中国科学院国家天文台
NATIONAL ASTRONOMICAL OBSERVATORIES, CAS

Atomic data for Solar Physics Applications

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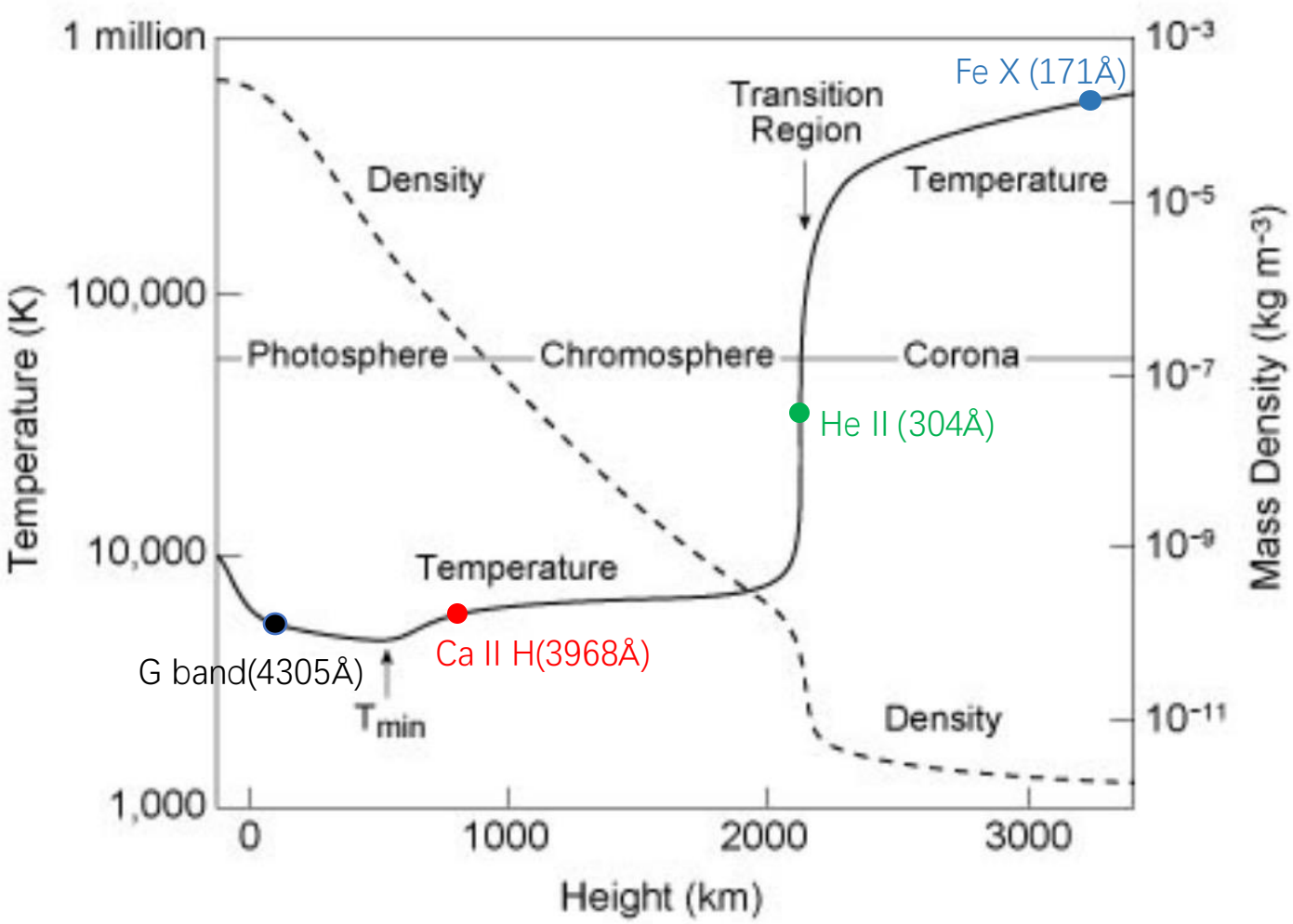
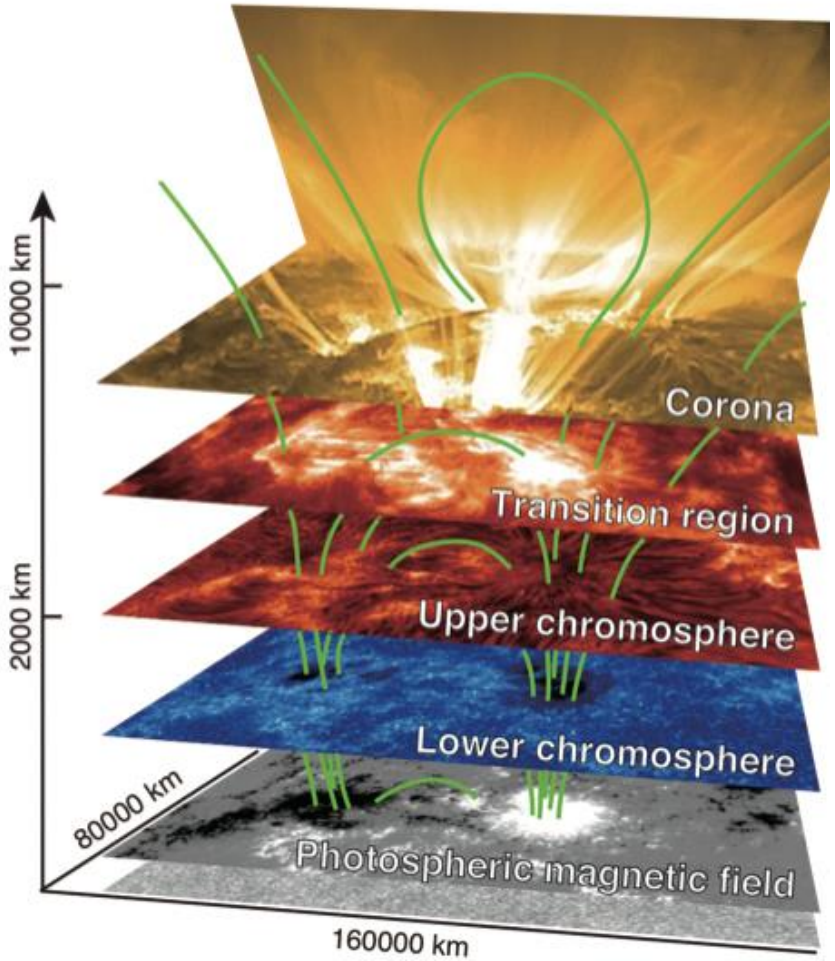
National Astronomical Observatories
Chinese Academy of Sciences

CompAS meeting, 2025.6.13, Lund, Sweden

Solar Atmosphere

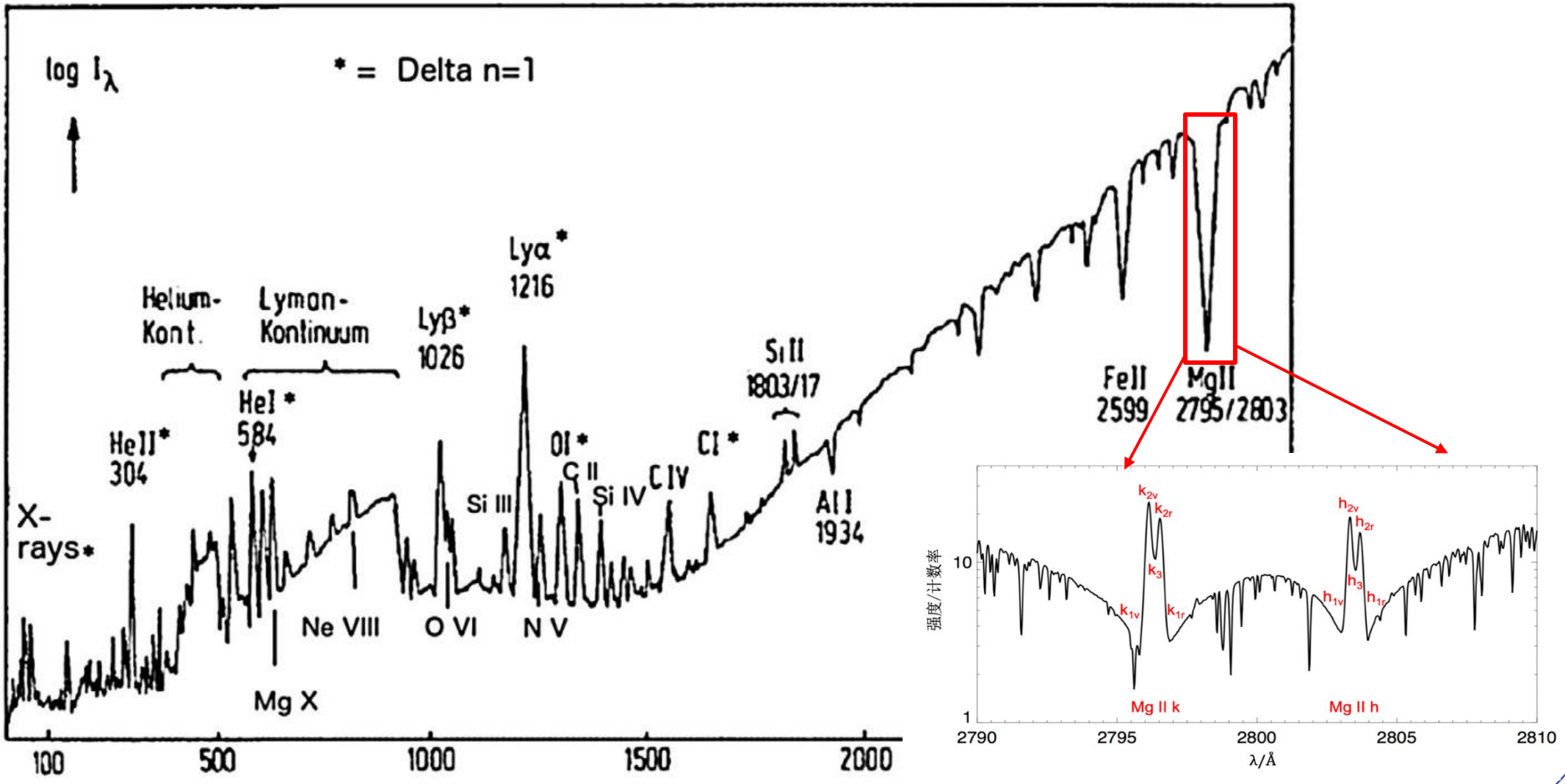


Source: Rajhans 2022



Credit: NAOJ/JAXA, NASA

Solar Spectra



Source: Judge 2019

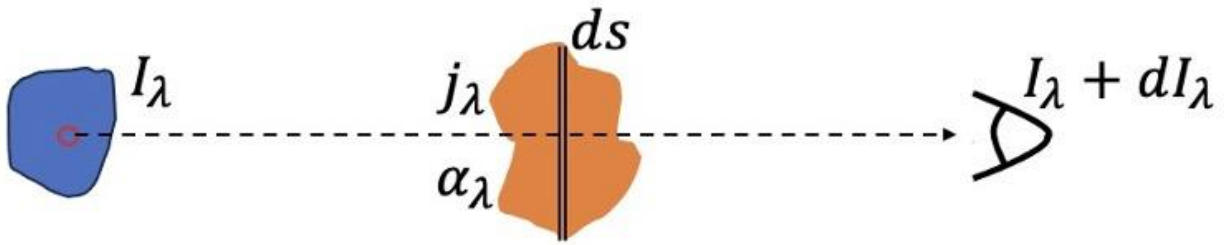
Solar Spectra Lines

Optical thin lines:

$$I(\lambda_{ji}) = \frac{h\nu_{ji}}{4\pi} \int N_j(Z^{+r})\, A_{ji}\, ds \quad (\mathrm{erg\,cm^{-2}\,s^{-1}\,sr^{-1}})$$

$$N_j(Z^{+r}) \equiv \frac{N_j(Z^{+r})}{N(Z^{+r})} \frac{N(Z^{+r})}{N(Z)} \frac{N(Z)}{N_H} \frac{N_H}{N_e} N_e$$

Optical thick lines:



emission absorption

$$dI_\lambda(s) = j_\lambda(s)\rho ds - \kappa_\lambda(s)\rho I_\lambda(s) ds$$

statistical equilibrium

+

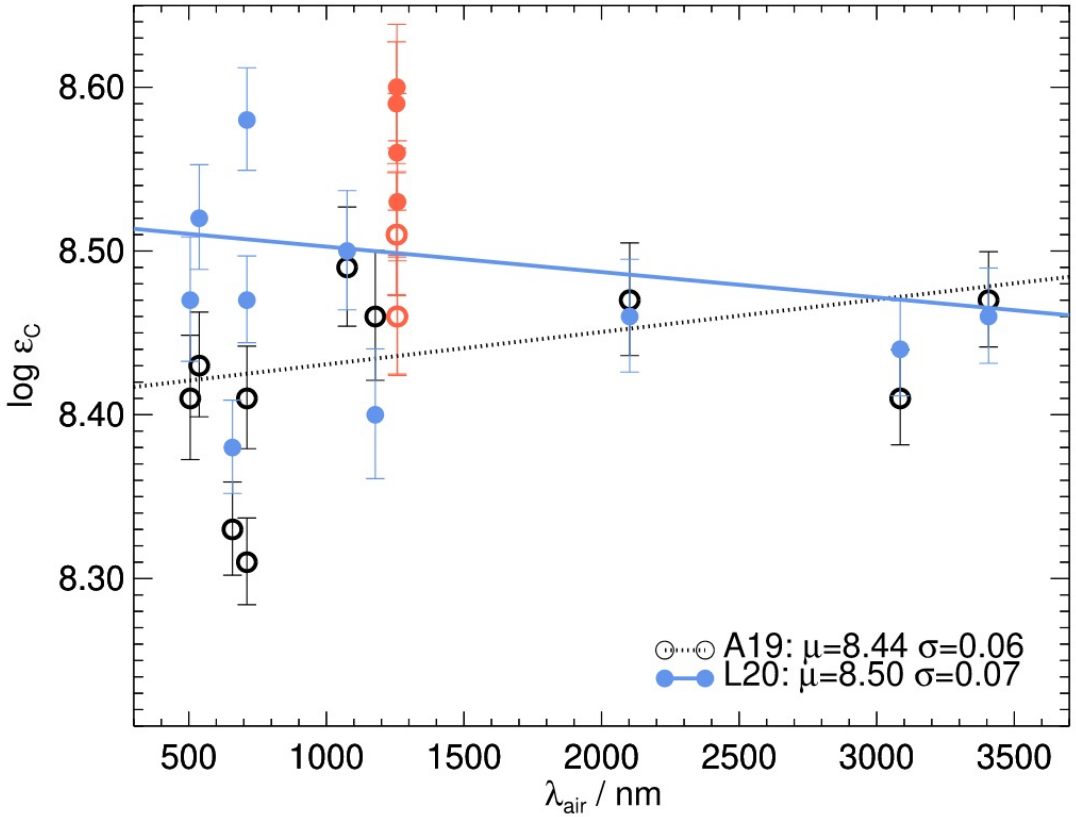
radiative transfer

Atomic data

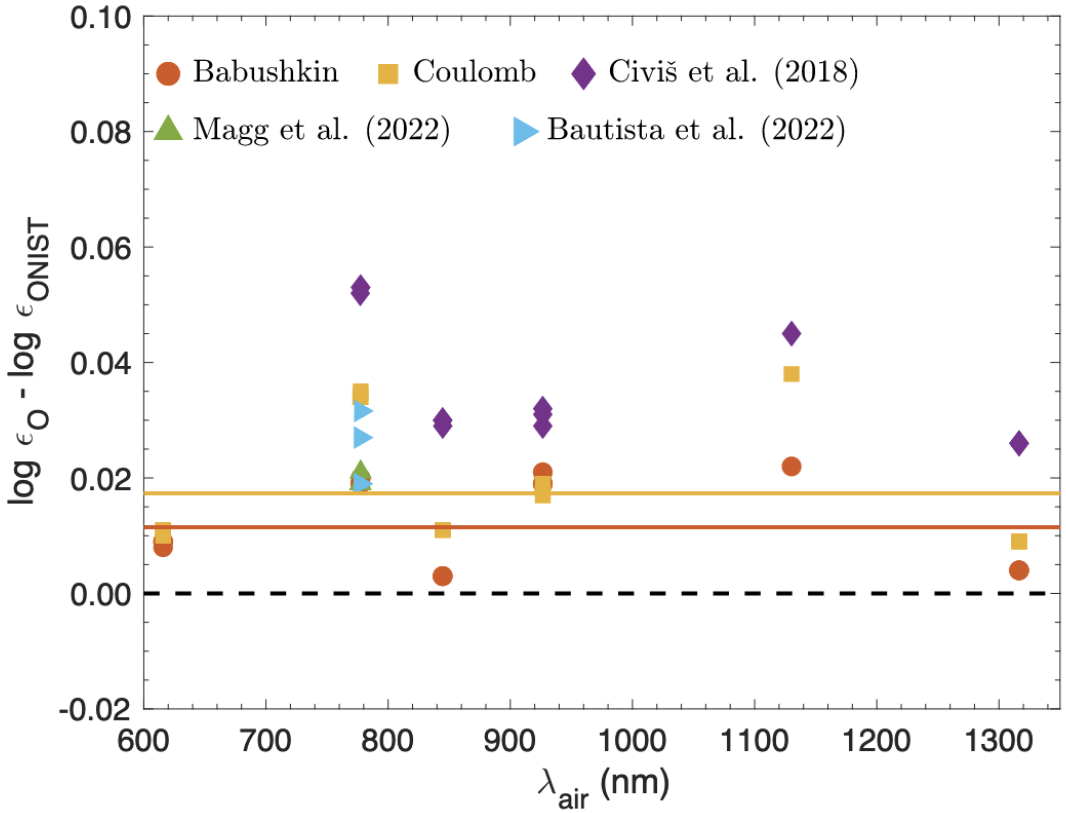
- wavelength
- radiative data A/log gf
- collisional cross section
- photoionization cross section
- hyperfine and isotopic splitting
- ……

GRASP calculations for radiative transitions

Collaborated with Anish Amarsi, Per Jönsson, Meichun Li on C, N, O, S atoms and atomic ions



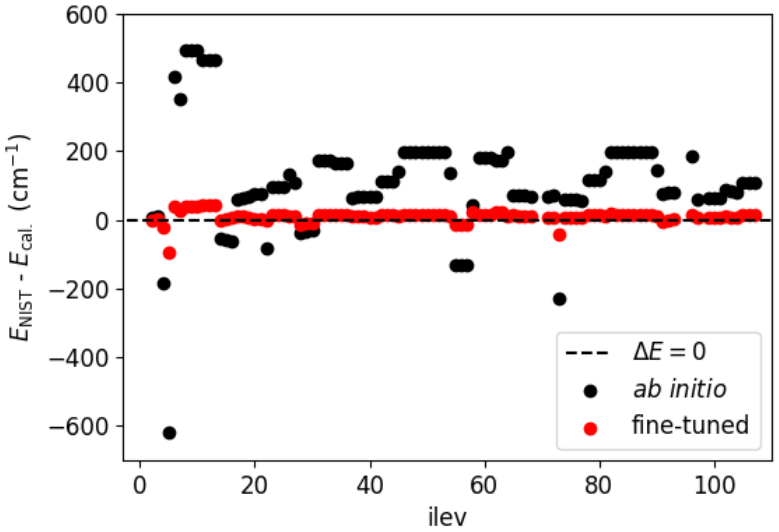
C abundance analysis
(Li et al. 2021)



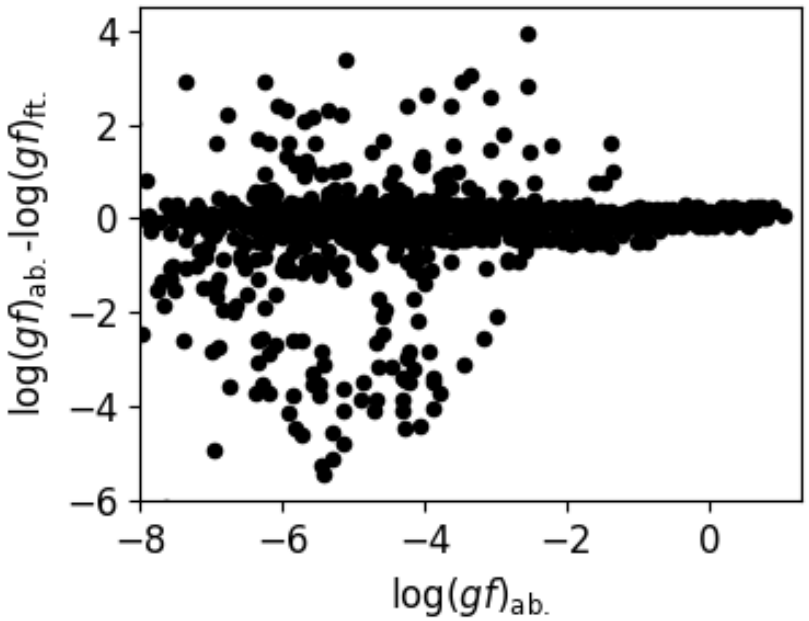
O abundance analysis
(Li et al. 2023)

GRASP calculations for radiative transitions

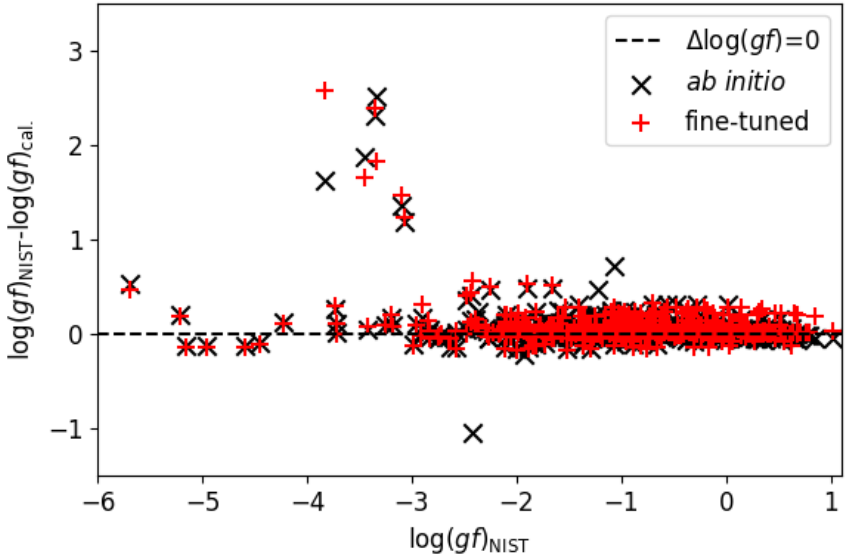
ab initio and fine-tuned energies and log(gf) for S I



ab initio and fine-tuned energies compared with NIST-ASD



Comparison *of ab initio* and fine-tuned log(gf)



ab initio and fine-tuned log(gf) compared with NIST-ASD

Fine-tuning method: Y. Li et al. 2023, Atoms

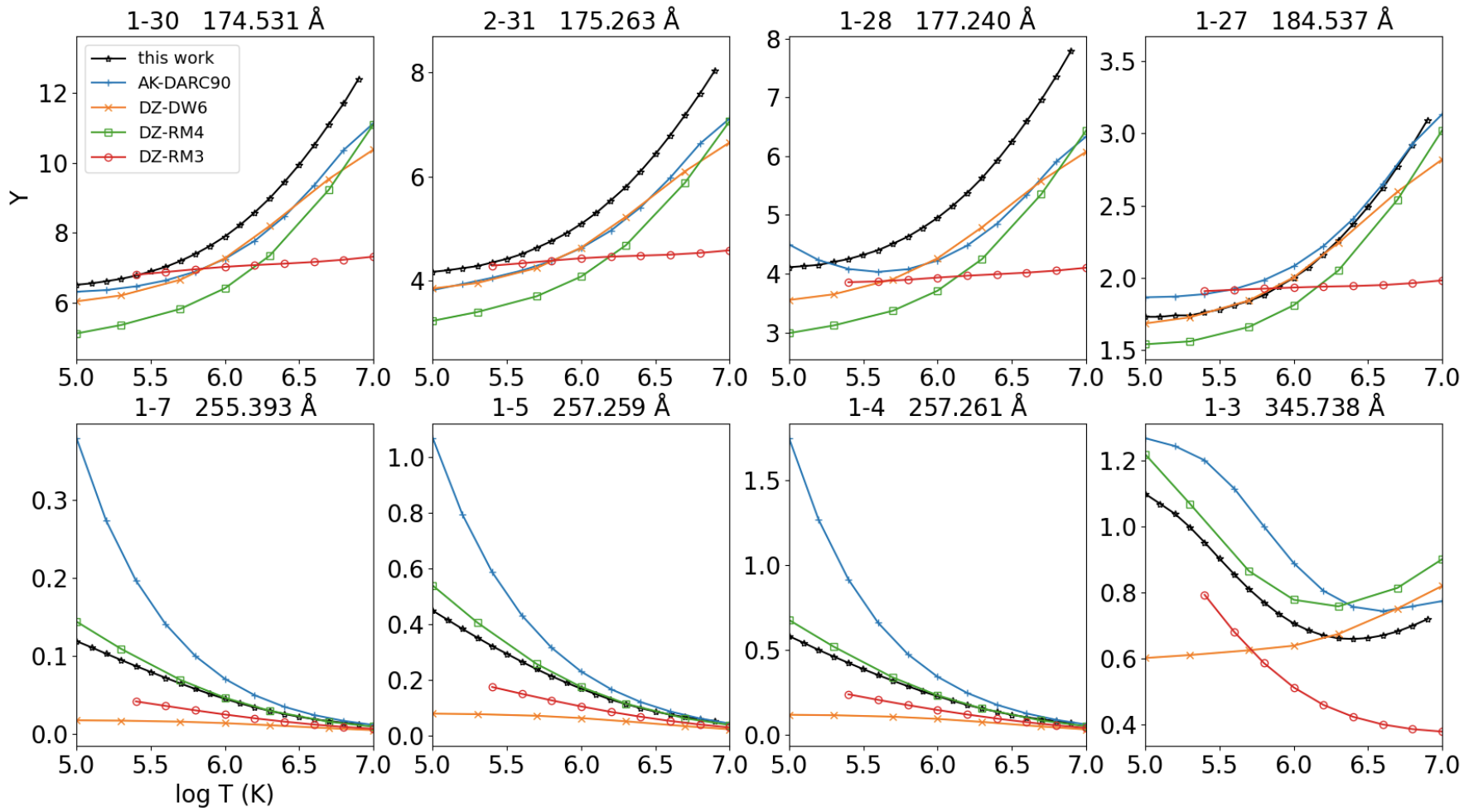
Theoretical calculations of collisional data

Collaborated with Connor Ballance and Tomas Brage
Atomic structure calculations: GRASP0 code
Scattering calculation: DARC codes based on the Dirac R-matrix method

				A (s^{-1})		
i-j	λ (Å)	Lower level	Upper level	CHIANTI V10.0[a]	MCDHF[b]	Ratio
1-30	174.531	$3s^2\ 3p^5\ {}^2P_{3/2}$	$3s^2\ 3p^4\ 3d\ {}^2D_{5/2}$	1.860e+11	1.807e+11	0.97
2-31	175.263	$3s^2\ 3p^5\ {}^2P_{1/2}$	$3s^2\ 3p^4\ 3d\ {}^2D_{3/2}$	1.750e+11	1.697e+11	0.97
1-28	177.240	$3s^2\ 3p^5\ {}^2P_{3/2}$	$3s^2\ 3p^4\ 3d\ {}^2P_{3/2}$	1.540e+11	1.466e+11	0.95
1-27	184.537	$3s^2\ 3p^5\ {}^2P_{3/2}$	$3s^2\ 3p^4\ 3d\ {}^2S_{1/2}$	1.220e+11	1.249e+11	1.02
1-7	255.393	$3s^2\ 3p^5\ {}^2P_{3/2}$	$3s^2\ 3p^4\ 3d\ {}^4D_{1/2}$	3.080e+06	3.453e+06	1.12
1-5	257.259	$3s^2\ 3p^5\ {}^2P_{3/2}$	$3s^2\ 3p^4\ 3d\ {}^4D_{5/2}$	3.330e+06	6.077e+06	1.82
1-4	257.261	$3s^2\ 3p^5\ {}^2P_{3/2}$	$3s^2\ 3p^4\ 3d\ {}^4D_{7/2}$	5.640e+01	5.748e+01	1.02
1-3	345.738	$3s^2\ 3p^5\ {}^2P_{3/2}$	$3s\ 3p^6\ {}^2S_{1/2}$	3.820e+09	2.996e+09	0.78

EUV lines in Fe X used for density, temperature and magnetic strength diagnostics

Theoretical calculations of collisional data

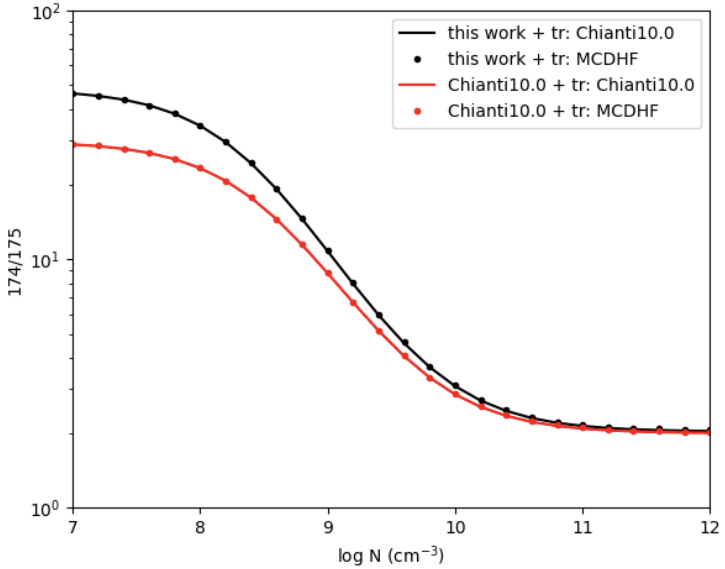


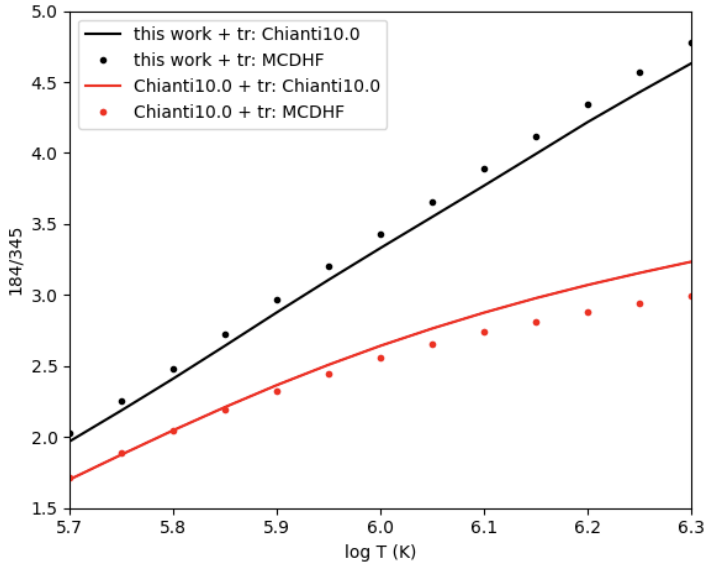
AK-DARC90: DARC R-matrix calculation from Aggarwal & Keenan (2005);
DZ-DW6: distorted wave calculation from Del Zanna et al. (2012);
DZ-RM4: R-matrix calculation from Del Zanna et al. (2012);
DZ-RM3: R-matrix calculation from Del Zanna et al. (2004);
This work: DARC calculation

Thermally-averaged effective collision strengths for Fe X lines, from different calculations.

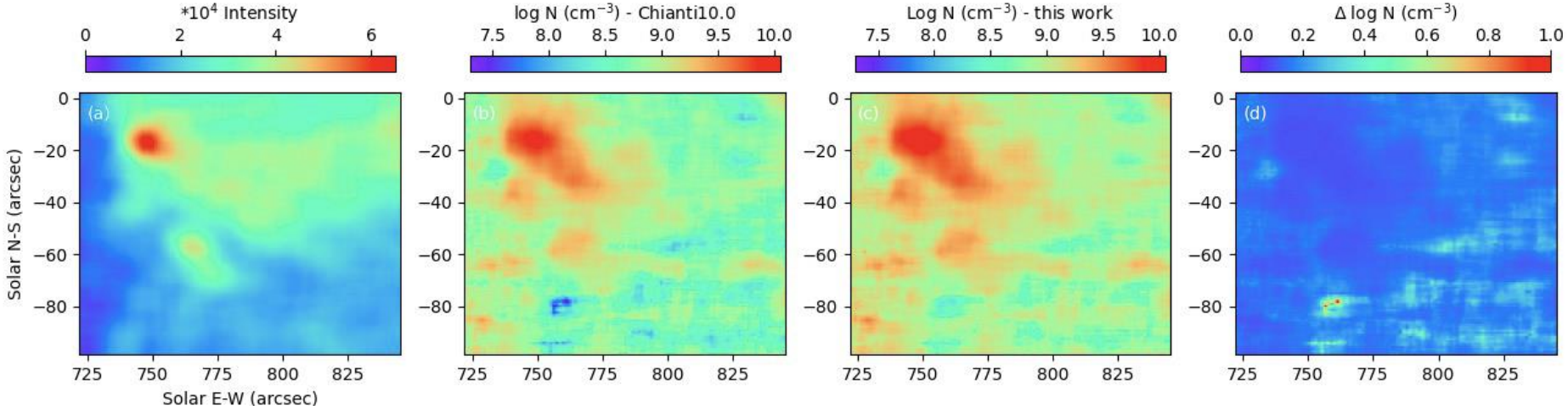
Theoretical calculations of collisional data

174/175 ratio as a function of electron density at temperature of 10^6 K →



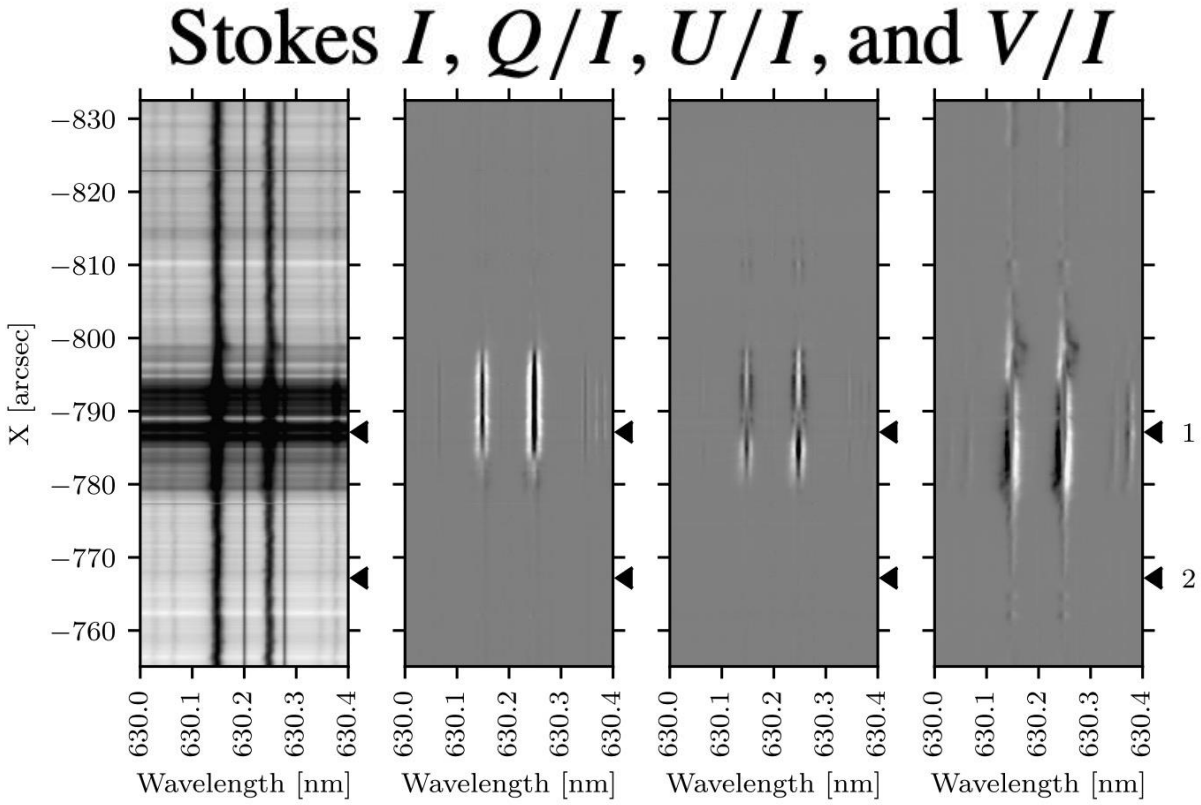


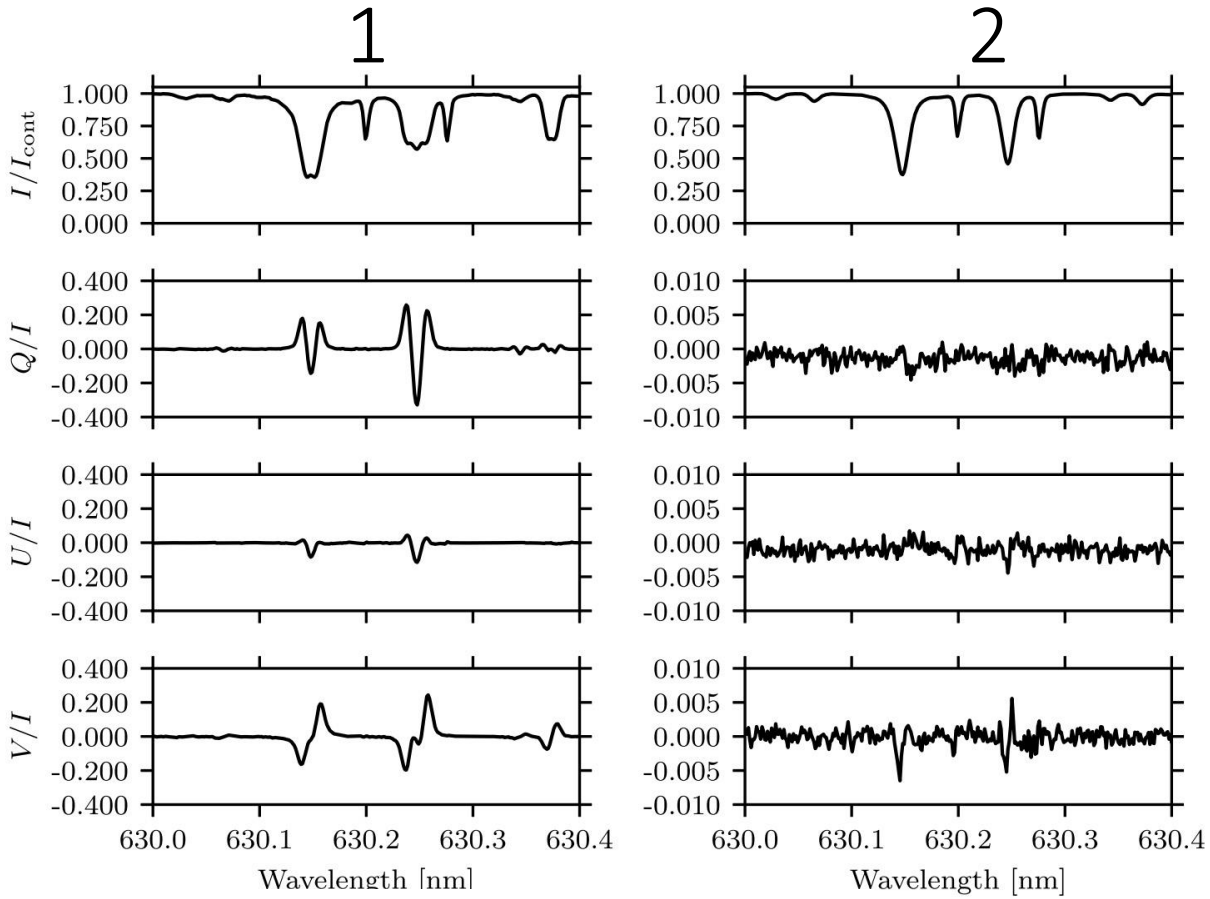
←184/345 as a function of temperature at electron density of 10^{10} cm^{-3}



Density map obtained with different collisional data

Spectropolarimetry: solar magnetic measurement





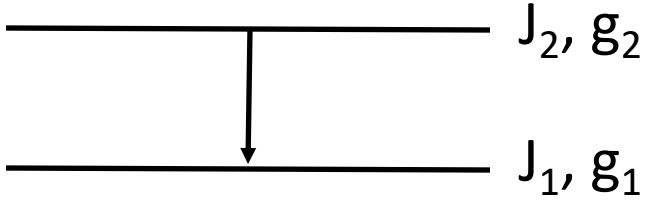
Fe I@630.2 nm from DKIST/ViSP

(Solar Physics, 2022, 297:22)

Landé factor

LS coupling, Zeeman induced polarization

"weak-field" approximation



$$\bar{g} = \frac{1}{2}(g_1 + g_2) + \frac{1}{4}(g_1 - g_2)d$$ ————circular polarization

$$\overline{G} = \bar{g}^2 - \delta$$ ————linear polarization

$$\delta = \frac{1}{80}\Delta^2(16s - 7d^2 - 4)\ ,$$

$$d = J_1(J_1+1) - J_2(J_2+1)\ ,$$

$$s = J_1(J_1+1) + J_2(J_2+1)\ ,$$

$$\Delta = g_1 - g_2\ .$$

Landi Degl'Innocenti & Landolfi 2004

Landé factor

LS coupling, Zeeman induced polarization

(1) Transitions with $\bar{g} \neq 0$ and $\bar{G} = 0$, which have zero *linear* polarization under the Zeeman effect;

$^4D_{1/2}$–$^{2S+1}L_{1/2}$,^{6} $G_{3/2}$–$^{2S+1}L_{1/2}$, where $^{2S+1}L \neq {}^4D$.

(2) Transitions with $\bar{g} = 0$ and $\bar{G} \neq 0$, which have zero *circular* polarization under the Zeeman effect;

$^6P_{3/2}$–$^4F_{5/2}$, $^5D_2$–$^3G_3$, $^7D_1$–$^5F_2$, $^8D_{5/2}$–$^6G_{7/2}$,
$^5F_2$–$^5H_3$, $^7F_2$–$^7H_3$, $^7F_3$–$^5H_4$, $^8F_{3/2}$–$^6G_{5/2}$.

(3) Transitions with $\bar{g} = \bar{G} = 0$, which have zero polarization under the Zeeman effect.

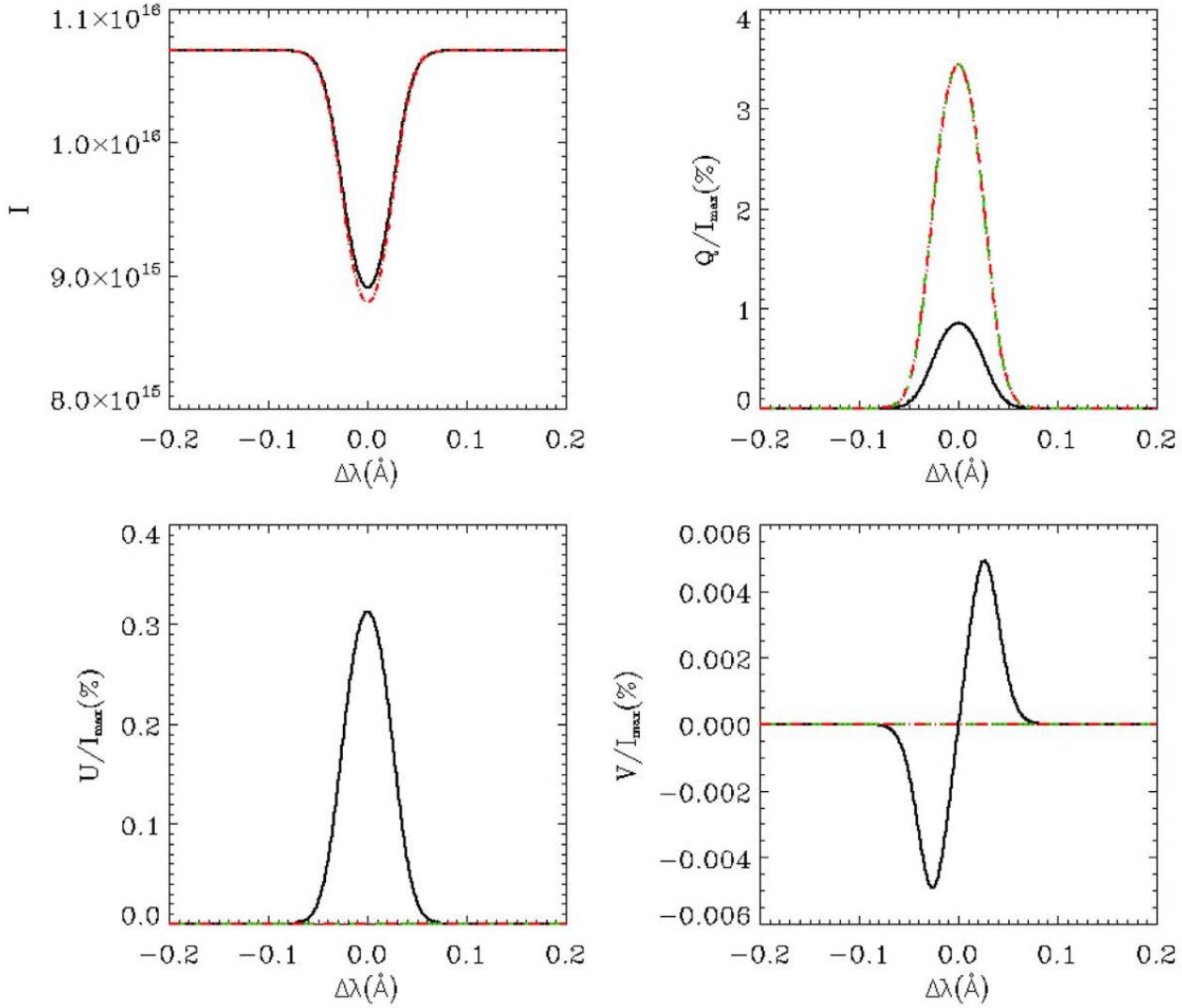
$^3P_0$–$^5F_1$, $^4D_{1/2}$–$^4D_{1/2}$, $^4D_{1/2}$–$^6G_{3/2}$, $^5D_0$– $^5F_1$,
$^5F_1$–$^5F_1$, $^5F_1$–$^7F_0$, $^5F_1$–$^7H_2$, $^6G_{3/2}$–$^6G_{3/2}$, $^7H_2$–$^7H_2$.

Transitions with large landé factor

$\bar{g}_{LS} \geq 3$					
$^4P_{\frac{1}{2}} - {}^6D_{\frac{1}{2}}$	3.	$^6D_{\frac{1}{2}} - {}^8F_{\frac{1}{2}}$	3.667	$^8D_{\frac{5}{2}} - {}^6G_{\frac{3}{2}}$	3.6
$^6P_{\frac{3}{2}} - {}^4D_{\frac{1}{2}}$	3.	$^7D_1 - {}^7D_1$	3.	$^8D_{\frac{7}{2}} - {}^6G_{\frac{5}{2}}$	3.
$^6P_{\frac{3}{2}} - {}^6F_{\frac{1}{2}}$	3.167	$^7D_1 - {}^7F_0$	3.	$^7F_3 - {}^7H_2$	3.
$^6P_{\frac{5}{2}} - {}^4F_{\frac{3}{2}}$	3.	$^7D_2 - {}^5F_1$	3.	$^7F_4 - {}^5H_3$	3.
$^7P_2 - {}^5F_1$	3.5	$^7D_2 - {}^7G_1$	3.25	$^8F_{\frac{1}{2}} - {}^8F_{\frac{1}{2}}$	4.
$^8P_{\frac{5}{2}} - {}^6F_{\frac{3}{2}}$	3.2	$^7D_3 - {}^5G_2$	3.167	$^8F_{\frac{5}{2}} - {}^6G_{\frac{3}{2}}$	3.
$^5D_0 - {}^7D_1$	3.	$^8D_{\frac{3}{2}} - {}^6F_{\frac{1}{2}}$	3.667	$^8F_{\frac{5}{2}} - {}^8H_{\frac{3}{2}}$	3.3
$^6D_{\frac{1}{2}} - {}^6D_{\frac{1}{2}}$	3.333	$^8D_{\frac{3}{2}} - {}^8G_{\frac{1}{2}}$	3.833	$^8F_{\frac{7}{2}} - {}^6H_{\frac{5}{2}}$	3.286

Landi Degl'Innocenti & Landolfi 2004; Li et al. 2017

Landé factor



Stokes profiles of Fe I transition $^5F_1^o$- $^5F_1$ at 7389.398 Å

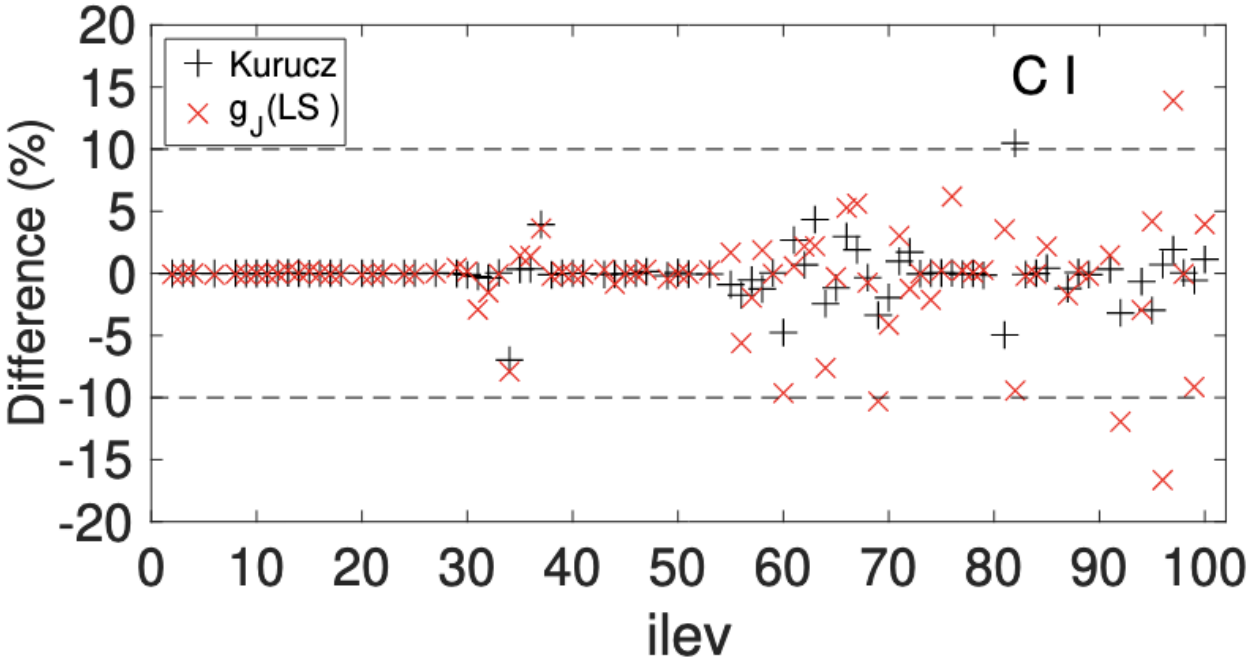
Red dashed curves: LS-coupling scheme g1=g2=0 , B=100 G.

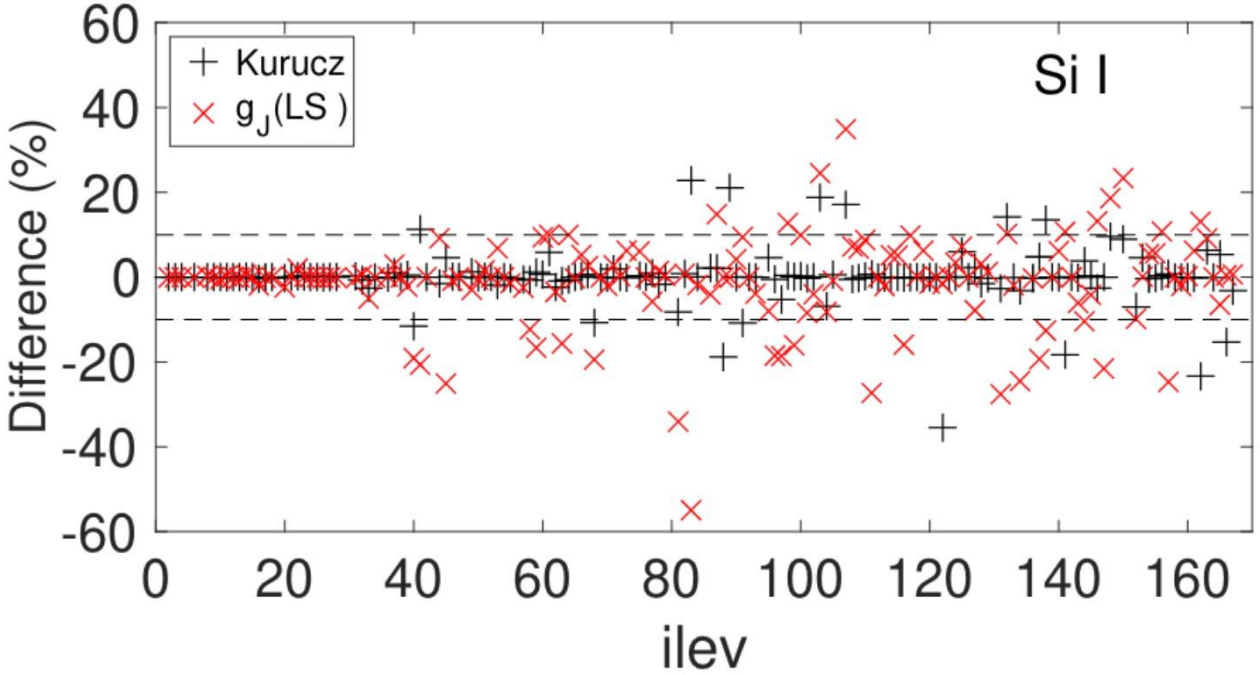
Green dashed curves: experimental g1= -0.016, g2= 0.007, B = 0 G

Black solid curves: experimental g1= -0.016, g2= 0.007, B = 100 G

Li et al. ApJ, 2017

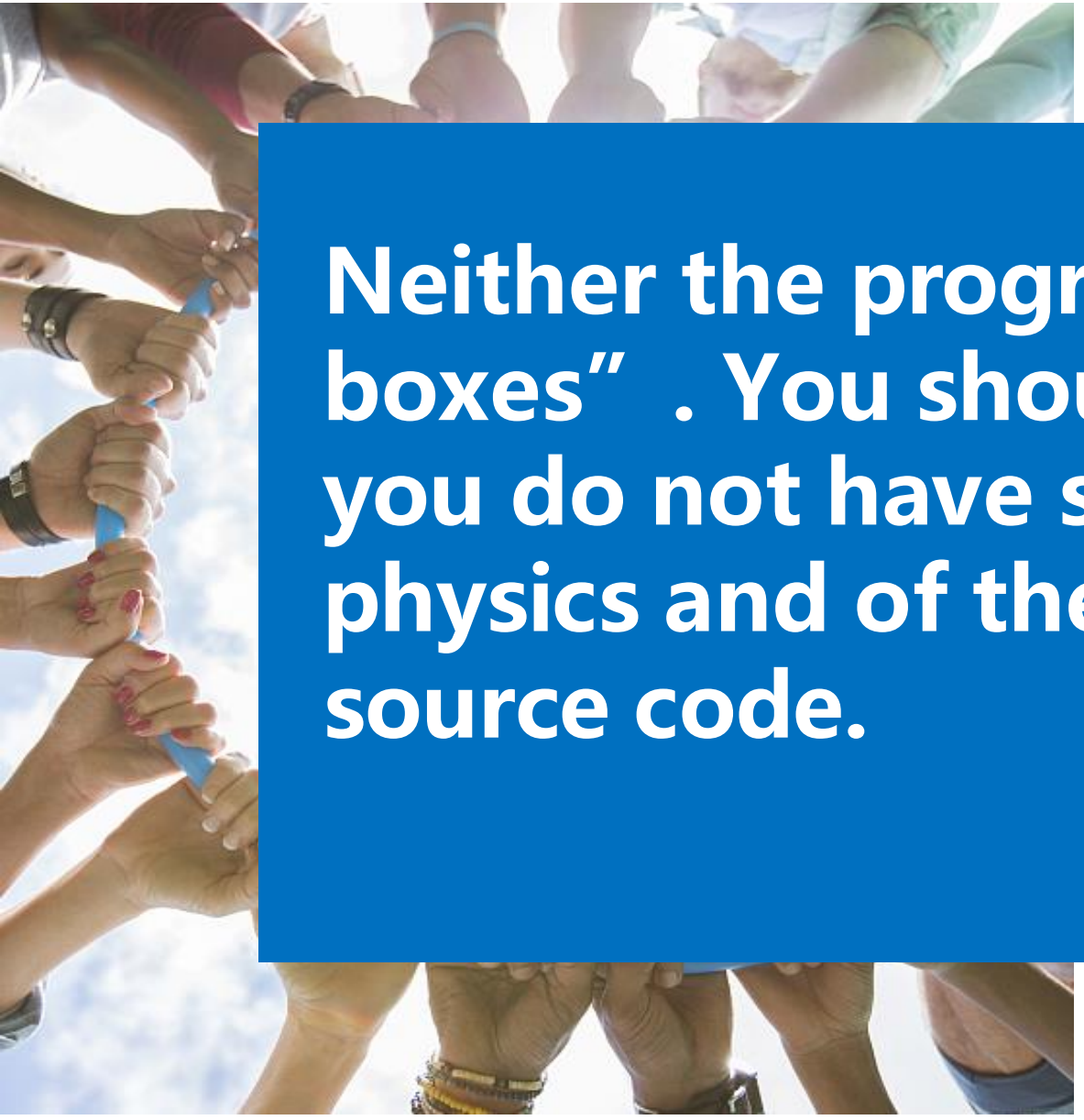
Landé factor calculations





MCDHF calculations of Landé factors compared with LS-coupling and Kurucz's database (http://kurucz.harvard.edu/atoms.html)

Li et al. , 2020



Neither the programs nor data are “black boxes”. You should not be using them if you do not have some understanding of the physics and of the programming in the source code.

--Robert L. Kurucz