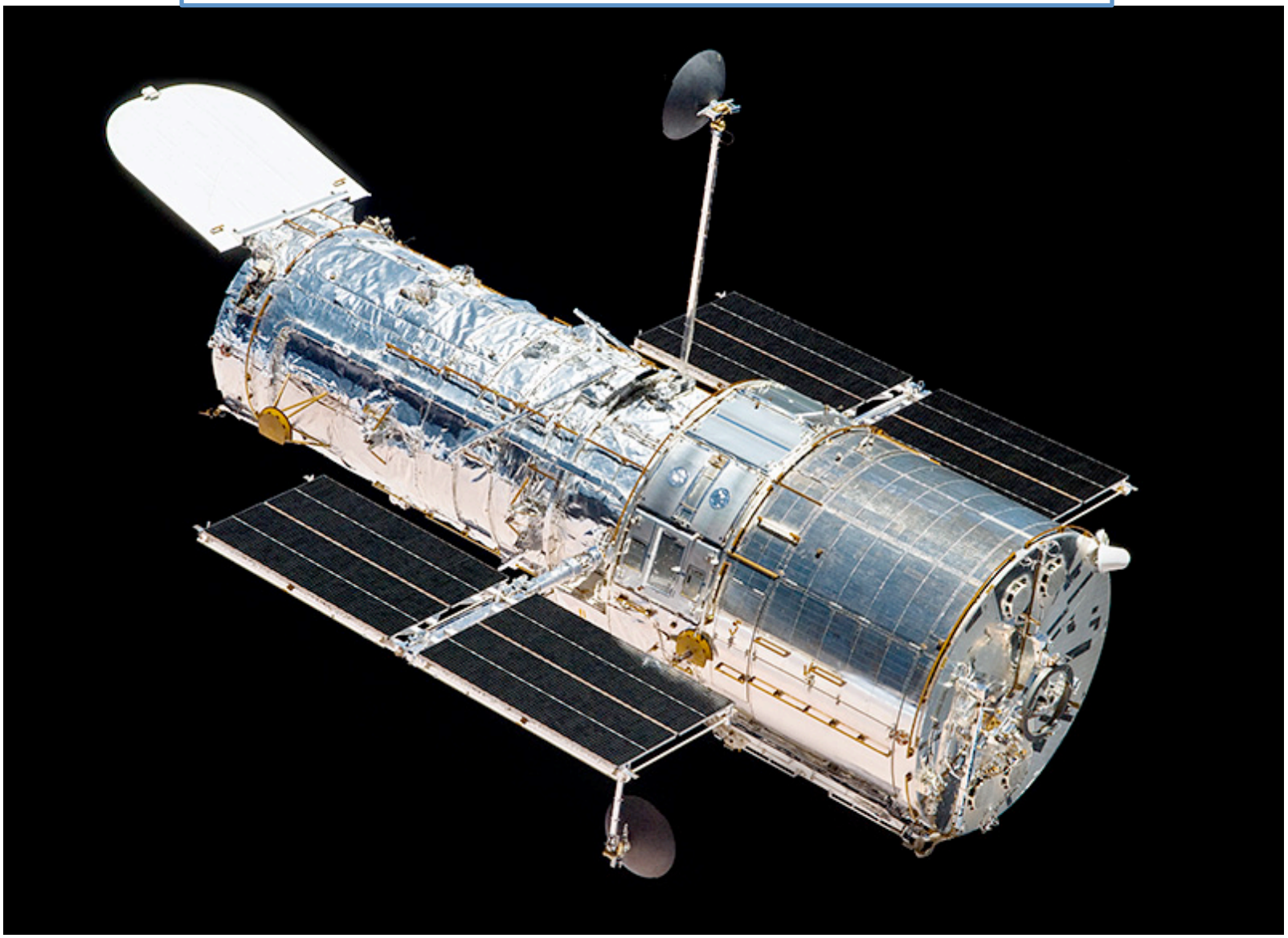
Theoreticians: many contributors around the world

See posters from NIST (15, 17, 19, 21), Toledo (46), Wisconsin (22), ICL (18)

People: (too few)

- University students, staff and faculty
- Government labs

Funding sources: (insufficient amounts)

- NASA lab-astro program
- NSF A&ARG and MRI programs
- NIST, DOE
- Industrial
- Education institutions
- Private Foundations (foreign)

Summary: Happy 20th Birthday to the *HST*