Atomic data for astrophysics. Calculations, benchmarking and distribution

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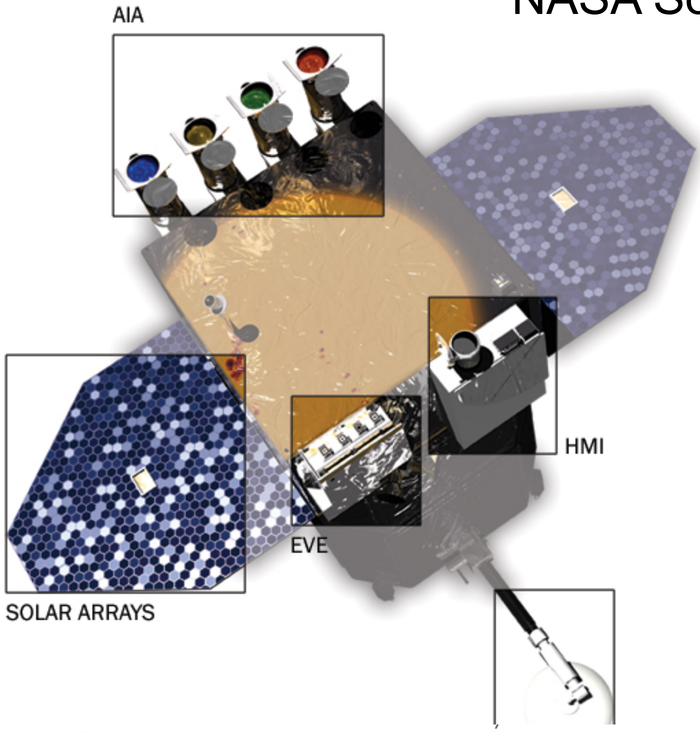
Science & Technology Facilities Council

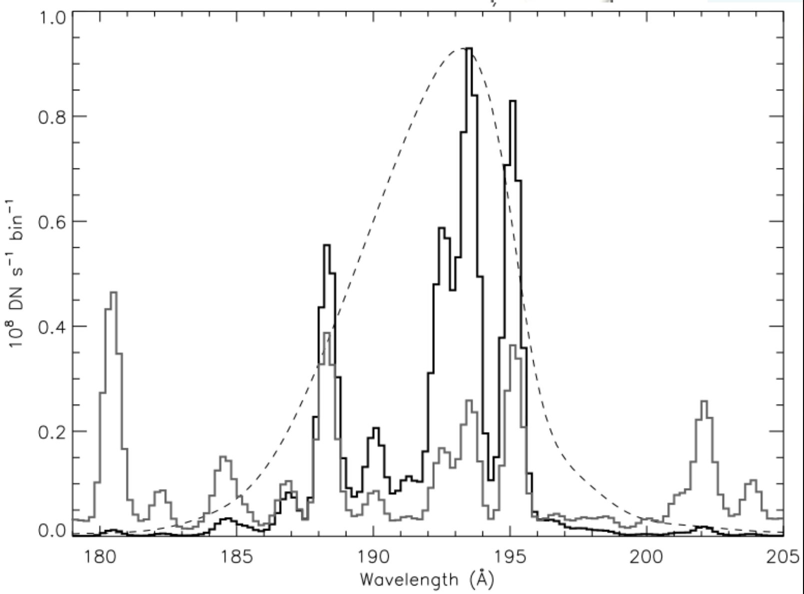
VAMDC Virtual Atomic and Molecular Data Centre

UNIVERSITY OF CAMBRIDGE

NASA Solar Dynamics Observatory (SDO) AIA

1 Tb/day, 7 EUV channels:
94, 132, 171, 195, 211, 304, 335 A
images every 12 seconds





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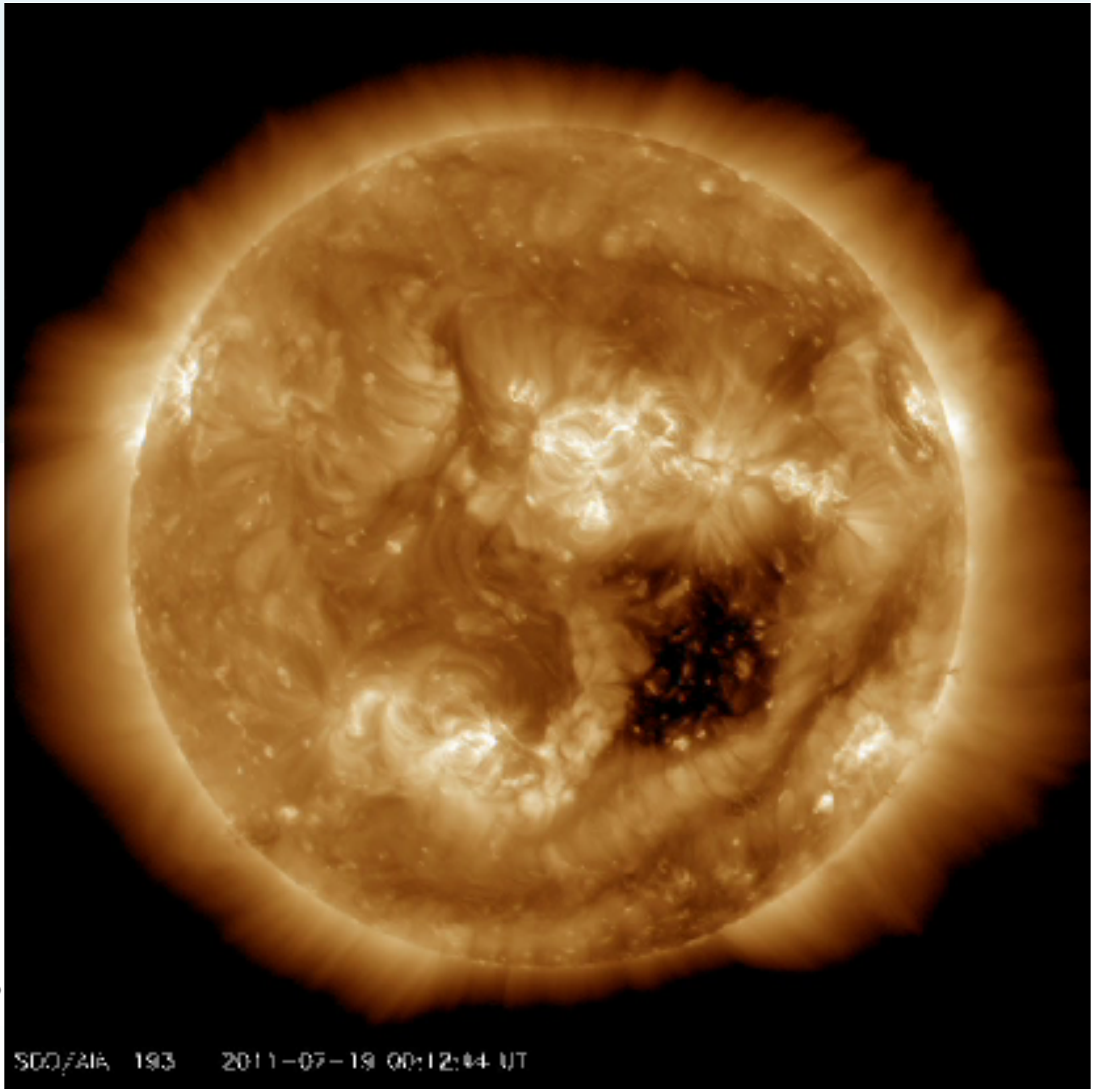
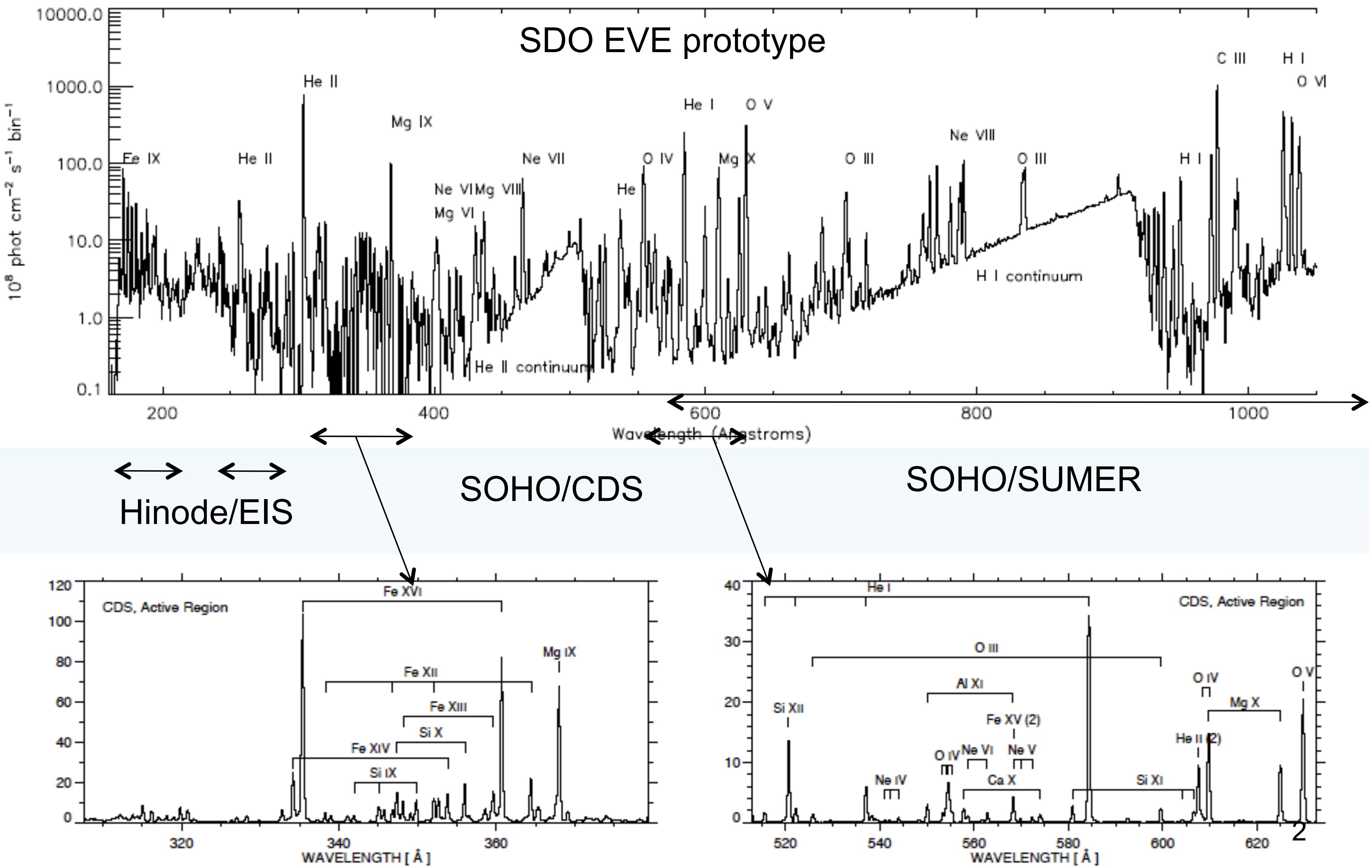
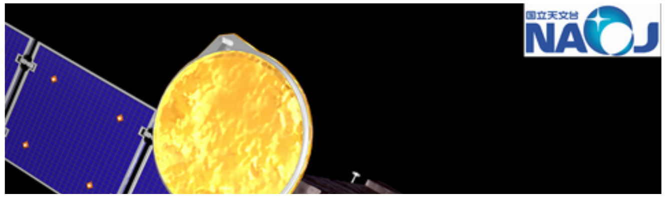


The solar EUV – UV

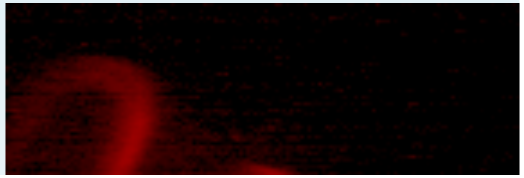
`You could spend a lifetime to understand this spectrum' (P. Storey)

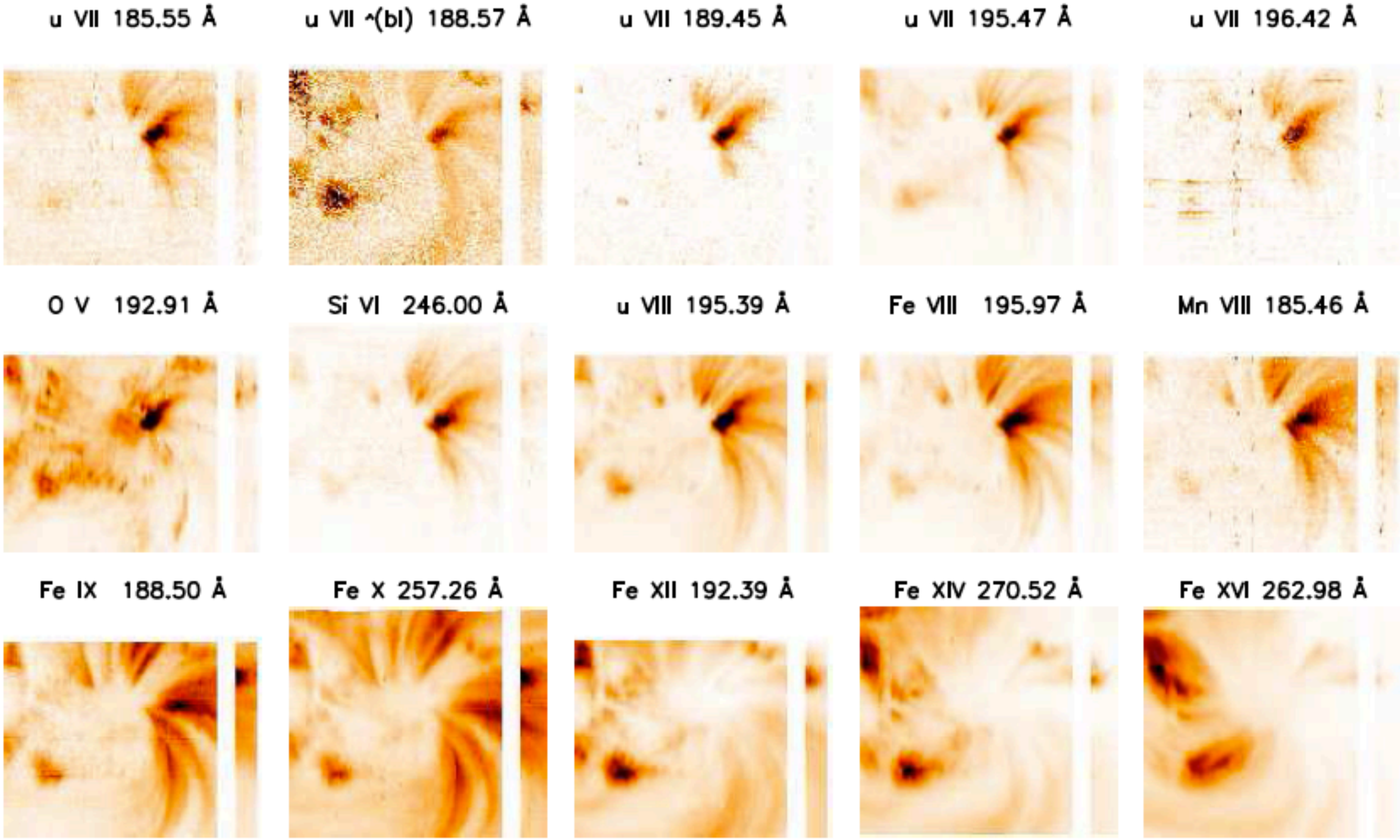


Hinode EUV imaging spectrometer (EIS)

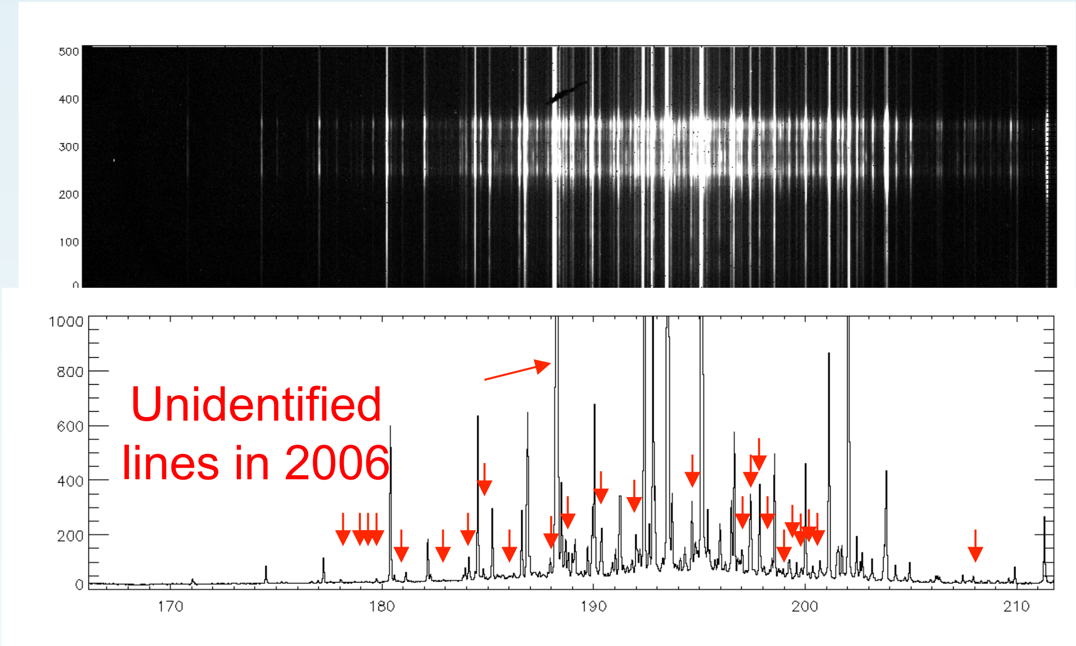


2D images are built up by
'rastering',i.e. moving the slit





Hinode EIS and B.Fawcett's plates



B.Fawcett 166 – 212 Angstroms

Resolution almost as good as B.Fawcett's plates.
5 m Angstroms accuracy in wavelengths.

Atomic data

In optically-thin plasmas line intensities are proportional to:

$$I \sim n_j\, A_{ji} = \frac{N_j(X^{+m})}{N(X^{+m})}\, A_{ji}\, \frac{N(X^{+m})}{N(X)}\, \frac{N(X)}{N(H)}\, \frac{N(H)}{N_e}\, N_e$$

A-value

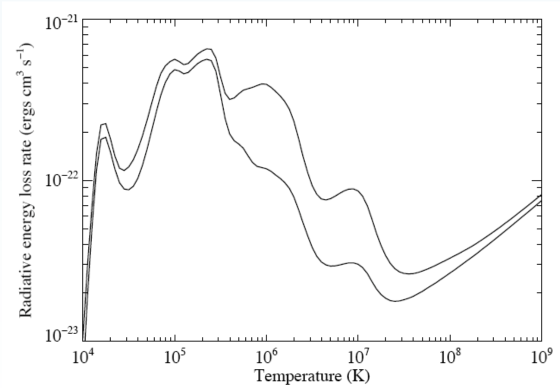
Level population (Ne,Te)

Ion abundance (Te, Ne)

El. abundance

- Measure electron densities, temperatures, emission measures and elemental abundances from spectra.

- Forward modeling.
- Calculate radiative losses:



Calculations of electron excitation data

R-matrix **electron impact excitation**:

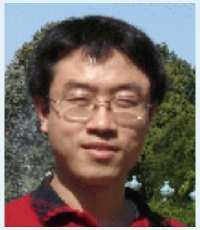
- developed over 30 years by various groups (UCL,QUB):
Seaton, Burke, Burgess, Storey, Eissner, Berrington, Badnell, etc.

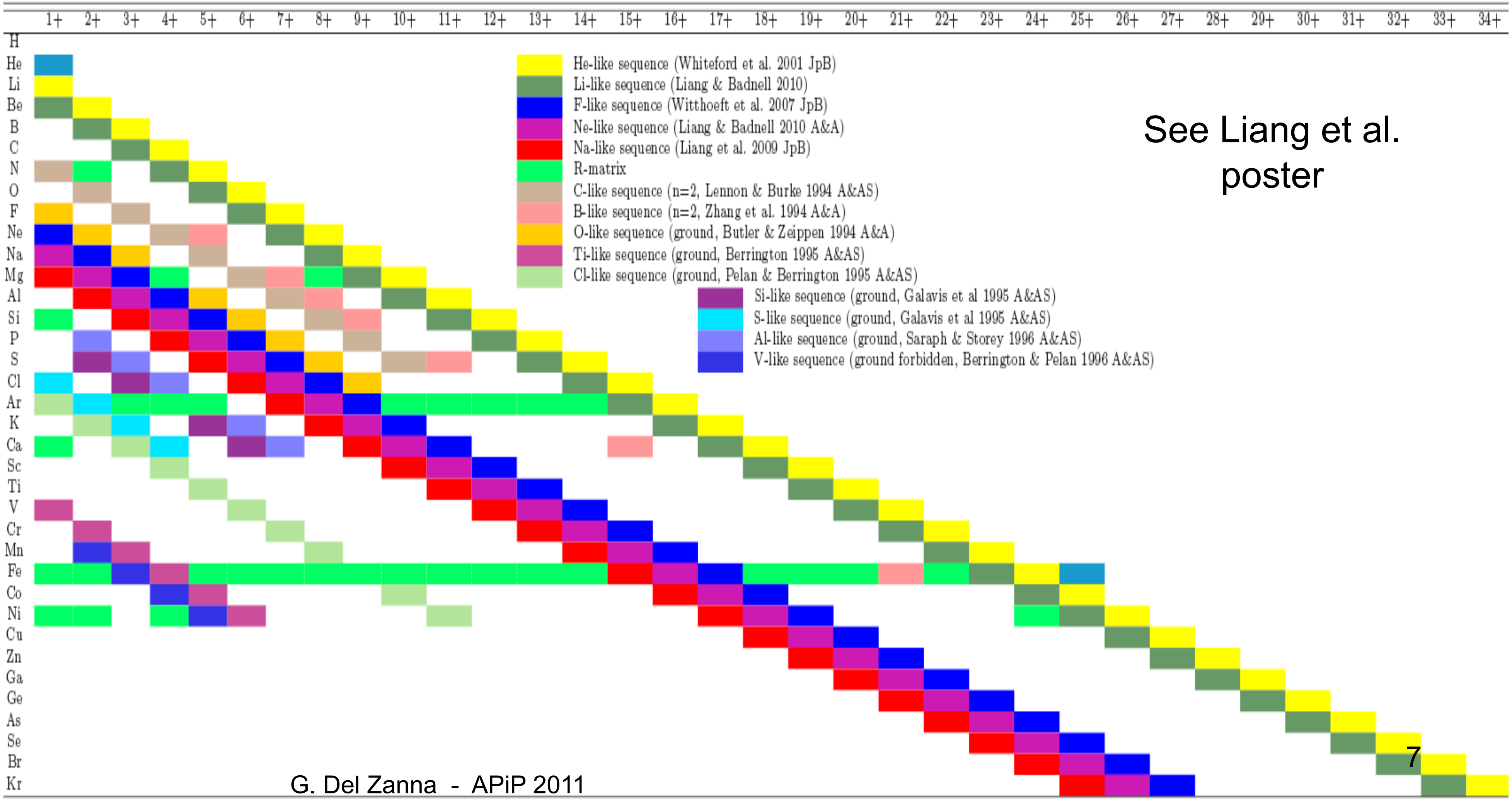
- Iron Project

- STFC-funded (UK) **APAP Network** http://www.apap-network.org/

R-matrix data for astrophysics (APAP data)

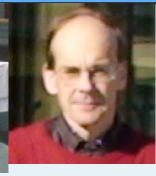
F-like: Witthoeft Whiteford Badnell (2007)
Na-like: Liang, Whiteford,Badnell (2009)
Ne-like: Liang et al. (2010, submitted)
Li-like: Liang & Badnell (2010)





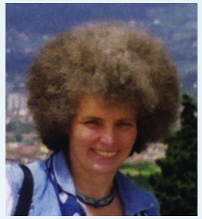
See Liang et al. poster

More R-matrix calculations of iron ions

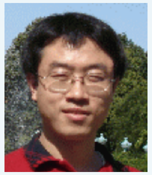



- Fe VII: Witthoeft et al. (2008)
- Fe VIII: Griffin et al. (2000)
  Del Zanna (2009)





- Fe IX: Storey et al. (2002)
- Fe X: Del Zanna, Berrington, Mason (2004)
- Fe XI: Del Zanna, Storey, Mason (2010)
- Fe XII: Storey et al. (2005)
- Fe XIII: Storey & Zeippen (2010)
- Fe XIV: Storey et al. (2000); Liang et al. (2010)
- Fe XV Berrington et al. (2005)



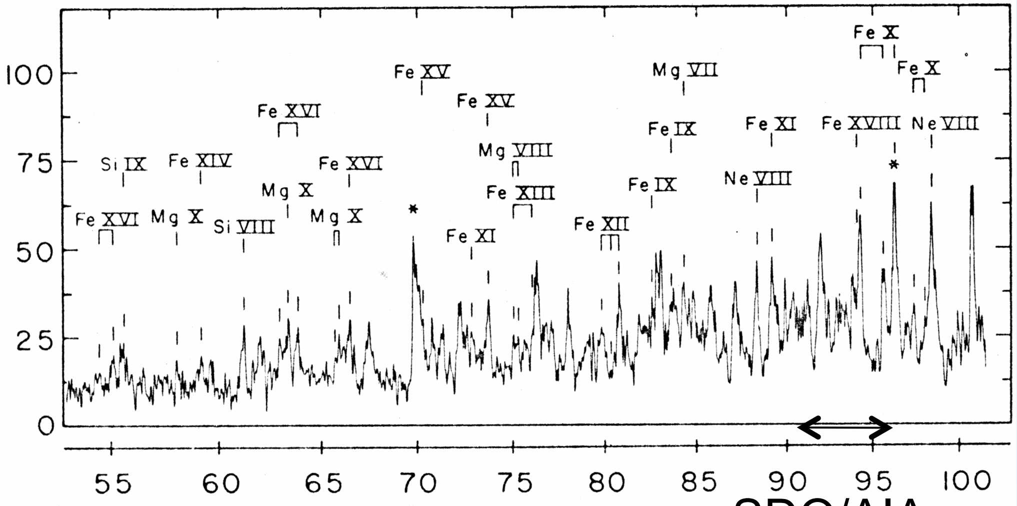
- Fe XVIII: Witthoeft et al.(2006).
- Fe XX: Witthoeft, Del Zanna, & Badnell (2007)
- Fe XXIII Chidichimo et al. (2005)

Data included in ADAS, ATOMDB, CHIANTI, etc.

Soft X-rays

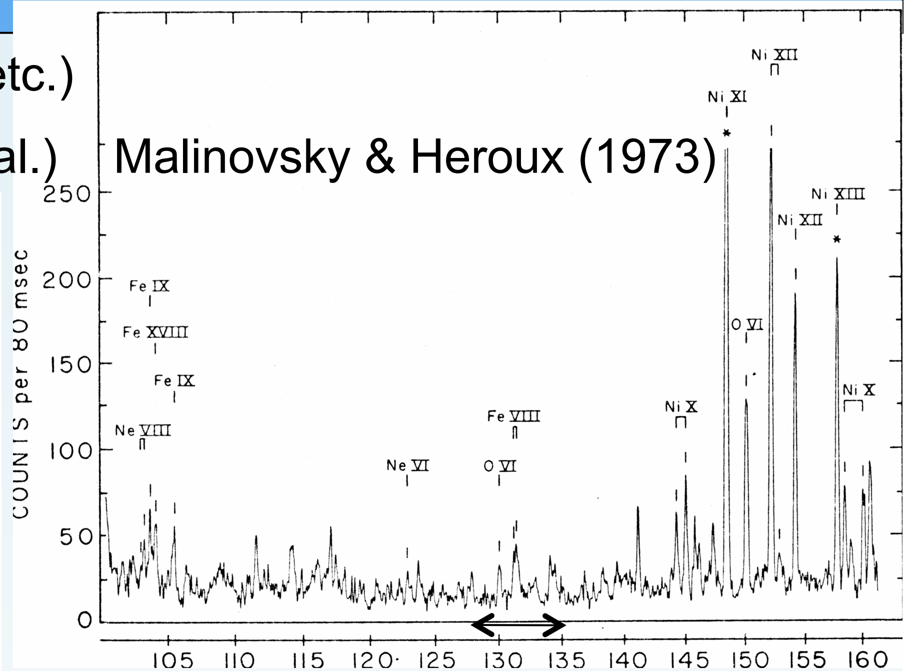
n=4-->3 transitions (Fawcett et al. 1968,1972,etc.)

Chandra LETG, EBIT (Beiersdorfer, Lepson et al.)

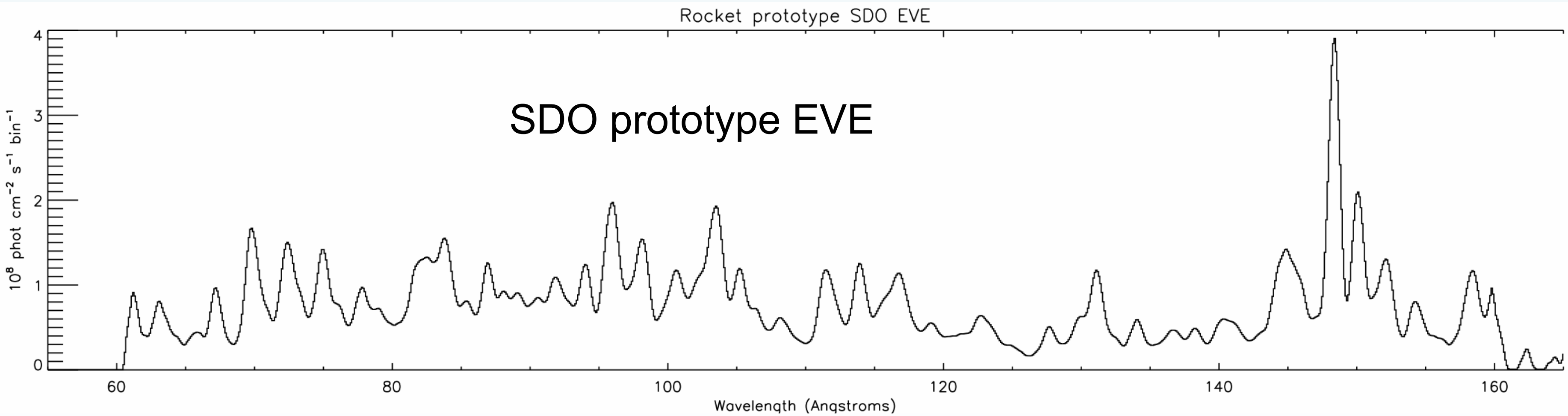


SDO/AIA

Malinovsky & Heroux (1973)



SDO/AIA



New distorted-wave code (Badnell 2011) to calculate Fe excitation data for n=4,5,6,7

CHIANTI atomic package

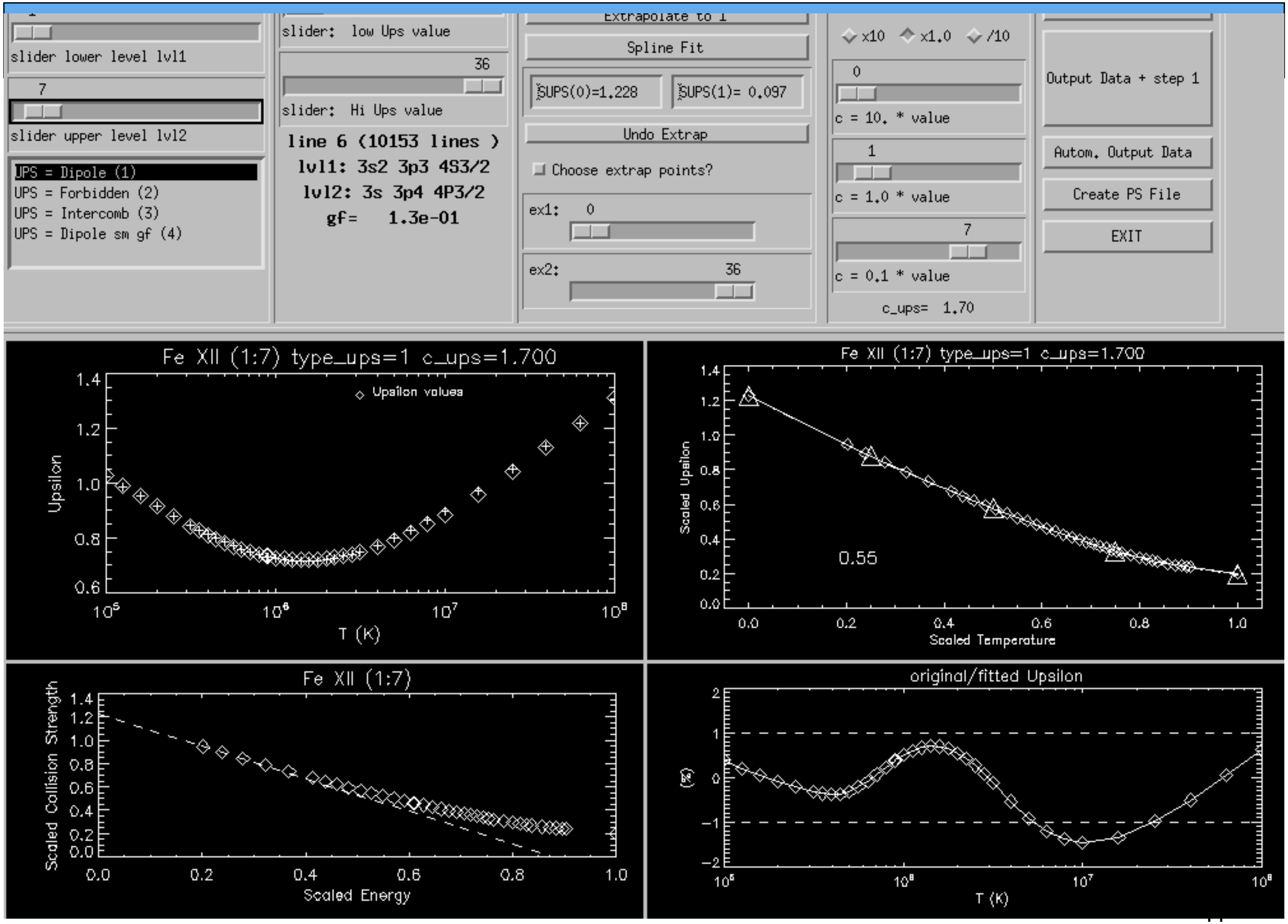
CHIANTI Provides all atomic data and IDL programs necessary for modelling spectra from collisionally-ionised plasmas for the XUV. Over 1000 direct citations.
No UK funding for 7 years.

~ 300 ion models
~ 300 000 spectral lines
http://www.chiantidatabase.org/
www.chianti.rl.ac.uk

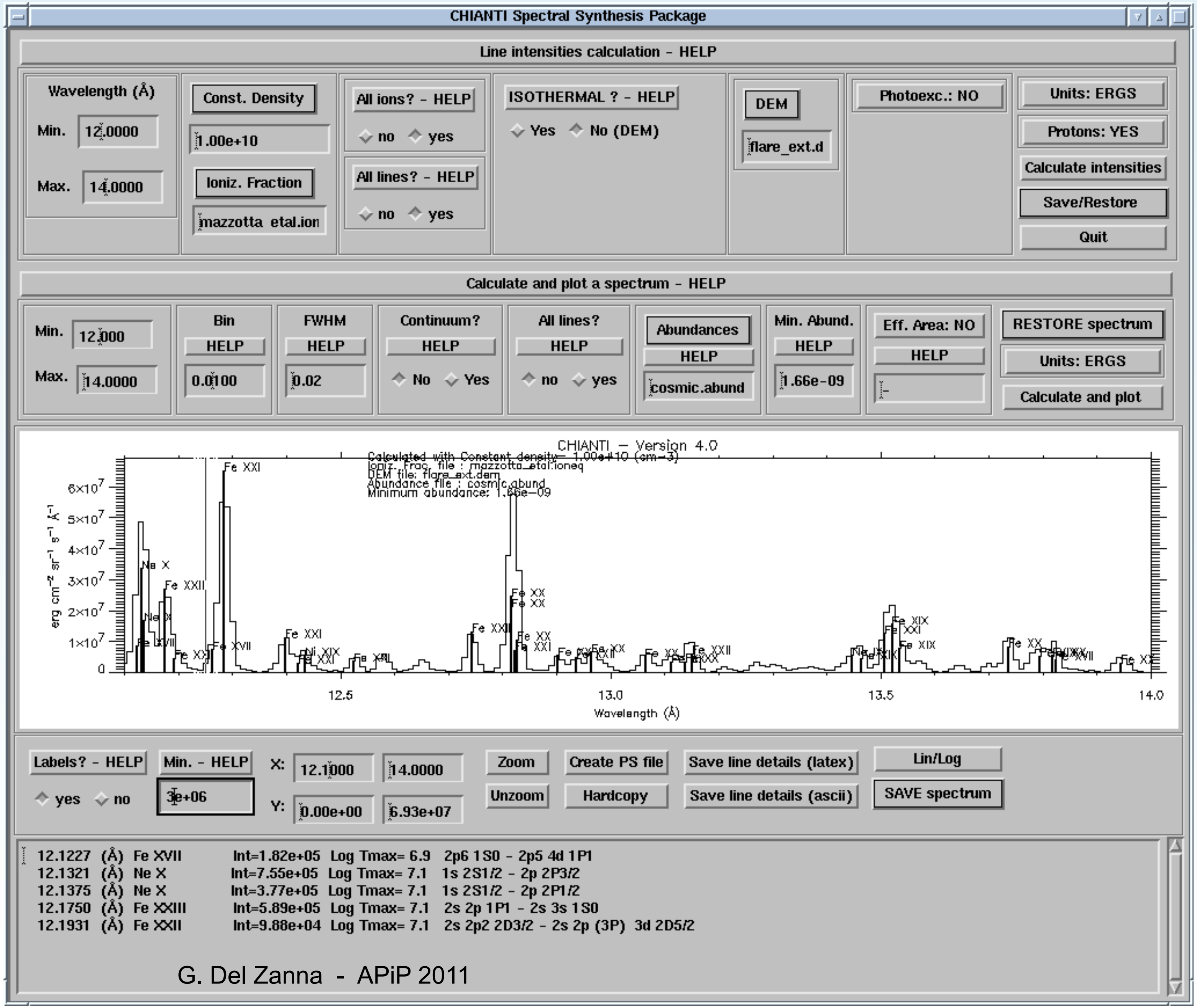
H	I																											
He	I	II																										
C		II	III	IV	V	VI																						
N	I	II	III	IV	V	VI	VII																					
O		II	III	IV	V	VI	VII	VIII																				
Ne		II	III	IV	V	VI	VII	VIII	IX	X																		
Na			III	IV	V	VI	VII	VIII	IX	X	XI																	
Mg		II		IV	V	VI	VII	VIII	IX	X	XI	XII																
Al		II	III		V	VI	VII	VIII	IX	X	XI	XII	XIII															
Si		II	III	IV	V	VI	VII	VIII	IX	X	XI	XII	XIII	XIV														
P					V		VII	VIII	IX	X	XI	XII	XIII	XIV	XV													
S		II	III	IV	V	VI	VII	VIII	IX	X	XI	XII	XIII	XIV	XV	XVI												
Cl		II								X	XI	XII		XIV		XVI	XVII											
Ar				IV			VII	VIII	IX	X	XI	XII	XIII	XIV	XV	XVI	XVII	XVIII										
K					V				IX		XI	XII	XIII	XIV	XV	XVI	XVII	XVIII	XIX									
Ca							VII	VIII	IX	X	XI	XII	XIII	XIV	XV	XVI	XVII	XVIII	XIX	XX								
Ti											XI	XII		XIV	XV	XVI	XVII	XVIII	XIX	XX								
Cr													XIII	XIV		XVI	XVII	XVIII	XIX	XX	XXI	XXII						
Mn															XV		XVII	XVIII	XIX	XX	XXI	XXII	XXIII					
Fe		II				VI	VII	VIII	IX	X	XI	XII	XIII	XIV	XV	XVI	XVII	XVIII	XIX	XX	XXI	XXII	XXIII	XXIV	XXV	XXVI		
Co																	XVII		XIX	XX	XXI	XXII	XXIII	XXIV	XXV			
Ni												XII	XIII		XV	XVI	XVII	XVIII	XIX	XX	XXI	XXII	XXIII	XXIV	XXV	XXVI	XXVII	XXVIII
Zn																				XX			XXIII	XXIV	XXV		XXVII	XXVIII

V.6 (Dere et al.2009) contained **new ionization and recombination rates**.
V.7 (Landi et al. 2011), Aug 2011, new atomic data for many ions.

Atomic data included other spectral codes. Photoionization (XSTAR, CLOUDY, MOCASSIN) and others (ATOMDB, XSPEC, ISIS, PINTofALE).


slider lower level lvl1
7
slider upper level lvl2
UPS = Dipole (1)
UPS = Forbidden (2)
UPS = Intercomb (3)
UPS = Dipole sm gf (4)
slider: low Ups value
36
slider: Hi Ups value
line 6 (10153 lines)
lvl1: 3s2 3p3 4S3/2
lvl2: 3s 3p4 4P3/2
gf= 1.3e-01
Extrapolate to 1
Spline Fit
SUPS(0)=1.228
SUPS(1)= 0.097
Undo Extrap
Choose extrap points?
ex1: 0
ex2: 36
x10
x1.0
/10
0
c = 10. * value
1
c = 1.0 * value
7
c = 0.1 * value
c_ups= 1.70
Output Data + step 1
Autom. Output Data
Create PS File
EXIT
Fe XII (1:7) type_ups=1 c_ups=1.700
Upsilon values
Upsilon
T (K)
Fe XII (1:7) type_ups=1 c_ups=1.700
Scaled Upsilon
0.55
Scaled Temperature
Fe XII (1:7)
Scaled Collision Strength
Scaled Energy
original/fitted Upsilon
(%)
T (K)

Spectral synthesis



Virtual Atomic and Molecular Data Center

• VAMDC aims at building an e-infrastructure for the exchange of atomic and molecular data. VAMDC involves 24 teams.

www.vamdc.org

• VAMDC is supported by the EU in the FP7 framework "Research Infrastructures - INFRA-2008-1.2.2 - Scientific Data Infrastructures" initiative.

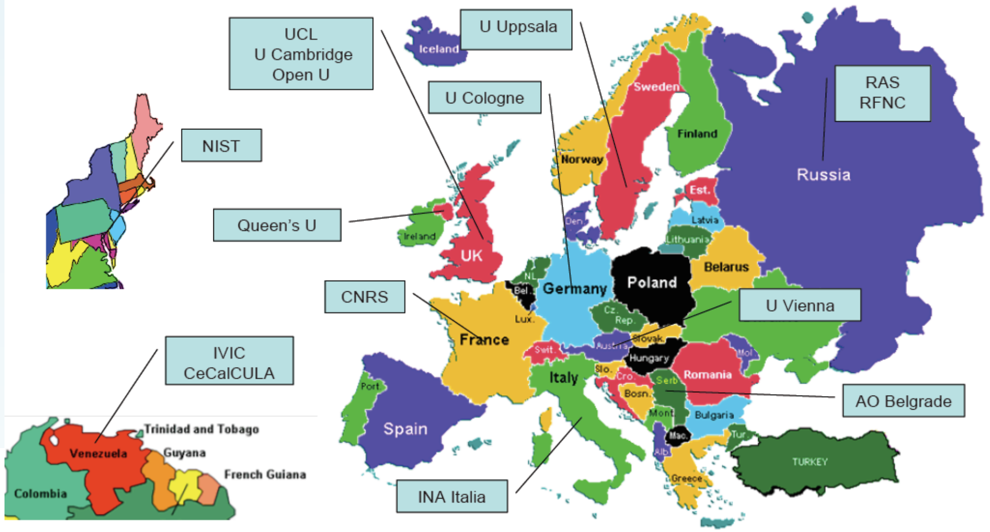
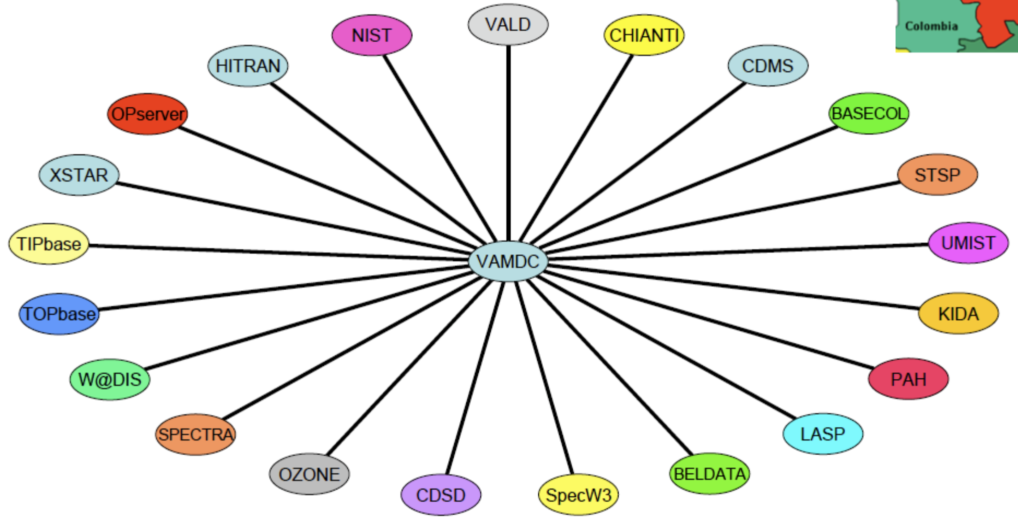


Figure from C.Mendoza



VAMDC Virtual Atomic and Molecular Data Centre

CHIANTI atomic data for VAMDC

-Giulio Del Zanna & Helen Mason (Cambridge) in collaboration with IoA and MSSL

-All the BASIC CHIANTI DATA: wavelength, A-value, gf-value, configuration, LSJ, observed, theoretical energies, excitation rates in MySQL
-Database can be queried via a web portal or workbench.

-DERIVED DATA (modelling): Python scripts to read the CHIANTI VAMDC

Various general issues:

How can different databases be easily compared ?
Multiple calculations. CHIANTI policy is to select one.

Appropriate references to original calculation lost.

Benchmarking atomic data (Del Zanna 2004-)

In a series of papers, I have calculated and benchmarked atomic data for the XUV using a `novel' approach.

Wern
Eissn

1)Find the best atomic structure with appropriate CI (and semi-empirical corrections)

2)Compare observed (beam-foil spectroscopy, Elmar Traebert et al.) and theoretical lifetimes and branching ratios.

3)Calculate e excitation rates (R-matrix) and build ion model to calculate line intensities.

4)compare observed and theoretical wavelengths and intensities for low- and high-densities using the emissivity ratios:

$$F_{ji}(N_e, T_e) = C \frac{I_{ob} N_e}{N_j(N_e, T_e)\, A_{ji}}$$

5)Try to identify all the brightest lines, using laboratory and astrophysical spectra.

RESULTS:

a large number of new identifications, new level energies, revised wavelengths (with uncertainties – (NIST EUV values often not accurate enough for current missions), new Ne, Te diagnostic applications

Benchmarking atomic data for Iron ions

- Fe VII: Del Zanna (2009a) 31/ 53 new EUV (160-300 A) IDs, new Te diagnostics
- Fe VIII: Del Zanna (2009b) 9/34 new EUV IDs, new Te diagnostics

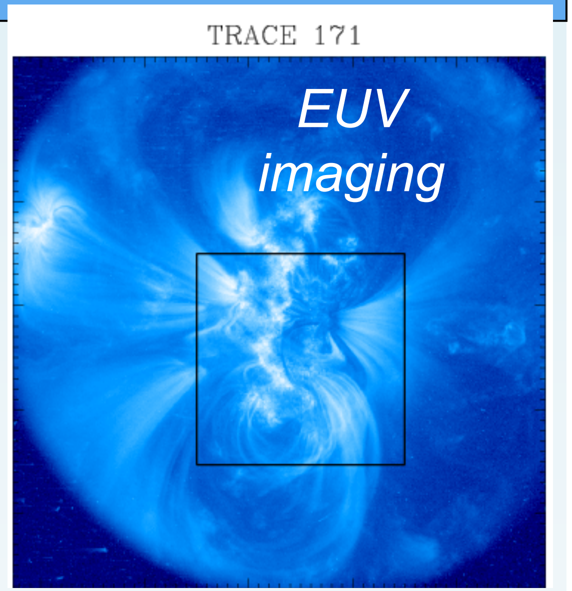
- Fe X: Del Zanna, Berrington, Mason (2004) 9/45 new IDs
- Fe XI: Del Zanna (2010) 31/60 new IDs, new Te diagnostics
- Fe XII: Del Zanna & Mason (2005) 21/58 new IDs
- Fe XIII: Del Zanna (2011a) 13/41 new EUV IDs

- Fe XIV: Del Zanna (2011b)
- Fe XVII: Del Zanna & Ishikawa (2009) 16/50 new IDs (40-400 A), Del Zanna (2011): new Te diagnostics

- Fe XVIII: Del Zanna (2006) new IDs, new Te diagnostics
- Fe XX: Witthoeft, Del Zanna, Badnell (2007)

- Fe XXIII Del Zanna et al. (2005) new Ne,Te diagnostics
- Fe XXIV Del Zanna (2006) new Ne,Te diagnostics
-

Ne in a solar active region



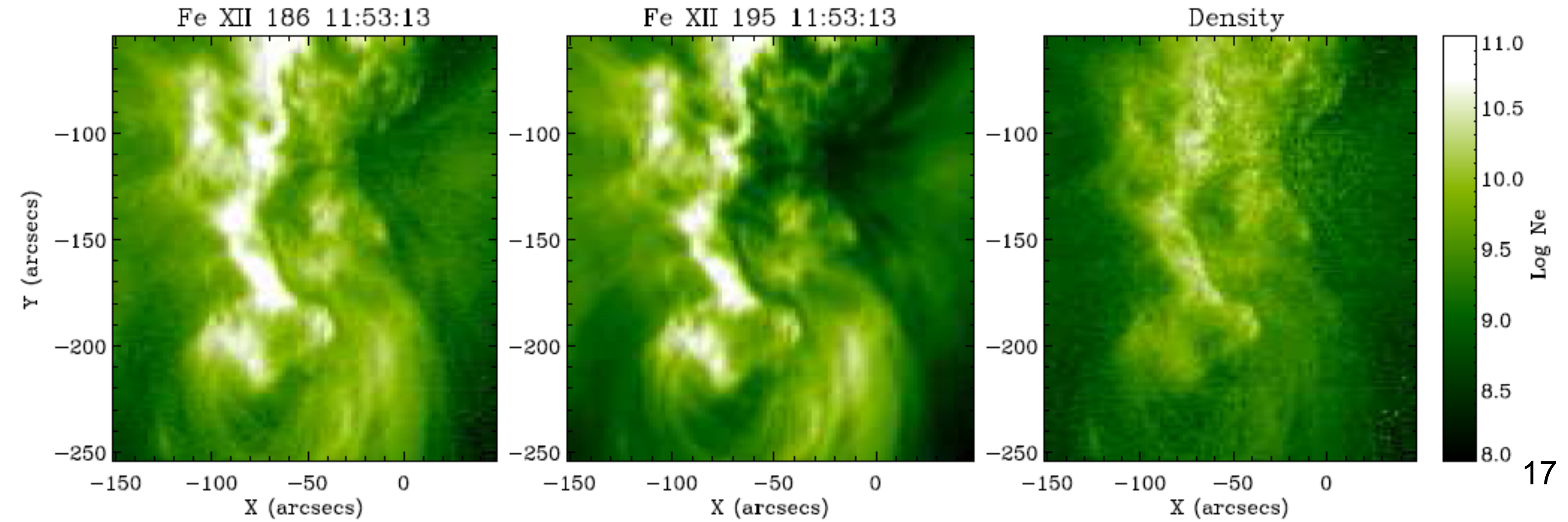
Hinode/EIS line ratios provide density maps

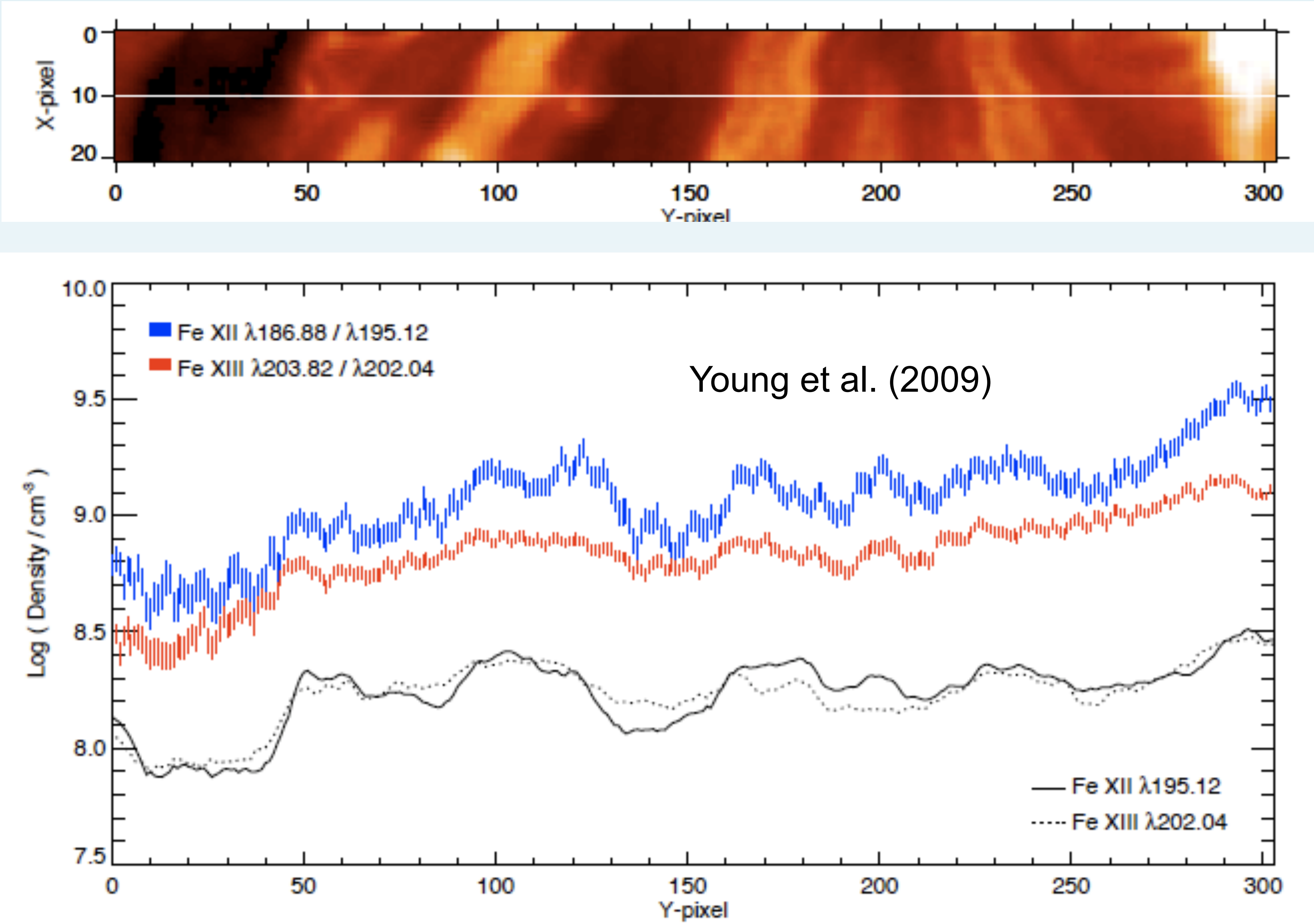
Self-blend decay to excited state

Self-blend decay to ground state

Tripathi et al. (2009)

First identified by Del Zanna & Mason (2005)

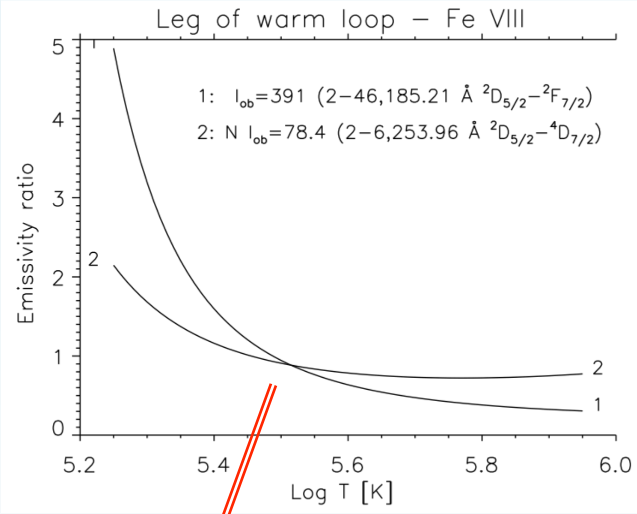


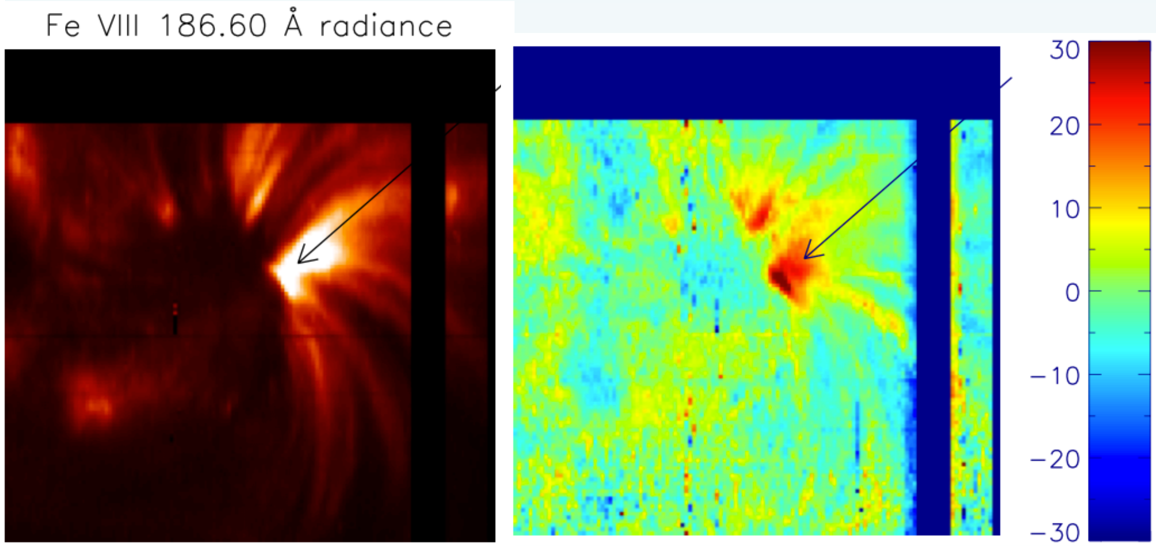

X-pixel
Y-pixel
Log (Density / cm^{-3})
Fe XII λ186.88 / λ195.12
Fe XIII λ203.82 / λ202.04
Young et al. (2009)
Fe XII λ195.12
Fe XIII λ202.04
Y-pixel

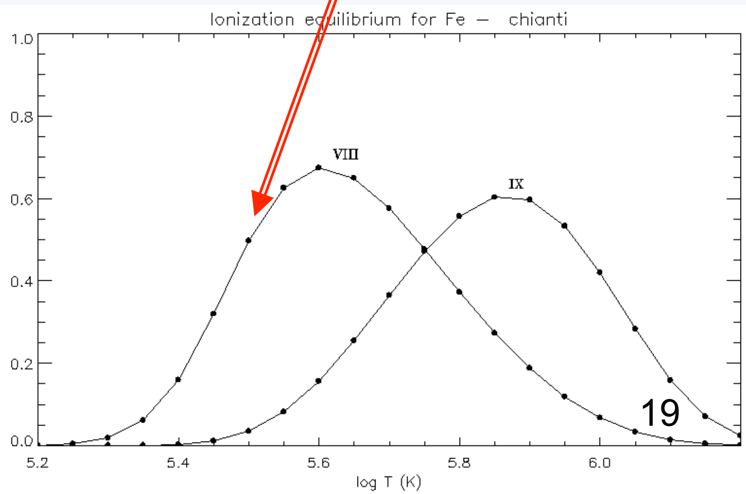
New EIS direct measurements of Te

Del Zanna (2009a,b, 2010):
new identifications of Fe VII, VIII lines providing direct Te.

Te different from T_{max} peak ion abundance in equilibrium.







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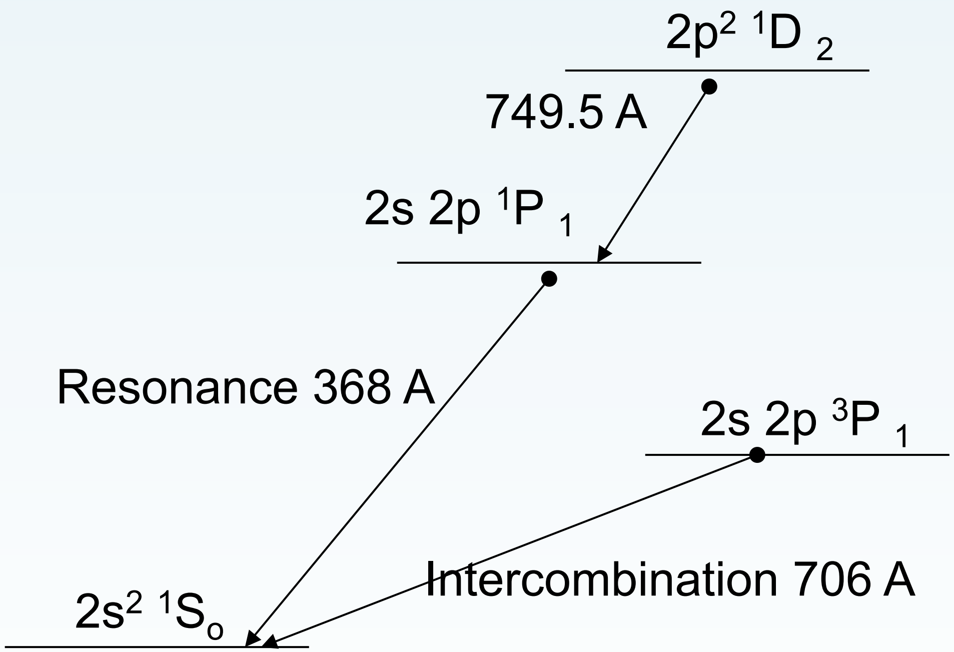
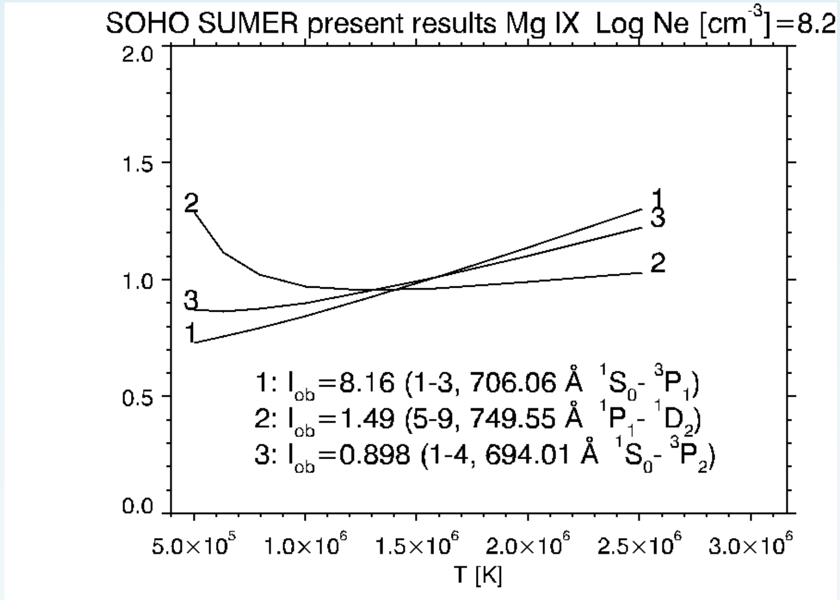
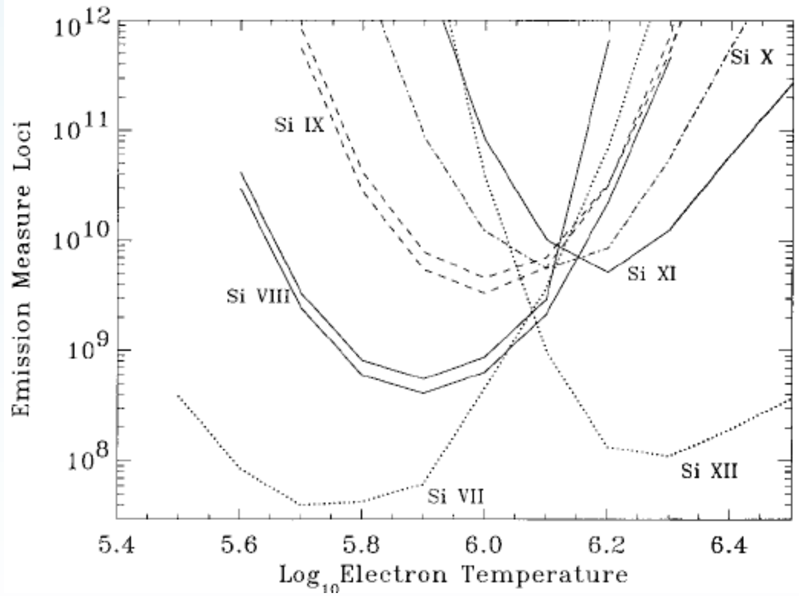
Te from Be-like Mg IX

First R-matrix calculation for Be-like Mg (Del Zanna Rozum Badnell 2008) resolved significant problems.

Best Te diagnostic for the 1 MK corona.
Te in CH underestimated by a factor of 2







Te=1.35 MK (Feldman et al. 1999)

Fe XI

i	Conf.	Lev.	E_{exp}	E_{NIST}
1	$3s^2\ 3p^4$	$^3P^e_2$	0	0
2	$3s^2\ 3p^4$	$^3P^e_1$	12667	12667 (0)
3	$3s^2\ 3p^4$	$^3P^e_0$	14306	14312 (-6)
4	$3s^2\ 3p^4$	$^1D^e_2$	37743	37743 (-1)
5	$3s^2\ 3p^4$	$^1S^e_0$	80831	80814 (16)
6	$3s\ 3p^5$	$^3P^o_2$	283551	283558 (-7)
7	$3s\ 3p^5$	$^3P^o_1$	293158	293158 (0)
8	$3s\ 3p^5$	$^3P^o_0$	299163	299163 (0)
9	$3s\ 3p^5$	$^1P^o_1$	361846	361842 (4)
10	$3s^2\ 3p^3\ 3d$	$^5D^o_0$	387544	-
11	$3s^2\ 3p^3\ 3d$	$^5D^o_1$	387726	-
12	$3s^2\ 3p^3\ 3d$	$^5D^o_2$	387940	-
13	$3s^2\ 3p^3\ 3d$	$^5D^o_3$	388268	-
14	$3s^2\ 3p^3\ 3d$	$^5D^o_4$	389227	-
15	$3s^2\ 3p^3\ 3d$	$^3D^o_2$	412856	-
16	$3s^2\ 3p^3\ 3d$	$^3D^o_3$	415426	-
17	$3s^2\ 3p^3\ 3d$	$^3D^o_1$	417049	-
18	$3s^2\ 3p^3\ 3d$	$^3F^o_2$	422844	-
19	$3s^2\ 3p^3\ 3d$	$^1S^o_0$	-	-
20	$3s^2\ 3p^3\ 3d$	$^3F^o_3$	426022	-
21	$3s^2\ 3p^3\ 3d$	$^3F^o_4$	430522	-
22	$3s^2\ 3p^3\ 3d$	$^3G^o_3$	-	-
23	$3s^2\ 3p^3\ 3d$	$^3G^o_4$	450211	-
24	$3s^2\ 3p^3\ 3d$	$^3G^o_5$	452416	-
25	$3s^2\ 3p^3\ 3d$	$^1G^o_4$	459218	-
26	$3s^2\ 3p^3\ 3d$	$^1D^o_2$	-	-
27	$3s^2\ 3p^3\ 3d$	$^3D^o_1$	-	-
28	$3s^2\ 3p^3\ 3d$	$^3P^o_0$	-	-
29	$3s^2\ 3p^3\ 3d$	$^3P^o_1$	484830	-
30	$3s^2\ 3p^3\ 3d$	$^3F^o_3$	485039	-
31	$3s^2\ 3p^3\ 3d$	$^3F^o_2$	-	-
32	$3s^2\ 3p^3\ 3d$	$^3F^o_4$	486413	-
33	$3s^2\ 3p^3\ 3d$	$^3D^o_2$	489378	-
34	$3s^2\ 3p^3\ 3d$	$^3P^o_2$	494013	496090 (-2077)
35	$3s^2\ 3p^3\ 3d$	$^3D^o_3$	497235	-
36	$3s^2\ 3p^3\ 3d$	$^1F^o_3$	525260	-
37	$3s^2\ 3p^3\ 3d$	$^3P^{o\dagger}_1$	531070	526480 (4590)
38	$3s^2\ 3p^3\ 3d$	$^3P^o_2$	531304	531290 (14)
39	$3s^2\ 3p^3\ 3d$	$^3S^{o\dagger}_1$	533445	533450 (-5)
40	$3s^2\ 3p^3\ 3d$	$^3P^o_0$	541777	541720 (57)
41	$3s^2\ 3p^3\ 3d$	$^3P^{o\dagger}_1$	541424	541390 (34)
42	$3s^2\ 3p^3\ 3d$	$^3D^o_3$	554321	554300 (21)
43	$3s^2\ 3p^3\ 3d$	$^3D^o_2$	561615	561610 (5)
44	$3s^2\ 3p^3\ 3d$	$^3D^o_1$	566396	566380 (16)
45	$3s^2\ 3p^3\ 3d$	$^1D^o_2$	578890	578860 (30)
46	$3s^2\ 3p^3\ 3d$	$^1F^o_3$	594047	594030 (17)
47	$3s^2\ 3p^3\ 3d$	$^1P^o_1$	623101	623080 (21)
48	$3p^6$	$^1S^e_0$	-	

Most 3d levels were not known.
Difficulty in the structure calculations.

Fe XI

i	Configuration (% purity)	Term	E_b	E_b-E_{NIST}	E_b-E_{CC}	E_b-E_{SS}
37	$3s^2\ 3p^3\ (^2D)\ 3d(8\%)$ +41(22%) +39(34%)	$^1P^o_1$	531070.0 ± 500	-2380	-55519	-71
38	$3s^2\ 3p^3\ (^2D)\ 3d(59\%)$ +6(c2 15%) +34(18%)	$^3P^o_2$	531304.0 ± 10	14	-40888	+60
39	$3s^2\ 3p^3\ (^2D)\ 3d(54\%)$ +9(c2 15%) +37(14%)	$^3S^o_1$	533476.0 ± 500	-7914	-18513	-1031
40	$3s^2\ 3p^3\ (^2D)\ 3d(71\%)$ +8(c2 17%)	$^3P^o_0$	541768.0 ± 500	48	-41771	-367
41	$3s^2\ 3p^3\ (^2D)\ 3d(43\%)$ +7(c2 10%) +9(c2 11%) +47(12%)	$^3P^o_1$	541424.0 ± 200	14944	-35936	-798

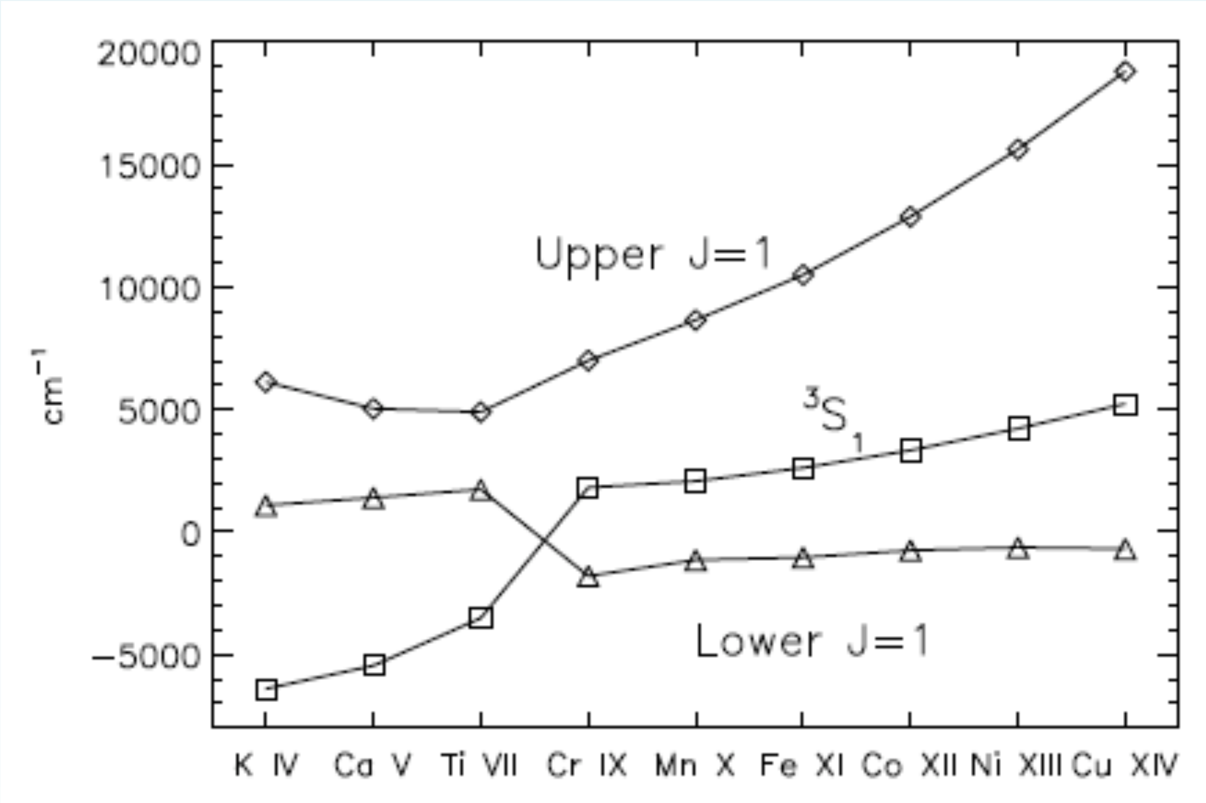
Main problems with three very mixed J=1 levels, giving rise to the strongest spectral lines observed in the EUV by Hinode

Found significant problems with all previous calculations.

Fe XI

Needed to study all ions along the sequence.

Ekefors (1931): K IV, Ca V best paper !

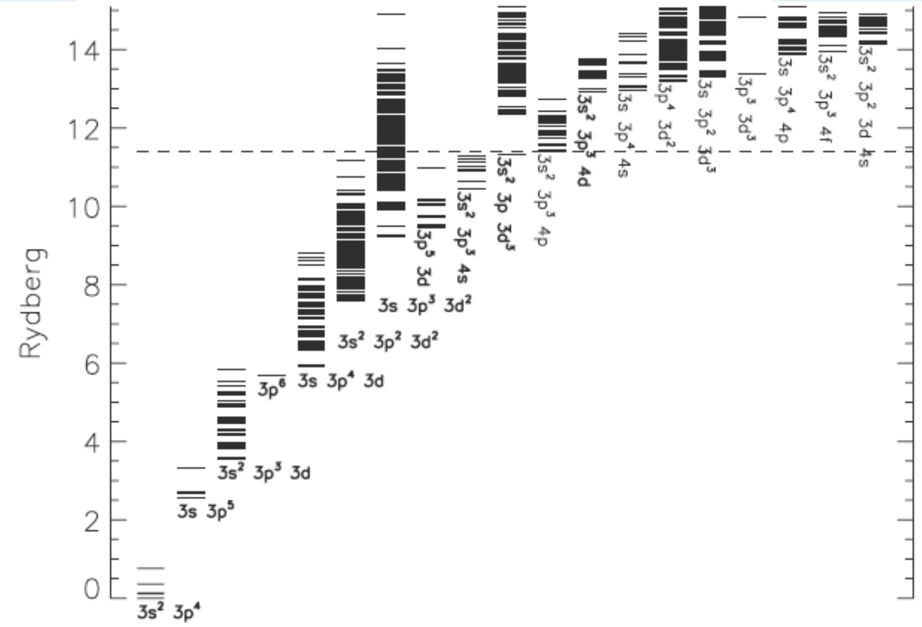


Fe XI

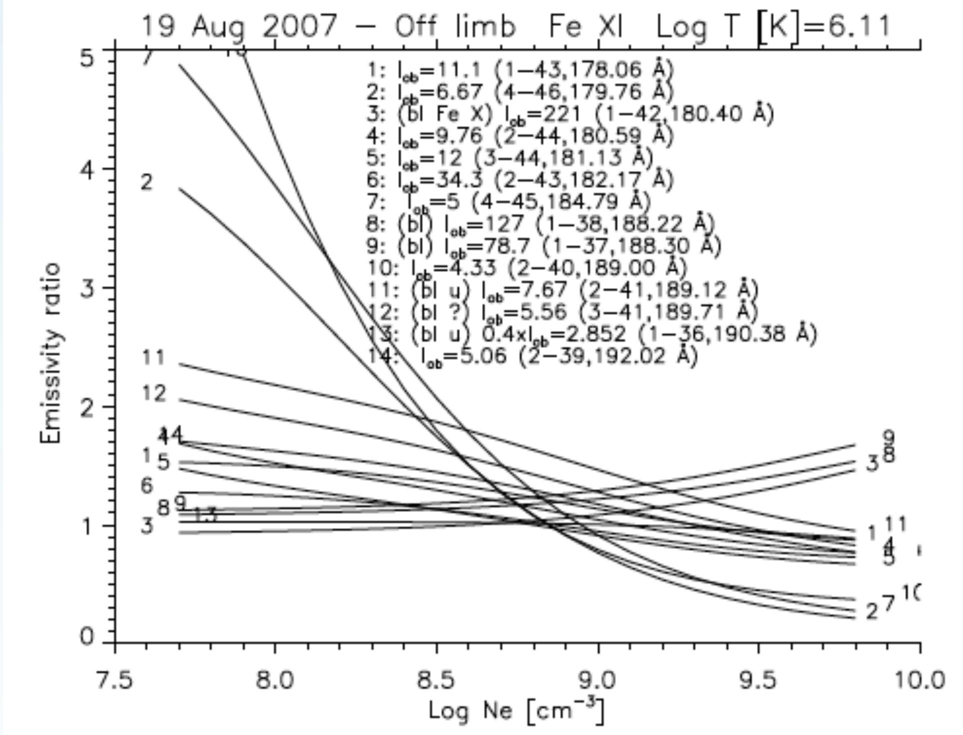
Atomic Data from the IRON Project

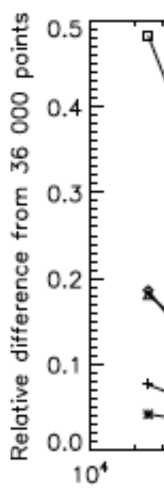
LXVIII. Electron impact excitation of Fe XI★

G. Del Zanna[1], P.J. Storey[2], and H.E. Mason[1]



Emissivity ratios





Conver

- ◆145 LS terms
- ◆ basis of 25 functions within the R-matrix boundary
- ◆partial wave expansion extended to *L = 16.*
- ◆outer region: ICFT

Fe XI – 6 years !

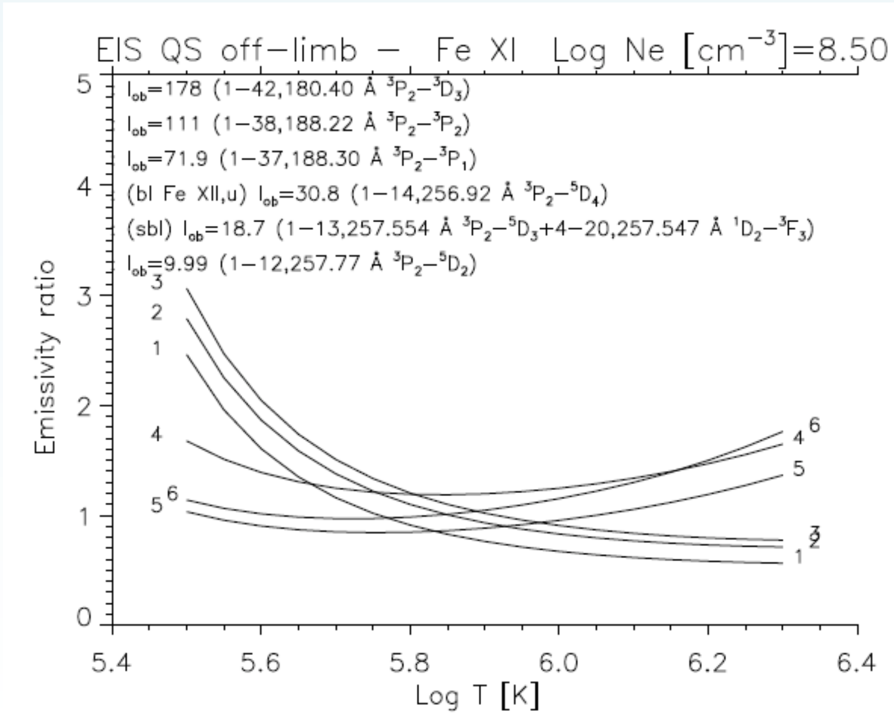
Table 3. Summary of line identifications for Fe xi.

i-*j*	λ_{exp} (Å)	λ_{obs} (Å)	ID	Diff. ID
6-103	168.929	? 168.929(10) Be76	N	
1-43	178.058	178.056(4) Be76	G66	
4-46	179.758	179.758(10) Be76	G66	
1-42	180.401	180.401(2) Be76 (bl)	G66	
2-44	180.594	180.595(4) Be76	F71	
3-44	181.130	181.131(10) Be76	G66	
2-43	182.167	182.167(2) Be76	G66	
4-45	184.793	184.793(10) Be76 (bl u)	FG66	
1-38	188.216	188.216(2) Be76	B77	F71 (188.299)
1-37	188.299	188.299(2) Be76	J93	B77(189.94)
2-41	189.123	189.123(4) Be76 (bl u)	B77	J93 (192.619)
3-41	189.711	189.723(5) N (bl)	B77	
1-36	190.382	190.382(5) N (bl u)	N	Be76 (S xi)
2-39	192.021	192.021(5) N (bl)	B77	
3-39	192.627	192.624(5) N (bl u)	B77	
2-38	192.813	192.811(5) N (bl O v, u)	F71	
3-37	193.512	- (bl Fe xii 193.509(2))		
4-41	198.538	198.555(10) Be76 (bl S viii)	B77	Be76, J93
1-35	201.112	201.112(5) N (bl Fe xiii)	N	
4-39	201.734	201.734(10) Be76 (bl Fe xii)	B77	
1-34	202.424	202.424(10) Be76 (bl u)	N	B77 (201.575)
4-38	202.609	- (bl S viii 202.608(10))		
4-37	202.705	202.710(10) Be76 (bl)		
1-30	206.169	206.169(10) Be76 (bl u)	N	
1-29	206.258	206.258(5) N	N	
2-34	207.751	207.749(5) N (bl u)	N	
2-33	209.771	209.771(5) N (bl u)		
1-20	234.730	234.73(2) D78	N	D78 (Fe xv)
1-18	236.494	236.494(10) Be76	N	
1-17	239.780	? 239.78(2) D78	N	
1-16	240.717	240.713(4) Be76 (bl Fe xiii)	N	
1-15	242.215	242.215(10) (bl) Be76	N	
4-21	254.596	254.600(5) N	N	
1-14	256.919	256.925(5) N (bl Fe xii)	N	
4-20	257.547	257.547(10) Be76 (sbl)	N	
1-13	257.554	257.547(10) Be76 (sbl)	J93	T98 (257.26 T)
1-12	257.772	257.772(4) Be76	J93	T98 (257.55 T)
1-11	257.914	257.914(5) N	N	T98 (257.78 T)
4-16	264.772	bl Fe xiv 264.787	N	
4-15	266.586	? 266.613(5) N (bl)	N	
21-79	266.759	266.755(5) N (bl u)	N	

Benchmark:
Del Zanna (2010)

31 (out of 60) new line identifications

New Te diagnostics



4-9	3
16-67	3
14-54	3
1-7	3
2-8	3
1-6	3
2-7	3
3-7	3
2-6	3
4-6	4
6-21	6
6-14	9
13-32	1
14-32	1
16-32	1
13-25	1
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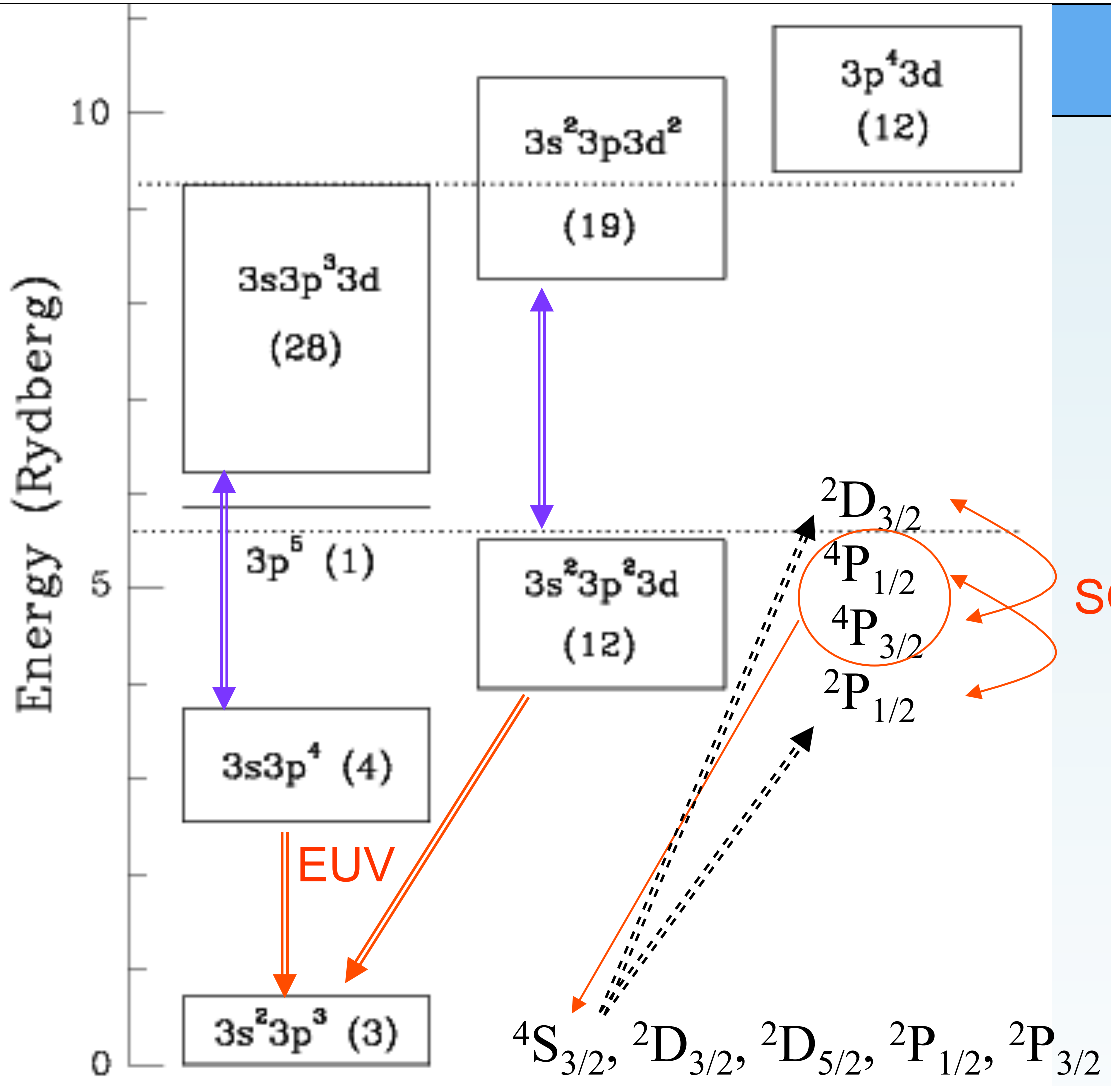
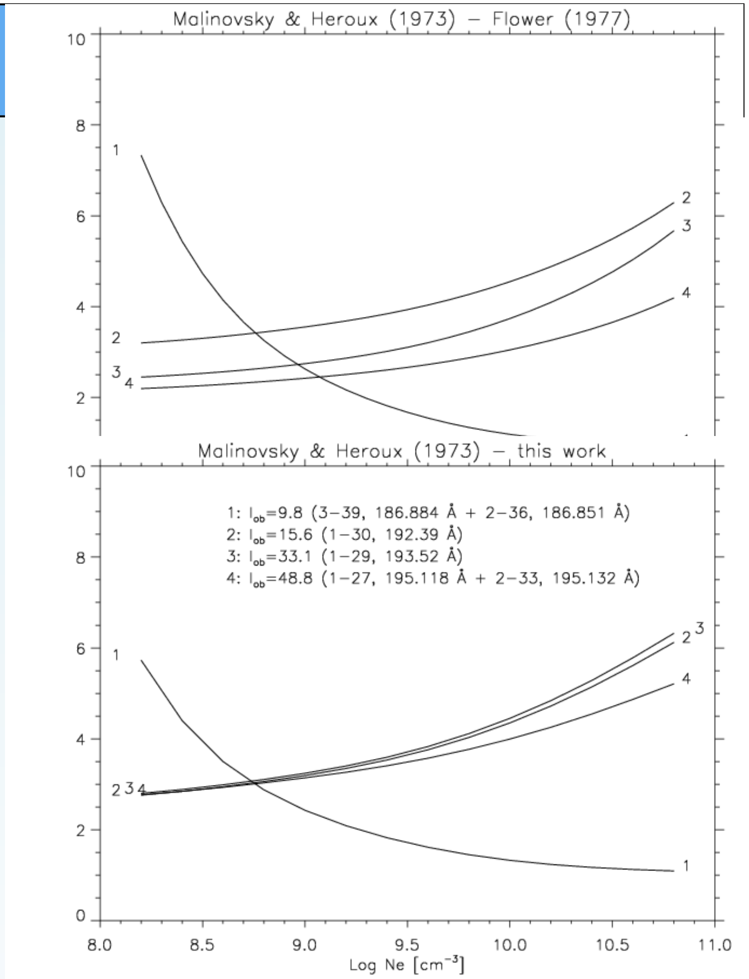
2-4	3
21-24	4
1-2	7



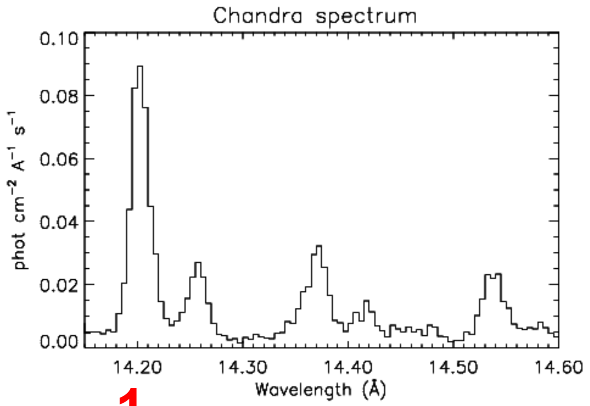


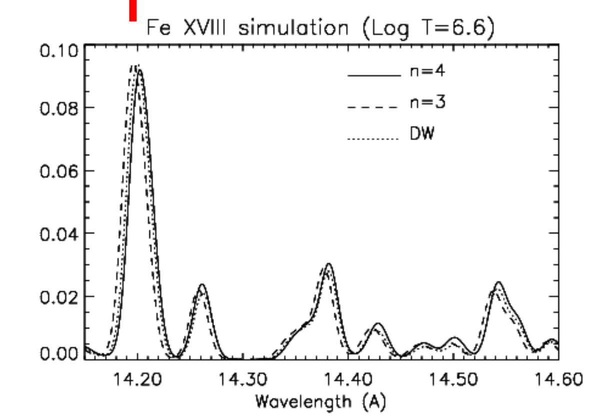
Serious problems only solved by Storey et al. (2005)

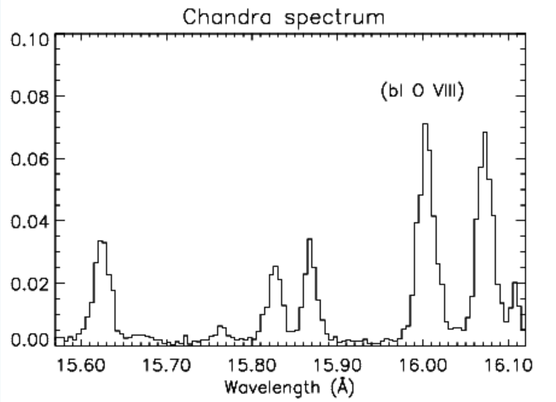
21/58 new transitions identified/revised (Del Zanna & Mason 2005)

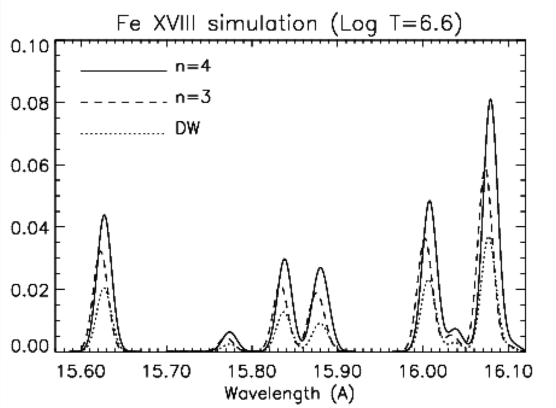
R-matrix makes a big difference! Fe XVIII

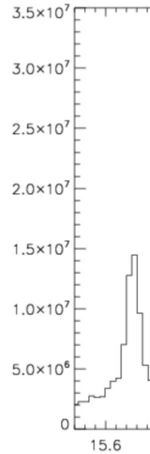
R-matrix e- scattering calculation by Witthoeft, Badnell, Del Zanna et al. (2006) solved the problem with the strong 3s--> 2p transitions .



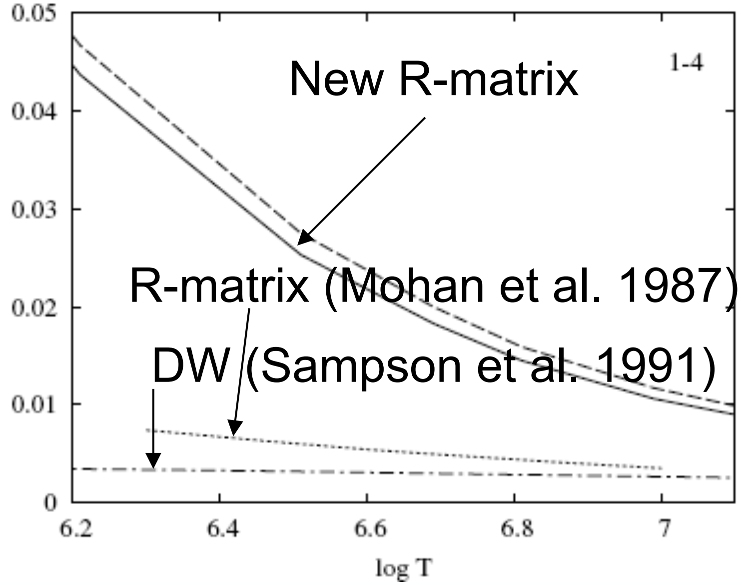








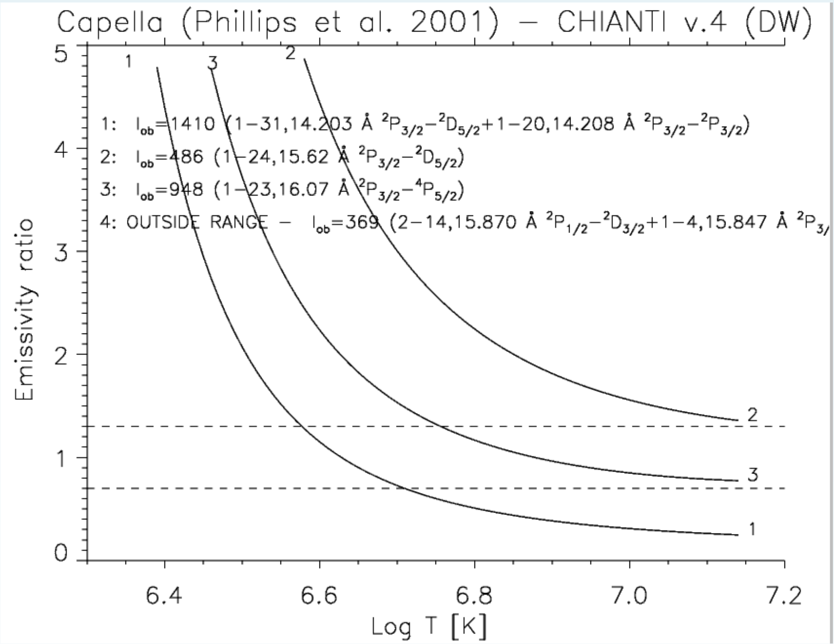
$2s^2\ 2p^4\ 3s\ ^4P_{5/2}$ --> $2s^2\ 2p^5\ ^2P_{3/2}$



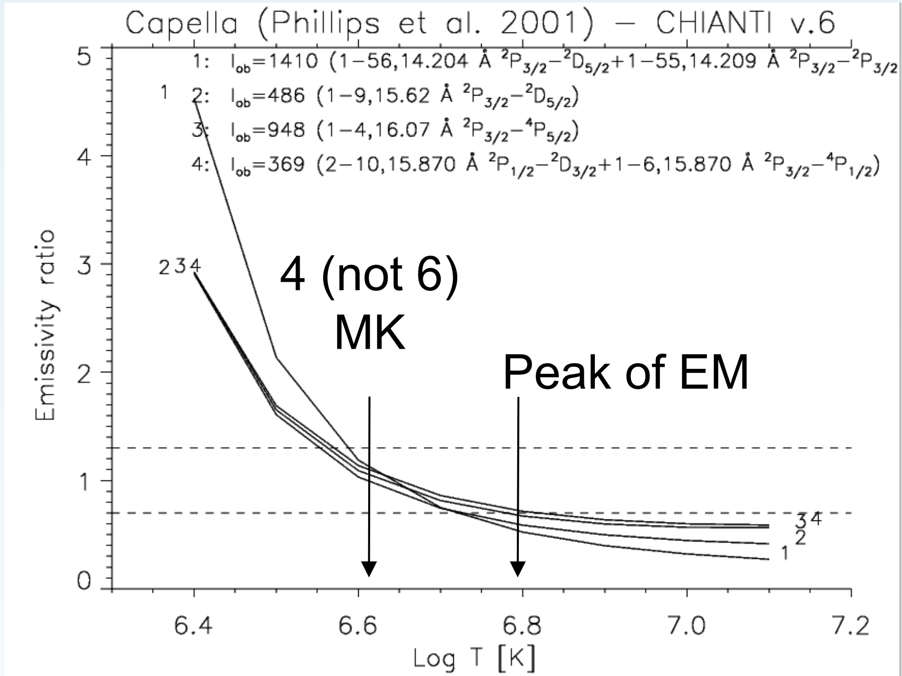
$2s^2\ 2p^4\ 3d$ --> $2s^2\ 2p^5$ $2s^2\ 2p^4\ 3s$ --> $2s^2\ 2p^5$

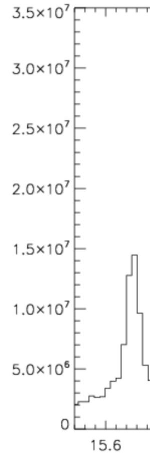
Fe XVIII

DW:



R-matrix:

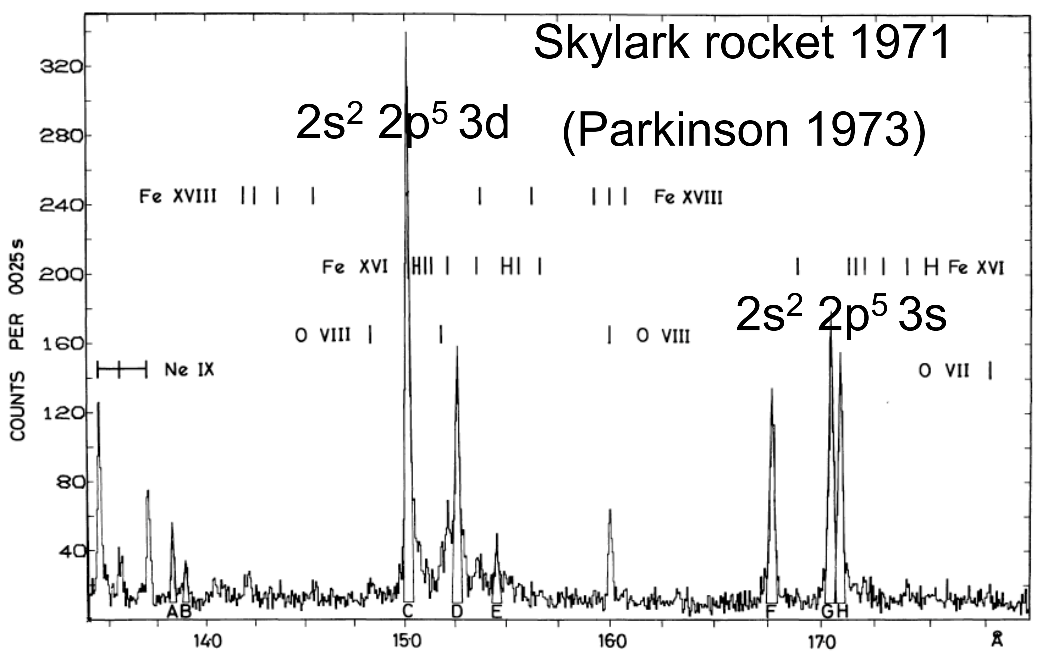


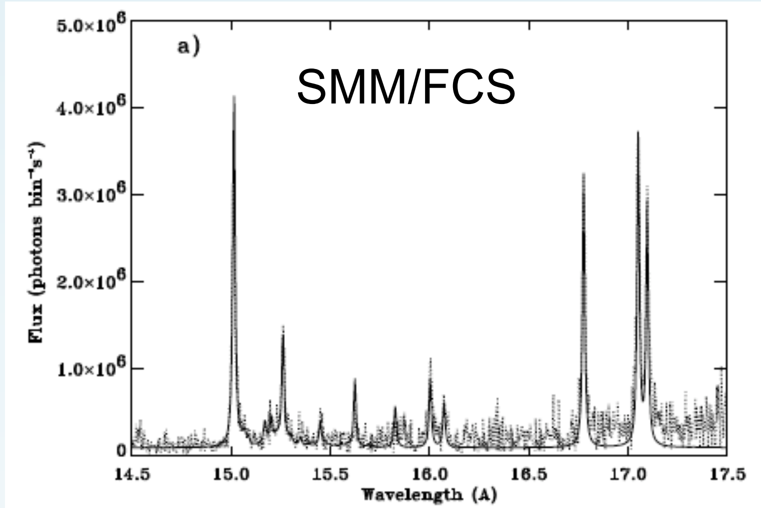


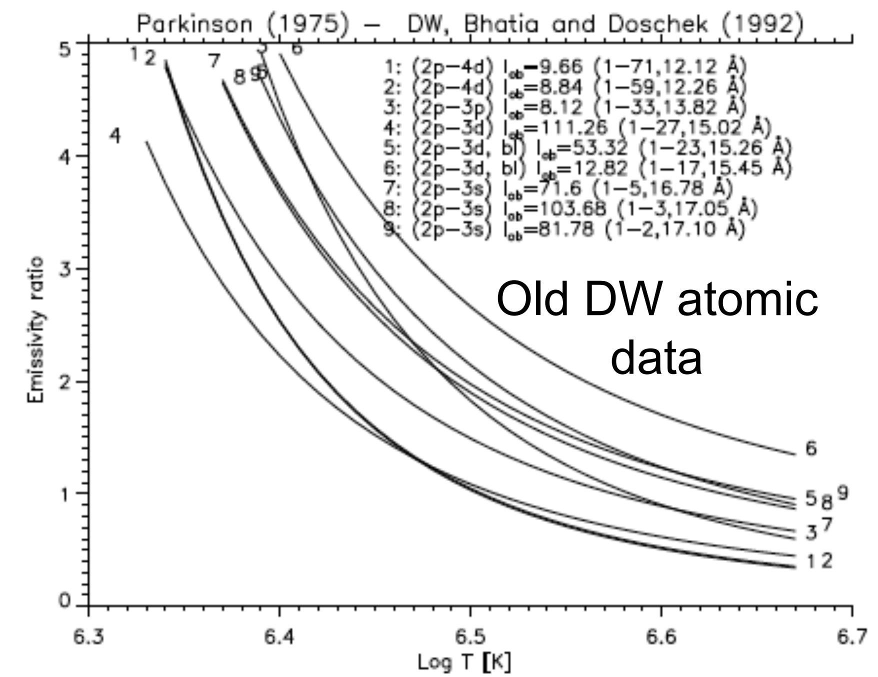
New diagnostics to measure electron temperatures and densities (Del Zanna 2006).

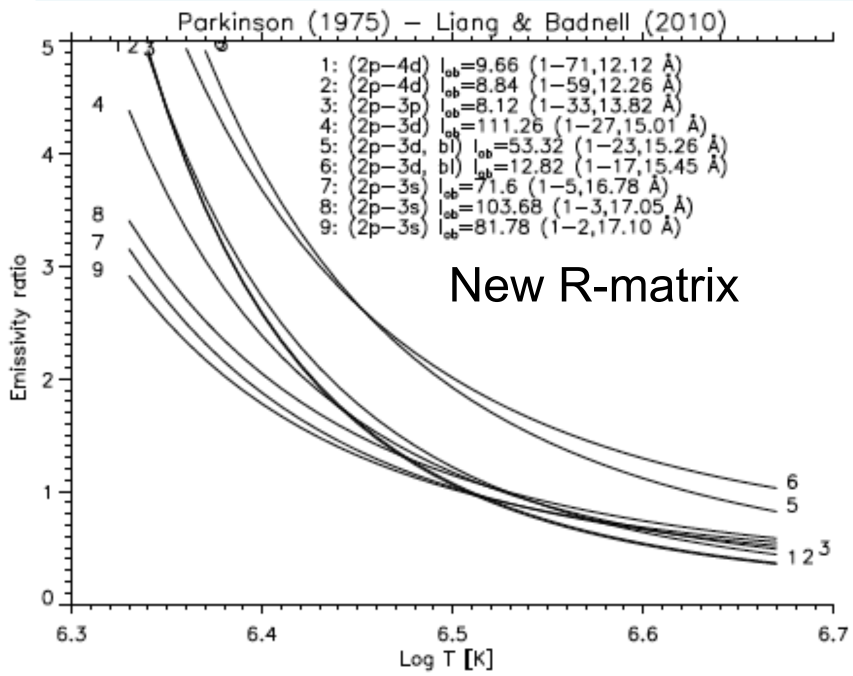
Same issues with Fe XVII. See benchmark paper on R-matrix calculations from Loch et al. (2006) and Liang & Badnell (2010): Del Zanna (2011).

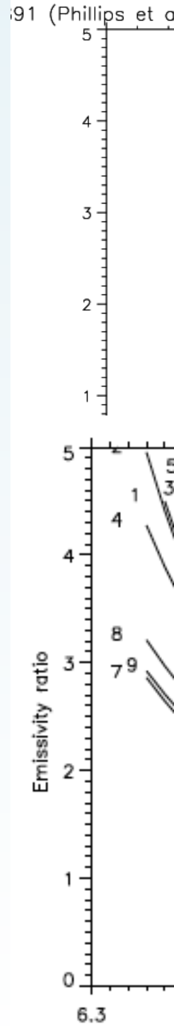
Te from Fe XVII – solar data (Del Zanna 2011)











Conclusions

High-resolution astrophysical spectroscopy in the XUV has shown the need for high-accuracy atomic data.

Excellent agreement (within 10%) between theoretical and observed line intensities for stellar coronae when R-matrix calculations are used.

A novel benchmark work has established a large number of new line identifications and spectral diagnostics.

We have made a great progress, but after 40 years, a large fraction of spectral lines remains unidentified..

A daunting amount of laboratory and theoretical work is still needed..

Thank you