CHIANTI and VAMDC

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OUTLINE:

Atomic Data Calculations – e.g. **APAP Network (UK):**

Atomic Databases: **CHIANTI and VAMDC**

Benchmark: Full assessment against astrophysical and laboratory spectra of line identifications and diagnostics (densities, temperatures from line ratios) in the XUV

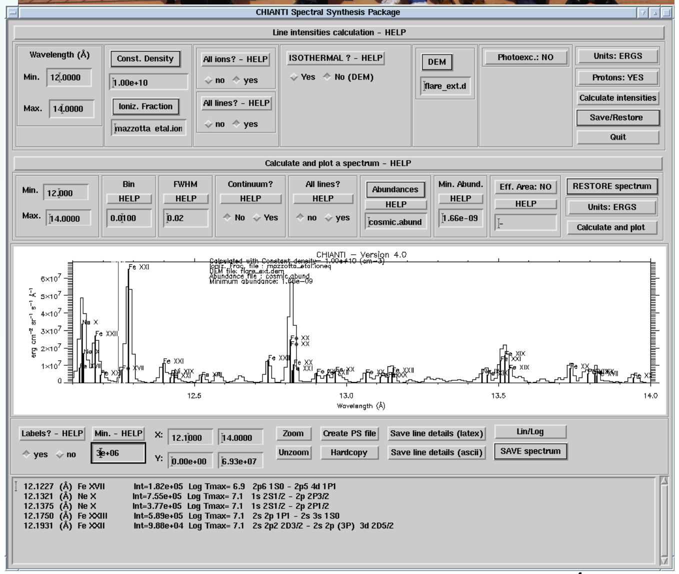
CHIANTI atomic package

VAMDC Virtual Atomic and Molecular Data Centre

CHIANTI Provides all atomic data and IDL programs necessary for modelling spectra from collisionally-ionised plasmas for the XUV. Over 1000 citations.
User base: solar physics, astrophysics, X-ray, EUV, UV

Ions included in CHIANTI
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 released (Dere et al.2009) contains **new atomic data and new ionization and recombination rates**

Basic atomic data from e.g. CHIANTI are included in many other spectral codes. Photoionization (XSTAR, CLOUDY, MOCASSIN) and others (ATOMDB, XSPEC, ISIS, PINTofALE).

CHIANTI data (ascii)

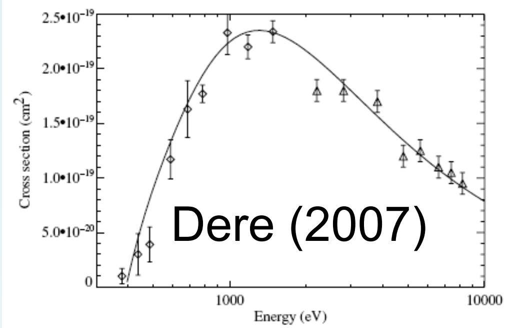
fe_12.elvlc	Energy levels (theoretical, observed), LSJ fro Fe XII (Fe^{11+})
fe_12.wgfa	Transition probabilities, gf values, theoretical, observed wavelengths
fe_12.splups	spline fits to Maxwellian-averaged e^- collision strengths. Only excitaton from ground+ kept. >90% of data are lost. Data from IP, APAP-Network, literature.
fe_12.psplus	Same but for protons.
.diparams .drparams .rrparams	DI, DR, RR total rates

- CHIANTI data and programs are distributed via
  + a tar file (www)
  + SolarSoft (IDL packages for Solar Physics).
  + (testing phase) Python interface (www)
- CHIANTI emissivities are currently calculated for plasmas in ionization equilibrium. Have photo-excitation but not photo-ionization.

Calculations of basic atomic data

1) **Direct-ionization by electron impact**:

Dere (2007) calculated ab-initio cross-sections of impact with ions and compared them with available experimental data for a large number of ions.



2) **Radiative recombination**: Badnell (2006).

3) **Dielectronic recombination**:
Badnell et al. (2003), a number of papers.

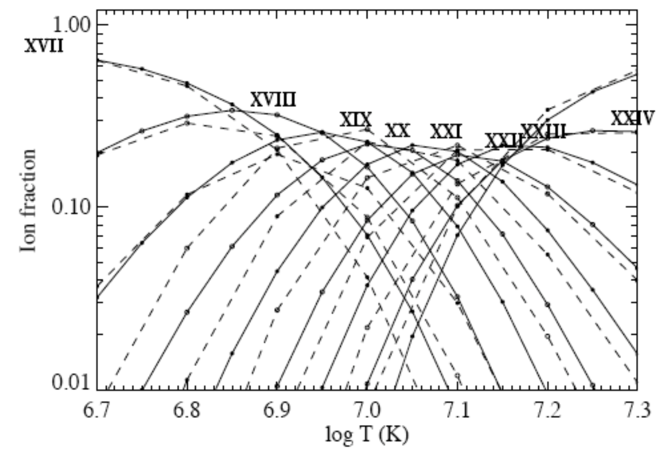


Fig. 3. Ionization equilibria for Fe XVII–XXIV. Full line - current calculations, dashed line = Mazzotta et al. (1998).

4) R-matrix **electron impact excitation**:

1) Iron Project
2) STFC-funded (UK)
APAP Network http://www.apap-network.org/
atomic structure and e- scattering data for all astrophysically-important ions, sequence by sequence.

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

Applications

- In optically-thin plasmas, line intensities are proportional to (e.g. Fe XII):

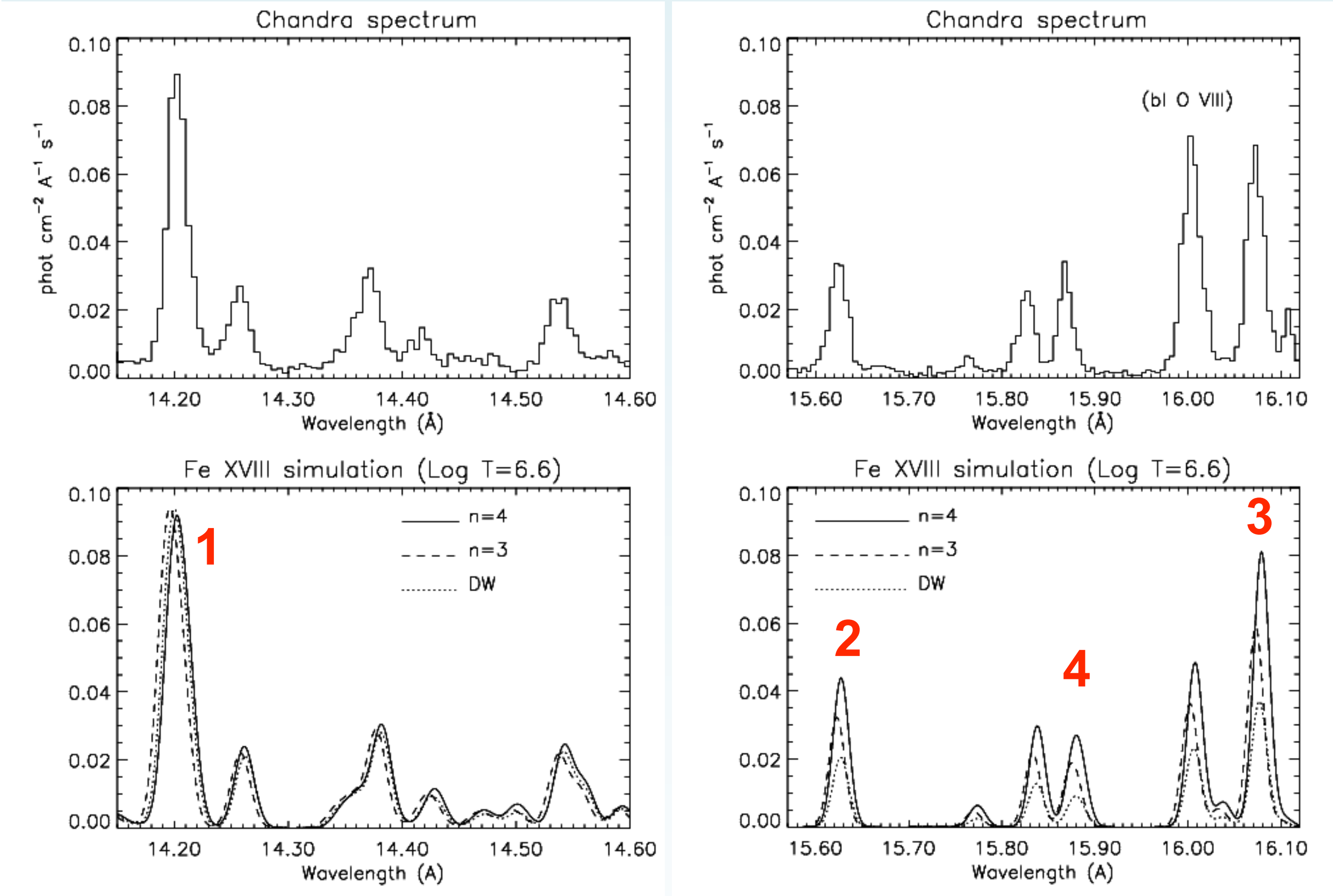
$$\varepsilon_{ij} = N_j A_{ji} = \frac{N_j}{N(\mathrm{Fe\,XII})} \frac{N(\mathrm{Fe\,XII})}{N(\mathrm{Fe})} \frac{N(\mathrm{Fe})}{N(\mathrm{H})} \frac{N(\mathrm{H})}{N_e} N_e A_{ji}$$

Ion ab. Yi A(Y)

- Obtain densities, temperatures and elemental abundances from spectra (and broad-band data).
- Create synthetic spectra to be compared to observed ones (requires links to instrument properties)
- Create synthetic broad-band images (X-ray, EUV)
- Calculate instrument response functions
- Calculate radiative losses

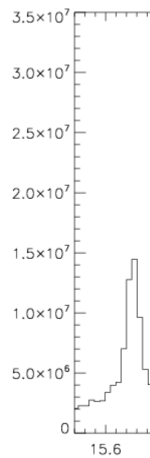
$$E_R \sim N^2 \times \sum_Y Ab(Y) \times \sum_{i=1}^{Z+1} Y_i \varepsilon_i$$

Atomic data do make a difference! Fe XVIII



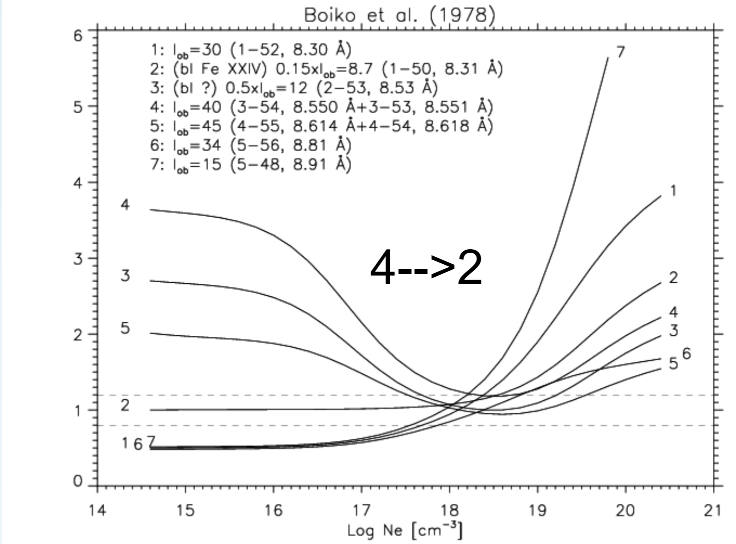
$2s^2\ 2p^4\ 3d \rightarrow 2s^2\ 2p^5$ 3s --> 2p

The large discrepancies between observed and theoretical intensities for the strong 3s--> 2p transitions are now resolved.



First R-matrix e- scattering calculation by Witthoeft, Badnell, Del Zanna et al. (2006).
Now available with CHIANTI v.6

Fe XXIII: Ne, Te

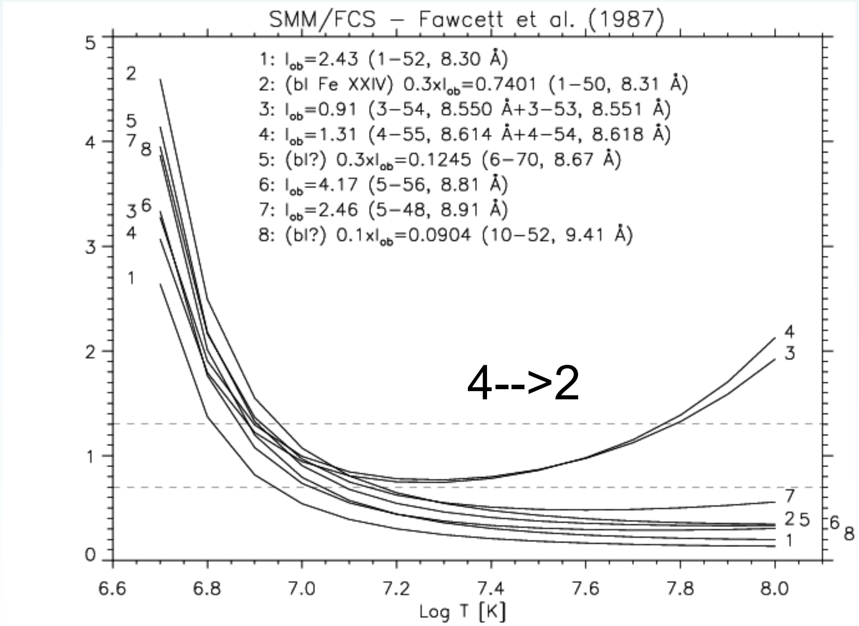


$$F_{ji}(N_e, T_e) = C \frac{I_{ob} N_e}{N_j(N_e, T_e)\, A_{ji}}$$

New electron impact excitation by Chidichimo et al. (2005).

Del Zanna et al. (2005):

New diagnostics to measure electron temperatures and densities.



Radiative lossess

$$\frac{\partial E}{\partial t} + \frac{\partial}{\partial s}[(E+P)v] = \rho v g_{\parallel} + \frac{\partial}{\partial s}\left(\kappa T^{\frac{5}{2}} \frac{\partial T}{\partial s}\right) + E_H(s,t) - E_R(s,t)$$

$$E = \frac{1}{2}\rho\, v^2 + \frac{P}{\gamma - 1}$$

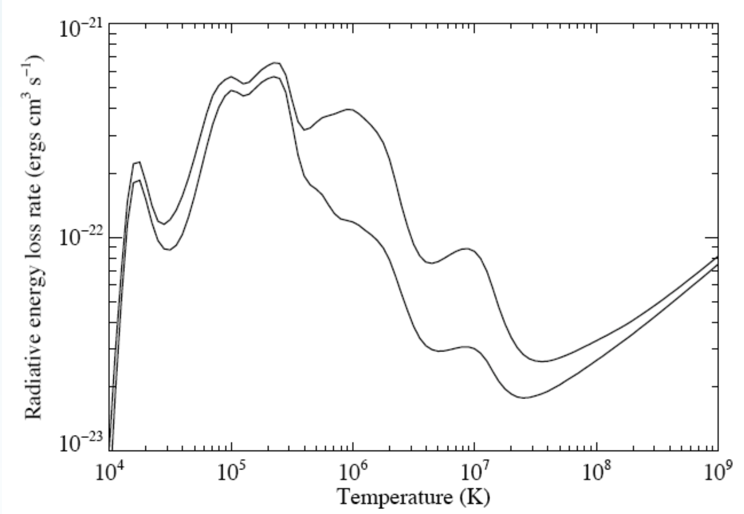
Hydrodynamic modelling
HYDRAD: Bradshaw & Mason (2003)

Radiative lossess in tabulated form
are needed by modellers

$$E_R = n^2 \times \sum_Y \Lambda_Y$$

$$\Lambda_Y = 0.83 \times Ab(Y) \times \sum_{i=1}^{Z+1} Y_i \varepsilon_i$$

Latest (v6) CHIANTI radiative losses
(coronal/photospheric abundances)



$$\frac{\partial Y_i}{\partial t} + \frac{\partial}{\partial s}(Y_i v) = n(I_{i-1}Y_{i-1} + R_i Y_{i+1} - I_i Y_i - R_{i-1} Y_i)$$

Time-dependent
ion populations

CHIANTI & Astrogrid (VO) - 2006

- CHIANTI data were imported into a MySQL database. (Silvia Dalla & Kevin Benson).

  Tables: SpectralLines and LineEmissivities. Link to the VO:

1. using ESAC DAL Toolkit to install a SLAP server (DMMapper can translate from CHIANTI data model to Line data model)
   Data appear automatically in VOSpec, once registered. -

2. by means of **AstroGrid:** **www2.astrogrid.org** DSA software: user can build ADQL queries on the CHIANTI tables via Workbench.

Spectral Lines table

Result of query to spectral lines table via AstroGrid DSA:

TOPCAT(1): Table Browser

File Subsets Help

Table Browser for 1: votable

	LINE_NU...	CHEMIC...	IONISAT...	TITLE	FINAL_L...	INITIAL_...	TRANSI...	WAVELENGTH_METE...	THEORETICAL...	WEIGHTED_O...	EINSTEIN_A	FINAL_
1	183728	26	14	Fe XV 180.0108 A	154	267	2	1.80011E-8	1.80011E-8	0.5414	1.59200E10	3d 4
2	17160	26	22	Fe XXIII 180.0180 A	15	36	1	1.80018E-8	1.81598E-8	0.	727.3	2s 3
3	201205	26	8	Fe IX 180.0318 A	11	106	2	1.80032E-8	1.80032E-8	1.935	5.68600E10	3s2
4	191364	26	11	Fe XII 180.0329 A	10	105	2	1.80033E-8	1.80033E-8	0.000879	2.79900E7	3s 3
5	197329	26	9	Fe X 180.0382 A	35	84	2	1.80038E-8	1.80038E-8	0.289	8.60800E9	3s 3
6	16620	26	22	Fe XXIII 180.0400 A	4	7	1	1.80040E-8	1.80481E-8	0.06407	4.39500E9	2s 2
7	168282	26	17	Fe XVIII 180.0506 A	196	238	2	1.80051E-8	1.80051E-8	0.001184	6.09200E7	2s2
8	48765	26	21	Fe XXII 180.0554 A	154	212	2	1.80055E-8	1.80055E-8	0.04897	5.03800E9	2s 2
9	186344	28	14	Ni XV 180.0558 A	3	23	1	1.80056E-8	1.75817E-8	0.2433	1.66900E10	3s2
10	1147	15	14	P XV 180.0569 A	14	19	1	1.80057E-8	1.80008E-8	0.1671	8.58900E9	4d
11	183746	26	14	Fe XV 180.0604 A	155	268	2	1.80060E-8	1.80060E-8	3.244	7.41500E10	3d 4
12	183857	26	14	Fe XV 180.0623 A	161	281	2	1.80062E-8	1.80062E-8	0.008523	3.50700E8	3p 5
13	116151	26	19	Fe XX 180.0665 A	355	473	2	1.80067E-8	1.80067E-8	0.007767	7.98900E8	2s2
14	118329	26	19	Fe XX 180.0710 A	627	703	2	1.80071E-8	1.80071E-8	0.03371	1.15600E9	2s 2
15	183696	26	14	Fe XV 180.0710 A	152	253	2	1.80071E-8	1.80071E-8	0.1018	1.90400E9	3d 4
16	187740	26	11	Fe XII 180.0783 A	5	47	2	1.80078E-8	1.80078E-8	0.	9248.	3s2
17	194770	26	11	Fe XII 180.0926 A	22	140	2	1.80093E-8	1.80093E-8	0.5435	1.75700E10	3s2
18	200097	26	9	Fe X 180.0928 A	86	168	2	1.80093E-8	1.80093E-8	0.00157	1.59000E8	3s2
19	200139	26	9	Fe X 180.0928 A	86	169	2	1.80093E-8	1.80093E-8	0.001221	6.18200E7	3s2
20	195445	28	12	Ni XIII 180.0948 A	2	34	2	1.80095E-8	1.80095E-8	0.03633	1.49400E9	3s2
21	27975	10	5	Ne VI 180.0997 A	12	40	1	1.80100E-8	1.80043E-8	3.67800E-6	3.78000E5	2p3
22	183745	26	14	Fe XV 180.1148 A	155	267	2	1.80115E-8	1.80115E-8	0.02654	7.79600E8	3d 4
23	169495	18	8	Ar IX 180.1250 A	15	55	1	1.80125E-8	1.75766E-8	0.02555	1.75000E9	2s2
24	117906	26	19	Fe XX 180.1342 A	554	654	2	1.80134E-8	1.80134E-8	0.00568	1.94600E8	2s2
25	117916	26	19	Fe XX 180.1339 A	556	657	2	1.80134E-8	1.80134E-8	0.0435	2.23500E9	2s 2
26	56793	16	10	S XI 180.1361 A	45	49	2	1.80136E-8	1.80136E-8	0.	42.	2s2
27	180762	26	14	Fe XV 180.1361 A	42	107	2	1.80136E-8	1.80136E-8	0.00119	2.44600E8	3s 4
28	201196	26	8	Fe IX 180.1386 A	11	105	2	1.80139E-8	1.80139E-8	0.08465	3.47800E9	3s2
29	118115	26	19	Fe XX 180.1445 A	586	674	2	1.80144E-8	1.80144E-8	0.4235	7.25400E9	2s 2
30	118114	26	19	Fe XX 180.1480 A	586	673	2	1.80148E-8	1.80148E-8	0.01876	4.81900E8	2s 2
31	75807	26	20	Fe XXI 180.1489 A	415	539	2	1.80149E-8	1.80149E-8	0.01088	4.47100E8	2s 2
32	181504	26	14	Fe XV 180.1486 A	64	170	2	1.80149E-8	1.80149E-8	0.004342	1.78500E8	3p 4
33	86746	20	13	Ca XIV 180.1600 A	11	15	1	1.80160E-8	1.76078E-8	0.000137	1.41200E7	2s 2

CHIANTI atomic data for VAMDC

- WP4 SA1 Giulio Del Zanna & Helen Mason (DAMTP, Univ. of Cambridge)

- Collaboration with IoA (Nic Walton, Guy Rixon)
- MSSL, UCL (Len Culhane, Kevin Benson, Peter Kuen)

- BASIC DATA: first table: wavelength, A-value, gf-value, configuration, LSJ, observed, theoretical energy of upper and lower levels.
  To do: add other basic atomic data (rates).
  Maintain identity of each database.
  Problem of multiple calculations. CHIANTI policy is to select one.
  Problem of upgrades (main once every 1-2 years)
  Essential to provide **appropriate references to original calculation in the literature ! Not simple to transfer info.**

- DERIVED DATA (modelling): second table: line emissivities in a grid of temperatures and densities.
- To do: write simple scripts to call CHIANTI routines via the MSSL server (IDL and CHIANTI installed). Alternatively, write Python programs.

See Kevin Benson's talk on wednesday

User base

1) Modellers, e.g. CLOUDY, XSTAR. Make ingestion of basic atomic data easier

2) General users that do not have IDL licence. Make the basic programs available via the www/ Python.

3) General users that are not bothered to install CHIANTI.

4) General users that want some derived products that are not readily available. Example: many users need CHIANTI radiative losses

- AHEAD EU proposal for next generation X-ray astrophysics. Emphasis is on spectroscopy and need for atomic data – links to VAMDC

- GDZ publicised VAMDC at the X-ray 2010 workshop (Utrecht)

END

Benchmarking atomic data

In a series of papers, I have calculated and benchmarked atomic data for the XUV using a `novel' approach: atomic structure calculations and comparisons between

- observed and theoretical wavelengths
- observed and theoretical line intensities for a wide range of astrophysical and laboratory plasmas using the emissivity ratios:

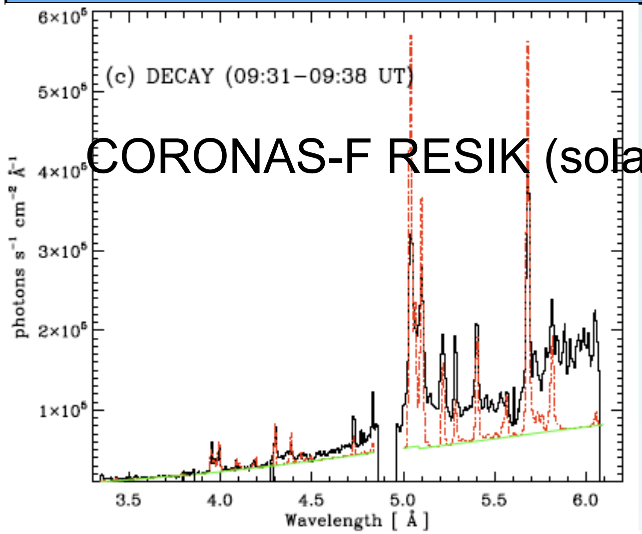
$$F_{ji}(N_e, T_e) = C \frac{I_{ob} N_e}{N_j(N_e, T_e)\, A_{ji}}$$

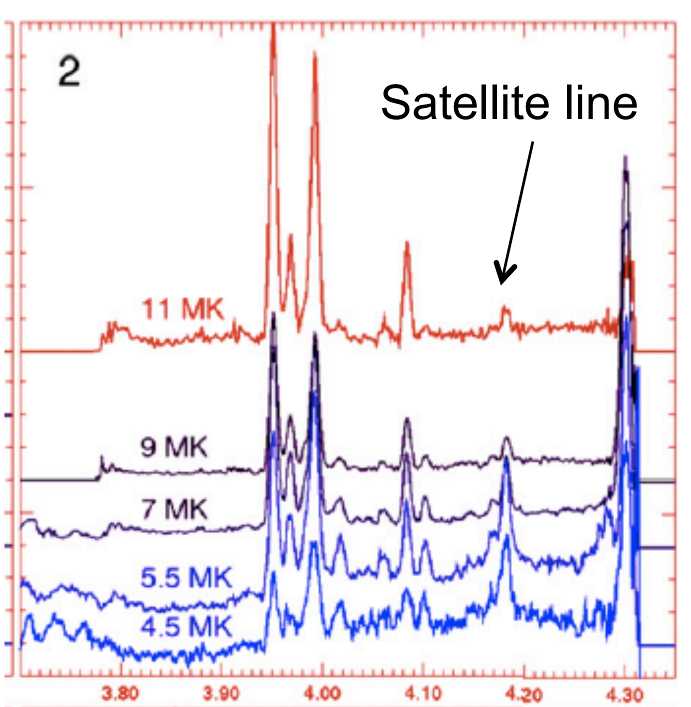
- lifetimes (beam-foil spectroscopy)

A large number of revised wavelengths, new identifications and new diagnostic applications.
For many ions NIST energies are not up-to-date. Not easy to trace original work.

Te from satellites and EM approach

CORONAS-F RESIK (solar)



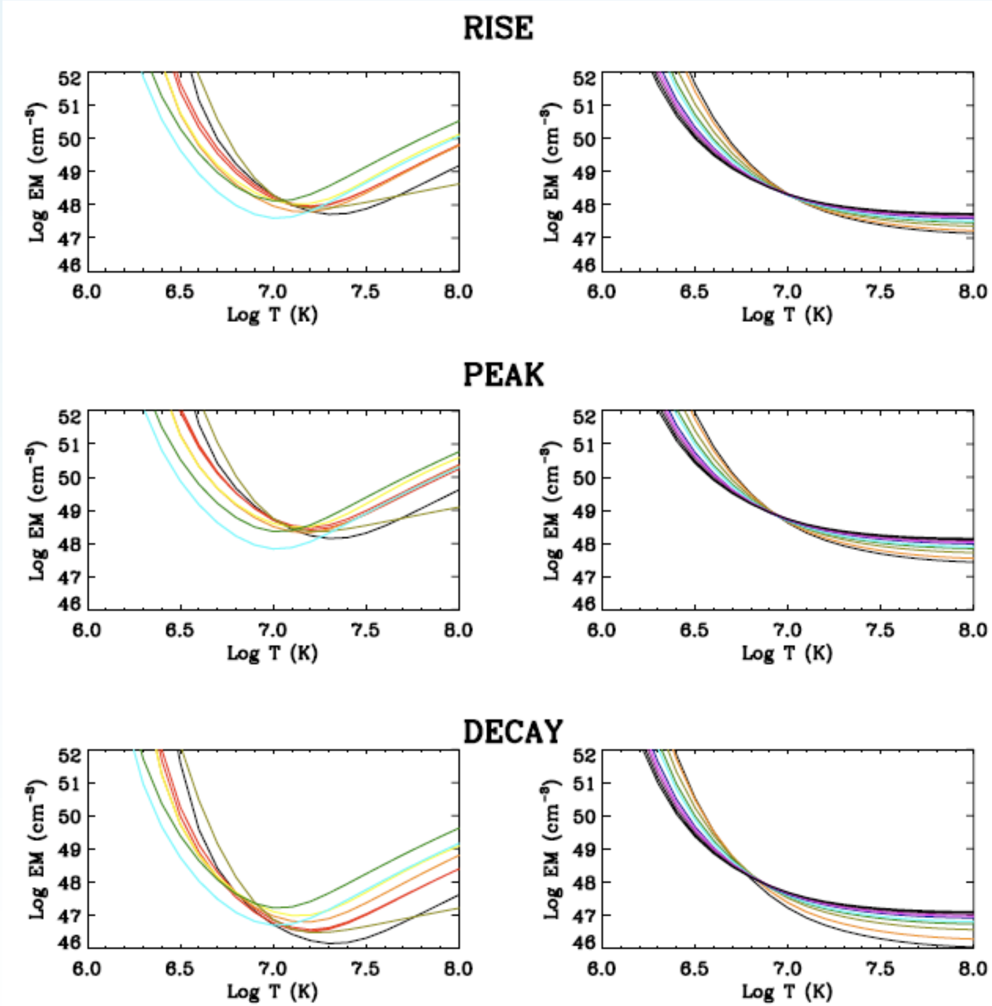


Sylvester et al. (2006)

Chifor Del Zanna et al. (2007)

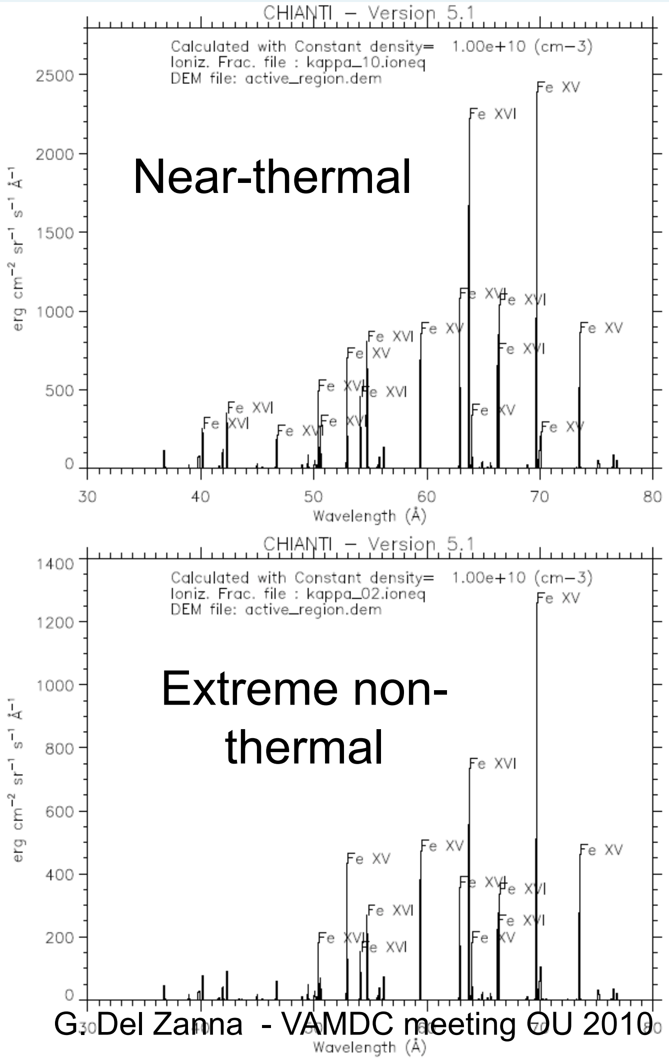
EM lines

EM continuum



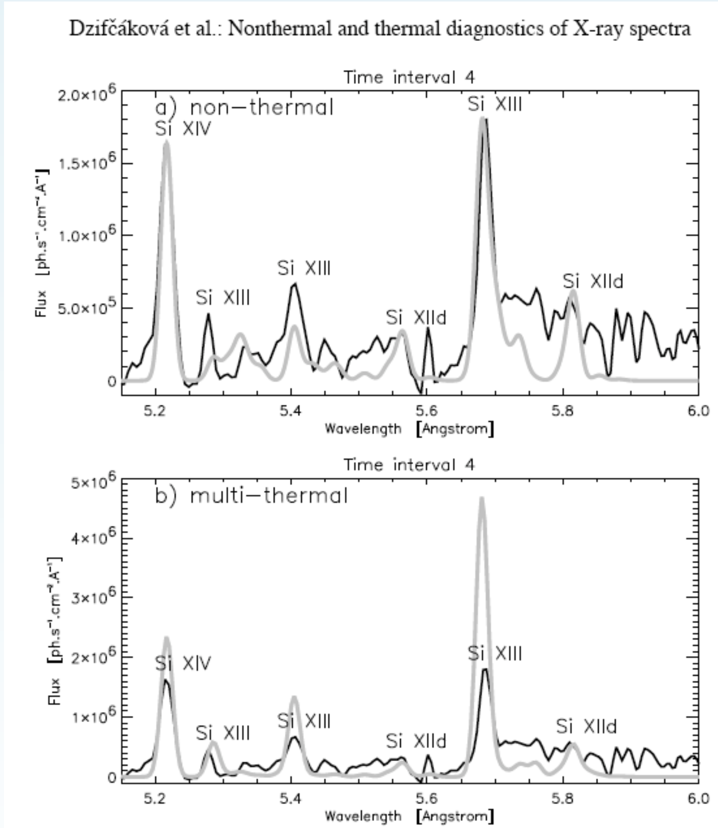
Non-thermal electron distributions

Calculate level population and ion abundances with non-Maxwellian e⁻ distributions (Dzifcakova & Mason 2008)



CORONAS-F RESIK SPECTRA

Dzifcakova et al. (2008)



Not implemented in CHIANTI yet.