X-RAY SPECTROSCOPY AND ATOMIC DATA

Current Status

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Collaborators

This work is a result of ongoing collaboration with the RGS consortium including teams from:

- Columbia University, New York (Kahn et al.)
- SRON, The Netherlands (Kaastra et al.)
- MSSL, UK (Branduardi-Raymont et al.)
- PSI, Switzerland (Güdel et al.)

… and laboratory measurements at LLNL California (Beiersdorfer et al.)

Outline

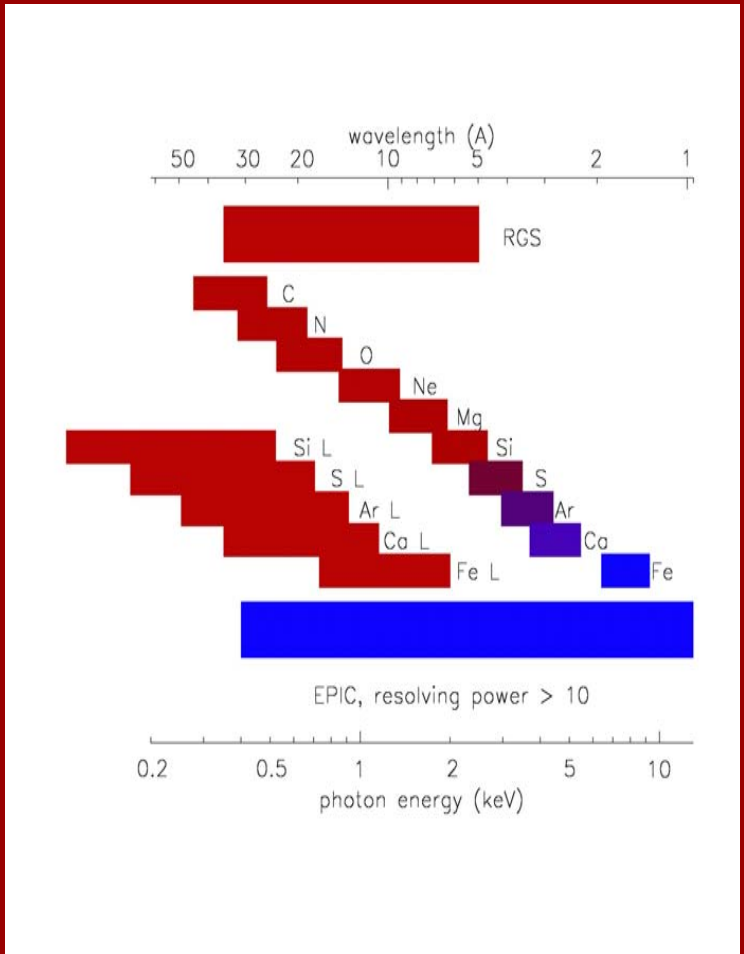
- ❖ Introduction:
  - **The Soft X-Ray Band with *Chandra* and *XMM-Newton***
- ❖ Measurements in Collisional Plasmas (stars, normal galaxies, clusters)
  - **Abundances**
  - **Temperature Structure**
  - **Beyond the Coronal Approximation**
    - ❖ **Transitions among excited levels (density and UV diagnostics)**
    - ❖ **Neighboring ion effects**
  - **Assessment of Fe-L Atomic Data**
  - **L-shells of Other Elements**
- ❖ Measurements in Photoionized Plasmas (active galaxies, x-ray binaries)
  - **Wavelengths (inner-shell phenomena)**
  - **Column Densities and Abundances**
  - **Atomic Data Status and Supporting Lab. Measurements**
- ❖ Conclusions

Introduction

- X-Ray Astronomy was born in 1962 with the discovery of Scorpius X-1.
- Over the years x-ray observatories have revealed a diverse collection of x-ray sources ranging from nearby stars to distant galaxies.
- However, it wasn’t until the recent launches (1999) of *Chandra* and *XMM-Newton* that x-ray line-resolved spectra have become available.
- With this recent achievement, the x-ray branch of astronomy now joins other wavebands in using spectroscopy to perform quantitative investigations of cosmic objects.

Features of the X-Ray Band: Highly Ionized Atoms

- The conventional (soft) x-ray band (1 to 100 Å or ~ 0.2 – 10 keV) comprises emission lines from many K-shell and L-shell ions pertaining to many elements (C – Ni).
- The x-ray band is uniquely compact, having several ions appear from each element and many lines present from each ion.
- The wealth of lines and ions allows for elaborate plasma diagnostics such as temperatures, densities, ionization state, and elemental abundances.



A New Era in X-Ray Astrophysics: *Chandra* and *XMM-Newton*

- *Chandra* (NASA):
  Launched July 23, 1999
  1 telescope
  2 CCD cameras
  2 transmission grating spectrometers (spectroscopy mode is alternative to imaging)

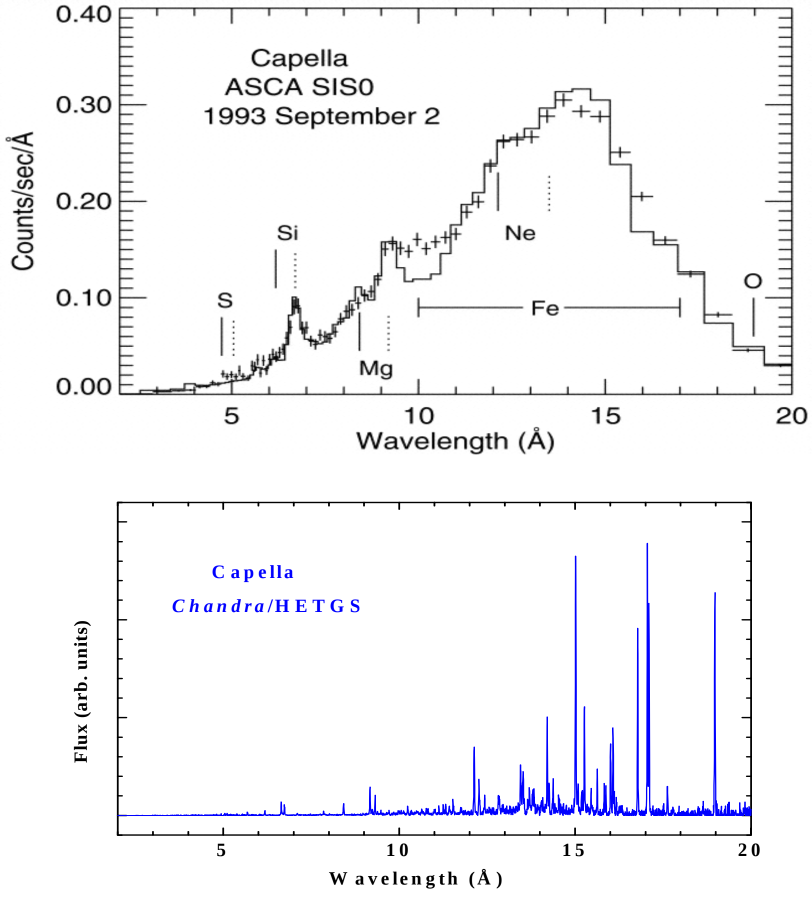
- *XMM-Newton* (ESA):
  Launched December 10, 1999
  3 telescopes
  2 reflection grating spectrometers
  1 Optical/UV monitor

The Difference High Spectral Resolution Makes (Capella)

- SIS0 CCD spectrum with ASCA

  (Brickhouse, Dupree, Edgar et al. 2000)

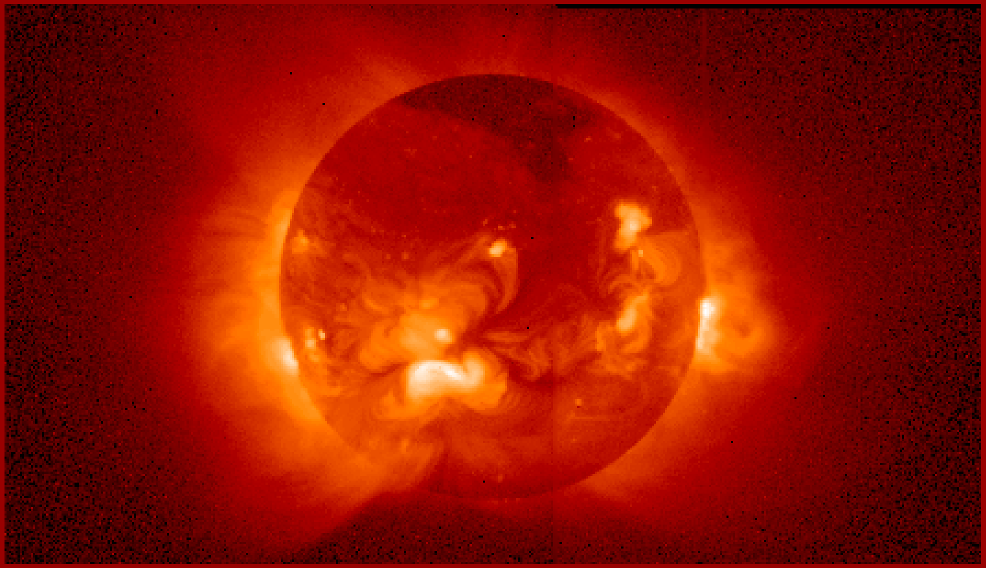
- HETGS grating spectrum with *Chandra*



Behar, Cottam, & Kahn 2001

Stellar Coronae: Hot, Collisional X-Ray Sources

- Physical environment:
  - Hot (*kT* ~ 0.1 – 3 keV)
  - Density ($n \sim 10^{10}$ cm^{-3})
  - Optically thin



- Ionization balance:
  - Standard electron-ion collisional processes: CI, RR, as well as EA and DR
- Line excitation:
  - Electron impact

Coronal Steady-State Approximations

- Excited level populations:

$$\frac{n_j}{n_{i(ground)}} = n_e Q_{ij}(T_e)/A_{ji}$$

- Individual-line emission-measure:

$$\int n_j A_{ji} dV \left(= F_{ji} 4\pi d^2\right) =$$

$$\int n_H \frac{n_Z}{n_H} \frac{n^{+q}}{n_Z} \frac{n_j}{n^{+q}} A_{ji} dV =$$

$$A_Z f^{+q}(T_e) Q_{ij}(T_e) \int n_H n_e dV$$

- Ionization balance:

$$\frac{n^{+q}}{n^{+(q+1)}} = \frac{n_e \alpha_{q+1 \rightarrow q}(T_e)}{n_e S_{q \rightarrow q+1}(T_e)}$$

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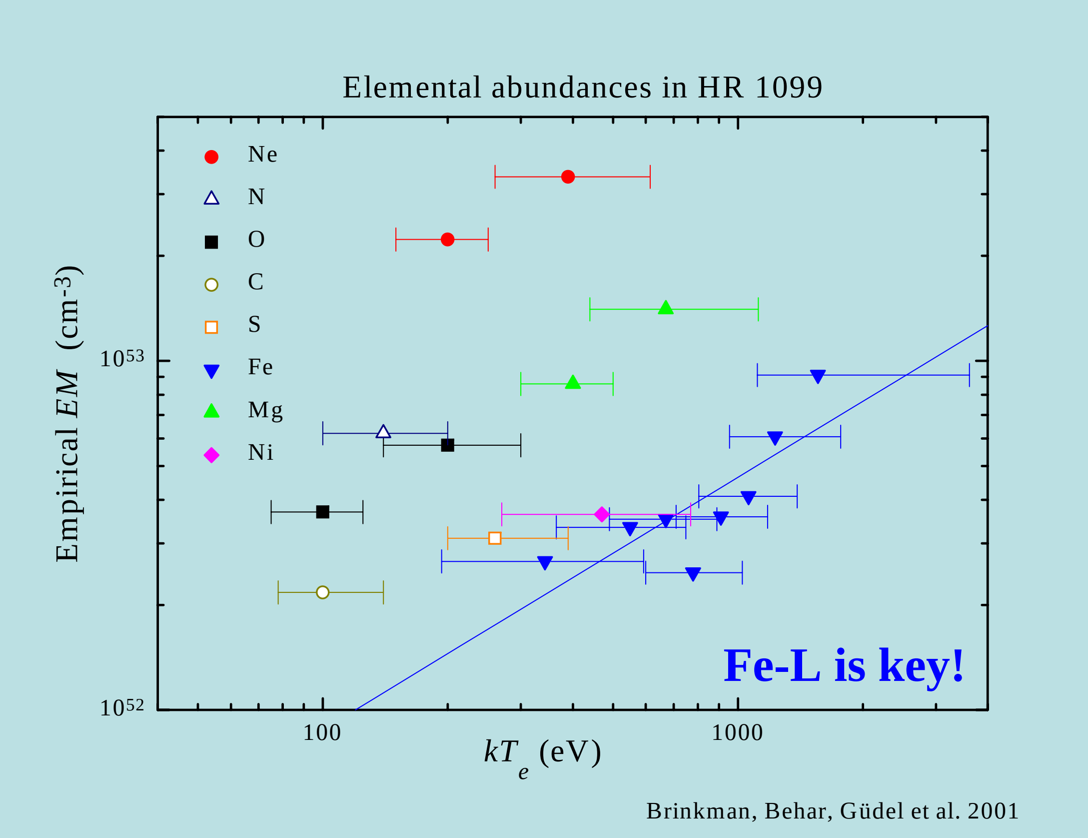
- Ionization balance:

$$\frac{n^{+q}}{n^{+(q+1)}} = \frac{n_e \alpha_{q+1\rightarrow q}\left(T_e\right)}{n_e S_{q\rightarrow q+1}\left(T_e\right)}$$

Stellar Coronae (cont.): Temperatures and Abundances



Brinkman, Behar, Güdel et al. 2001

$$n_e n_H V = \frac{4\pi d^2 F_{ji}}{A_Z P_{ji} f^{+q}}$$

F_{ji} – measured

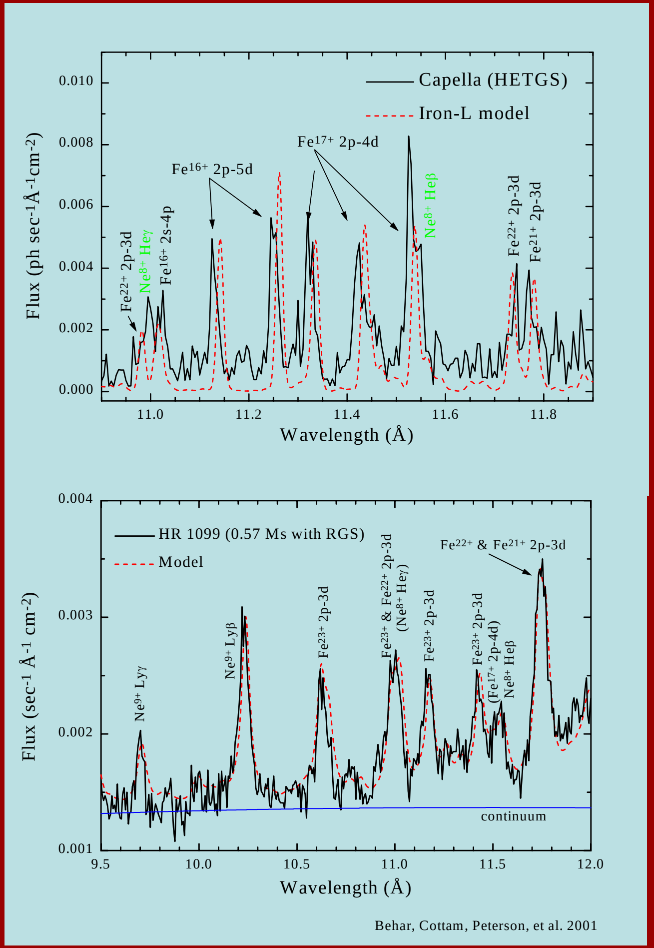
d – known

A_Z – assumed solar

P_{ji}, f_q – **atomic physics**

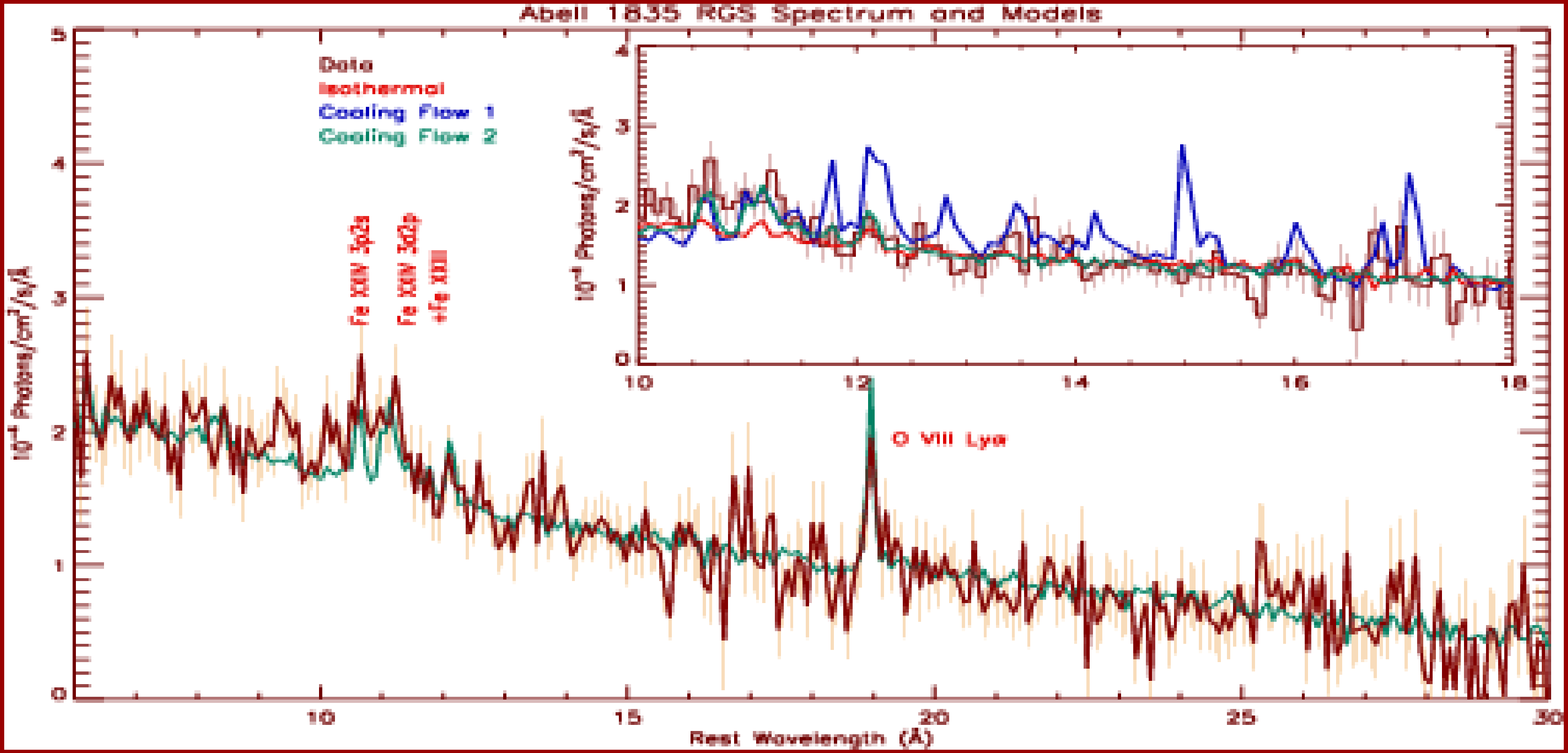
Coronal Abundances (cont)
Fe-L uncertainties most suspect

- Uncertainties in the EM stem from uncertainties in $\boldsymbol{P_{ji} * f_q}$
- $\boldsymbol{P_{ji}}$ actually seems in pretty good shape; multi-line ions are very powerful in constraining models
- $\Delta \boldsymbol{f_q}$ suffers directly from the uncertainties in $\alpha(T_e)$ and $S(T_e)$ – simple factor
- T_{max} is less affected: ($\Delta\alpha$ / α = ΔS / S)



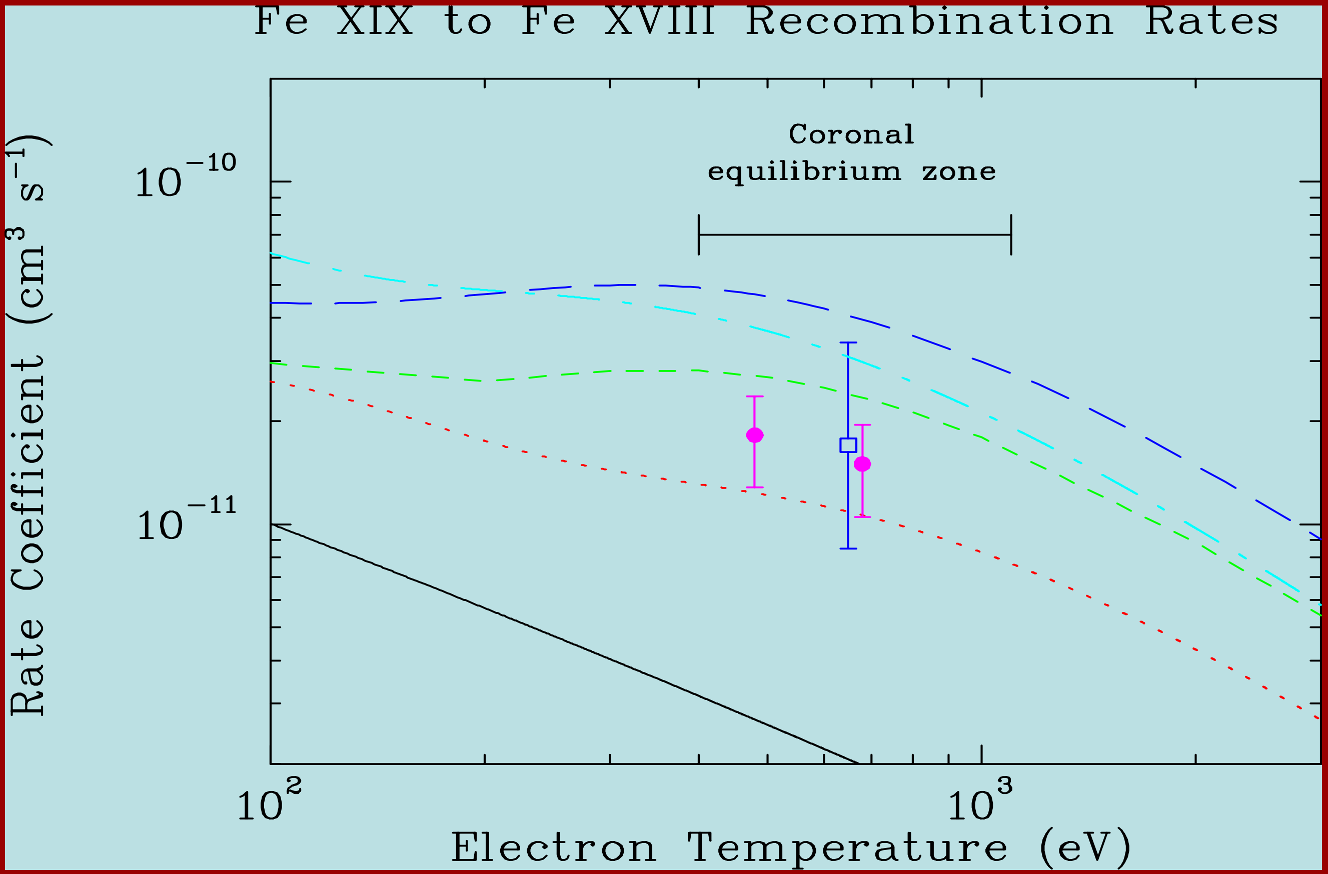
Behar, Cottam, Peterson, et al. 2001

Galaxy Clusters: Absence of the Cooling Flows



Peterson, Paerels, Kaastra et al. 2001

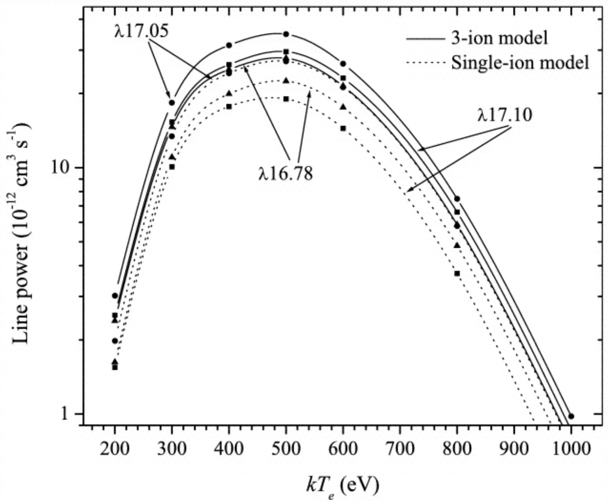
Dielectronic Recombination (DR): The weak link in the ioniz. balance

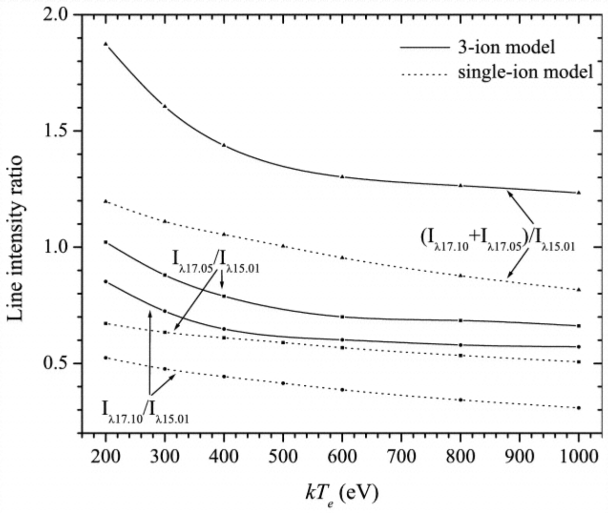


Courtesy of Daniel Savin

When the coronal approximation breaks down …

- The 2p-3s lines in some L-shell ions have the annoying habit of being populated by a variety of processes, not only CE, but also RE, and DR, and to a lesser extent also CI and RR (Doron & Behar 2002)
- Resonant absorption could (under special circumstances) affect these ratios: e.g., NGC 4636 (Xu, Kahn, Peterson, et al. 2002)



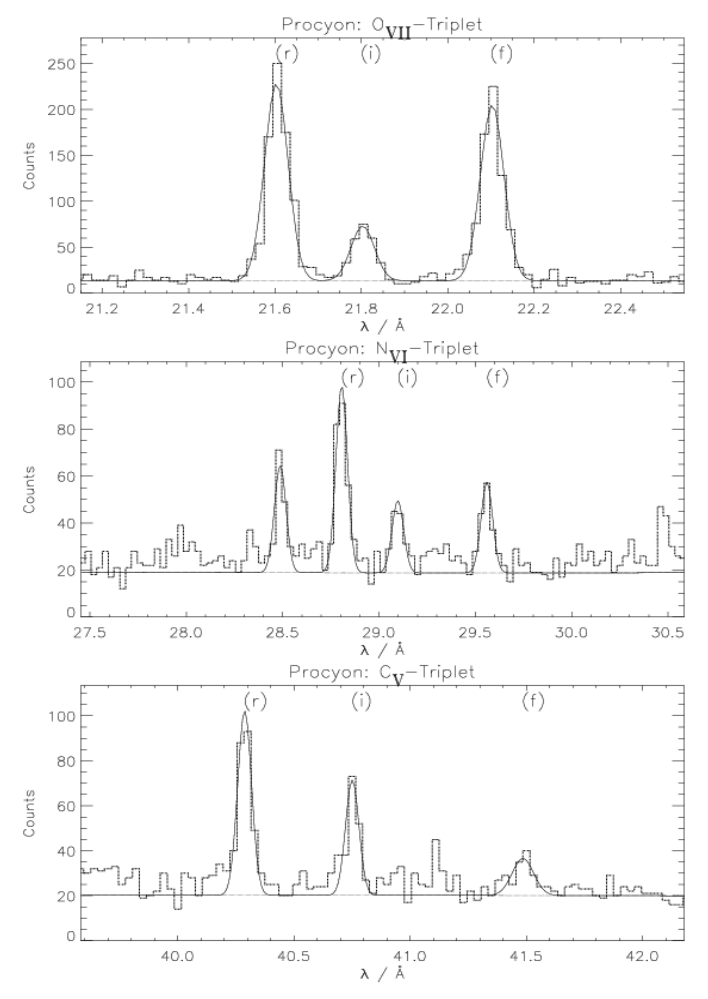


Beyond the Coronal Regime (cont.) Density Diagnostics

- ❖ Collisional depletion of the upper levels of forbidden lines

- ❖ Most popular are the He-like triplets (Gabriel & Jordan 1969). The 1s-2s forbidden line is suppressed at high densities.

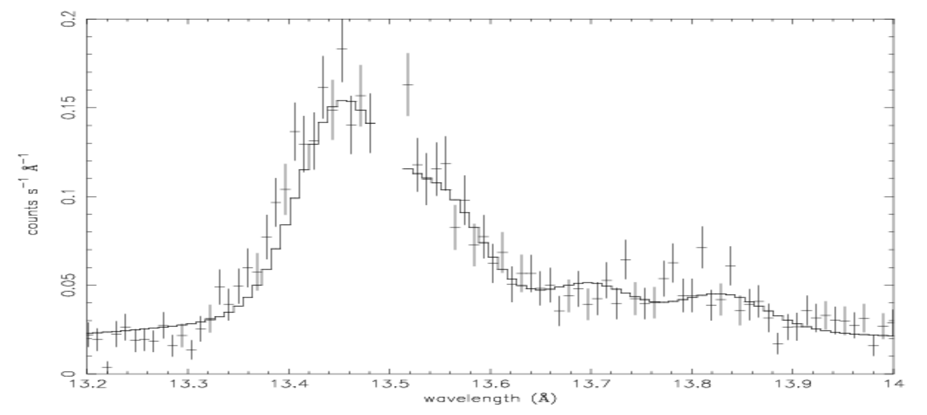
- ❖ Critical density increases with Z.



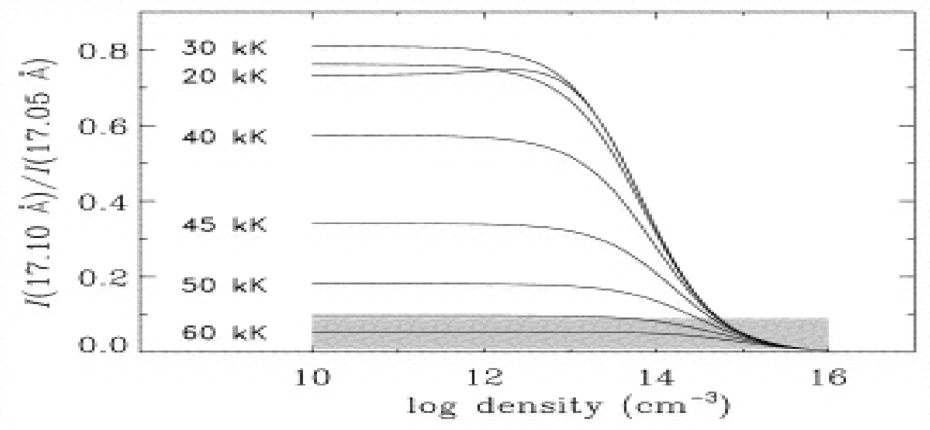
Ness, Mewe, Schmitt et al. 2001

Presence of UV Field

- UV depletion of excited levels mimics density effects
- Example: He-like triplets in ζ Pup
- Provides measurement of distance from photosphere
- Another example: 2p-3s forbidden line of Fe^{16+} in the magnetic CV (EX Hya)

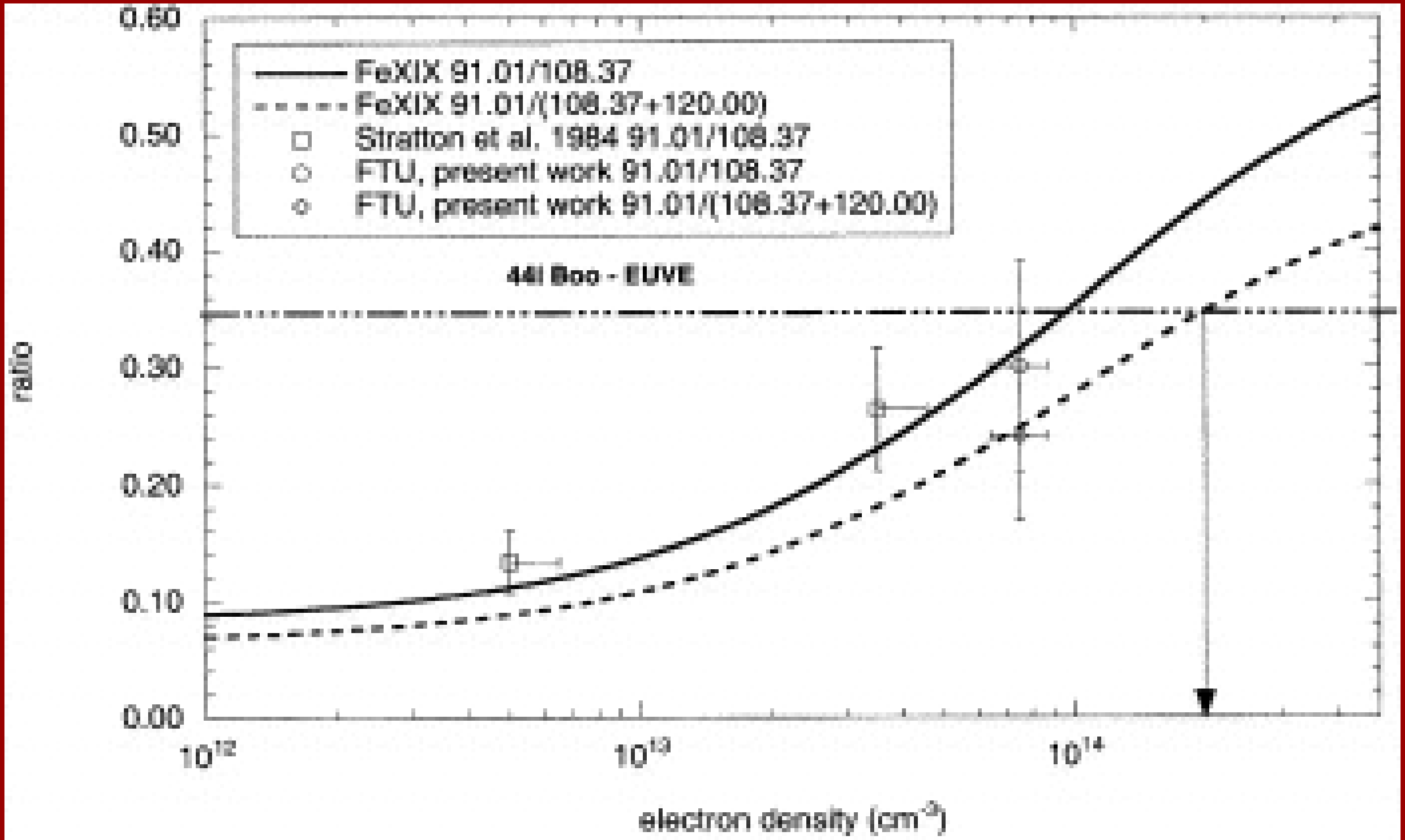


ζ Pup; Kahn, Leutenegger, Cottam, et al. 2001



Mauche, Liedahl, & Fournier 2001

Can we trust rates for transition among excited levels?



Fournier, May , Liedahl, et al. 2001

Fe-L – Quick Summary

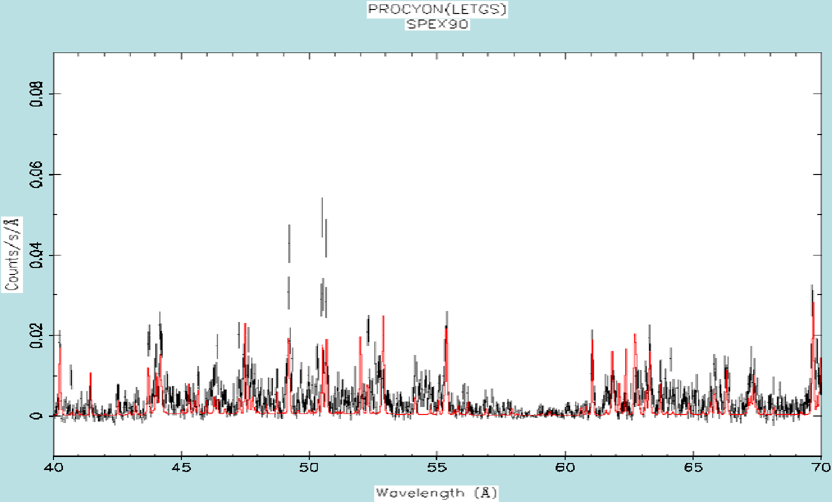
- The 2p-3d and 2p-3s lines of Fe^{16+} - Fe^{23+} dominate the soft x-ray spectrum of many sources.
- Lines of different Fe-L ions have been measured to high accuracy with LLNL EBIT and are easily discernible with contemporary grating spectrometers.
- Even within the simplified coronal approximation, Fe-L lines provide a powerful, robust tool for obtaining the (abundance-free) temperature structure (*EM*) of the source.
- For years, Fe-L was deemed uncertain and considered the nightmare and scapegoat of many x-ray astronomers. Unjustly so!
- The 2p – 3s line powers need to be treated more carefully.
- Where possible, it still makes a lot of sense to use single-ion models independent of the ionization balance.
- Testing of the rates for transitions among excited levels are encouraging.

There is Life After Fe-L …

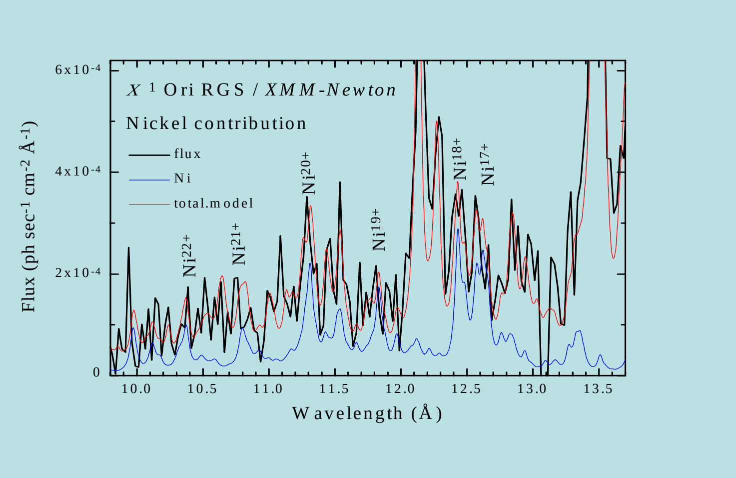
- Procyon with LETGS

  Raassen, Mewe, Audard, et al. 2002

  Si, S – L are inadequate in the commonly used databases

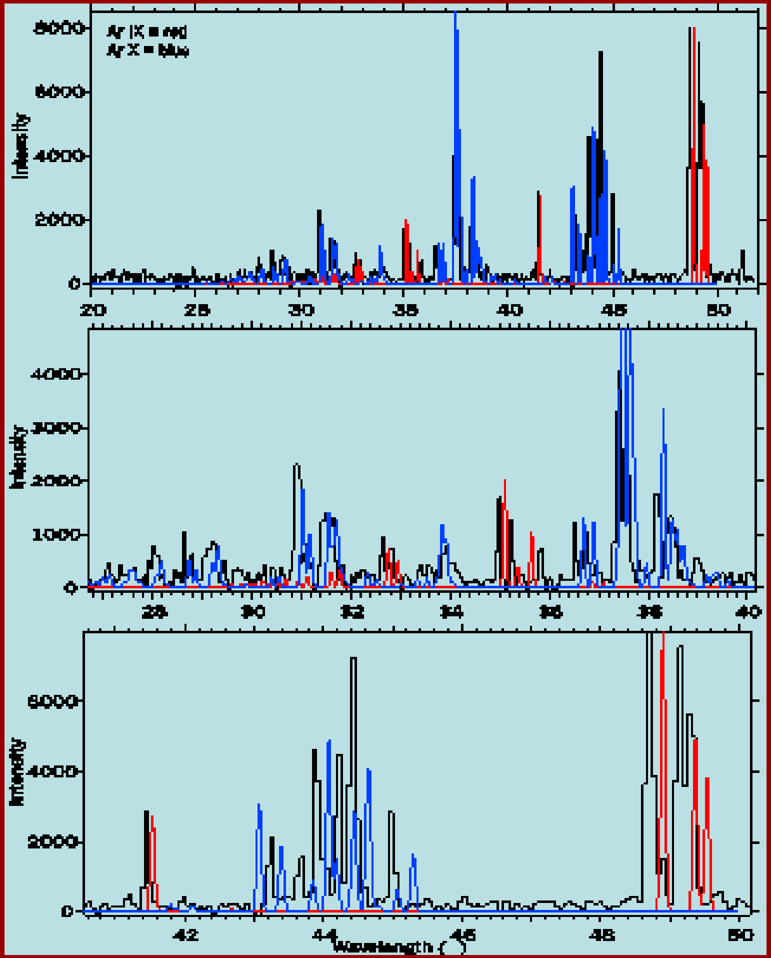


- *X^1* Ori (RGS): Noticeable Ni-L contribution



The world beyond Fe-L (e.g. Ar)

- **Ar IX & X,**
  EBIT LLNL measurements vs. HULLAC calculations



Lepson, Beiersdorfer, Behar, & Kahn 2002

Collisional Plasmas: Atomic Data Status

Expected Confidence Levels (Ball Park) and Experimental Benchmarking

Shell / Data	K	K (Fe)	L	L (Fe)
Wavelengths	0.01%	0.01%	0.5%	0.03%
Emissivities	10%	10%	50%	10-20%
Tot. Ionization	20%	20%	30%	30%
Tot. Recomb.	20%	20%	100%	50%
Transitions excited levels	50%	50%	50%	30%

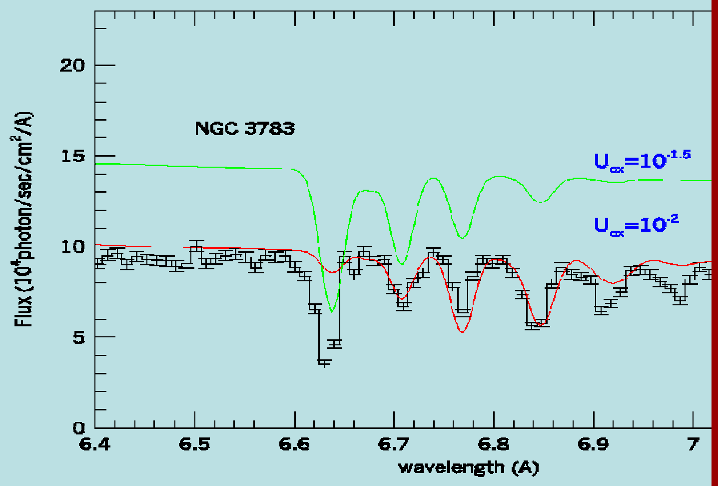
Spectroscopic Measurements in Photoionized Plasma

1. Outflow velocities, mass loss (wavelengths)
2. Electron temperatures (RRCs)
3. Optical depth => column densities
   via absorption (oscillator strengths) and emission
4. Elemental abundances
   (column density behavior as a function of
   ionization parameter $\xi = L/n_e r^2$)
5. Ionization balance (ξ), density (n_e) and position (r)
   (photo-ionization and recombination rates, including
   autoionization processes)

Note: X^2 is not a measurable astrophysical quantity!

1s-2p (Kα) Inner-Shell Absorption

- L-shell ions have vacancies in their 2p sub-shell and absorb by means of 1s-2p resonance lines
- Have been observed in many sources and for many elements
- Span wide range in ionization => very useful for probing the ionization state(s) of the plasma
- Autoionizing upper levels affect line shapes and ionization balance



Behar & Netzer 2002

1s-2p Inner-Shell Line Comparison

Wavelengths (in Å) and *f*-values

Code / Ion	R-Matrix (Pradhan et al)	HULLAC	Cowan (Raassen)	
O^{5+}	22.05 (*f*= 0.384,0.192)	22.01 (0.351,0.174)	22.05	
O^{4+}	22.35	22.33	22.38	
O^{3+}	22.73	22.73	22.77	
Fe^{23+}	1.860 (0.491) 1.864 (0.146)	1.861 (0.469) 1.864 (0.147)	---	

Inner-Shell Line Comparison

Wavelengths (in Å) and *f*-values

Code **Ion**	**R-Matrix (Pradhan et al)**	**HULLAC**	**Cowan (Raassen)**	**NGC 5548***
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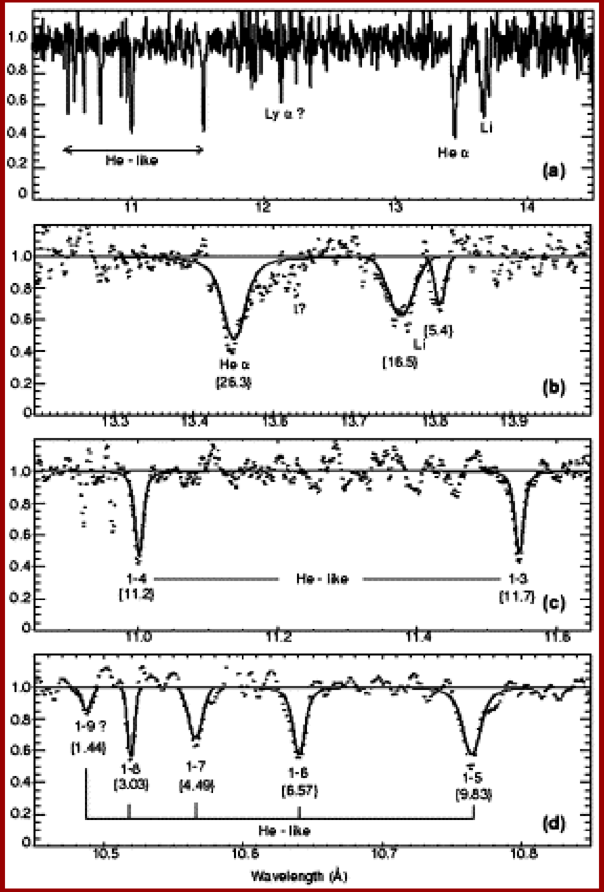
* Based on velocity of O^{6+} (± 0.01 Å); Courtesy of Jelle Kaastra

Uncertainty: 0.2% ~ 600 km/s
is of the order of the outflow velocities we want to measure in AGN!

Need for Laboratory Experiments
Z Pinch (& Laser Plasma)

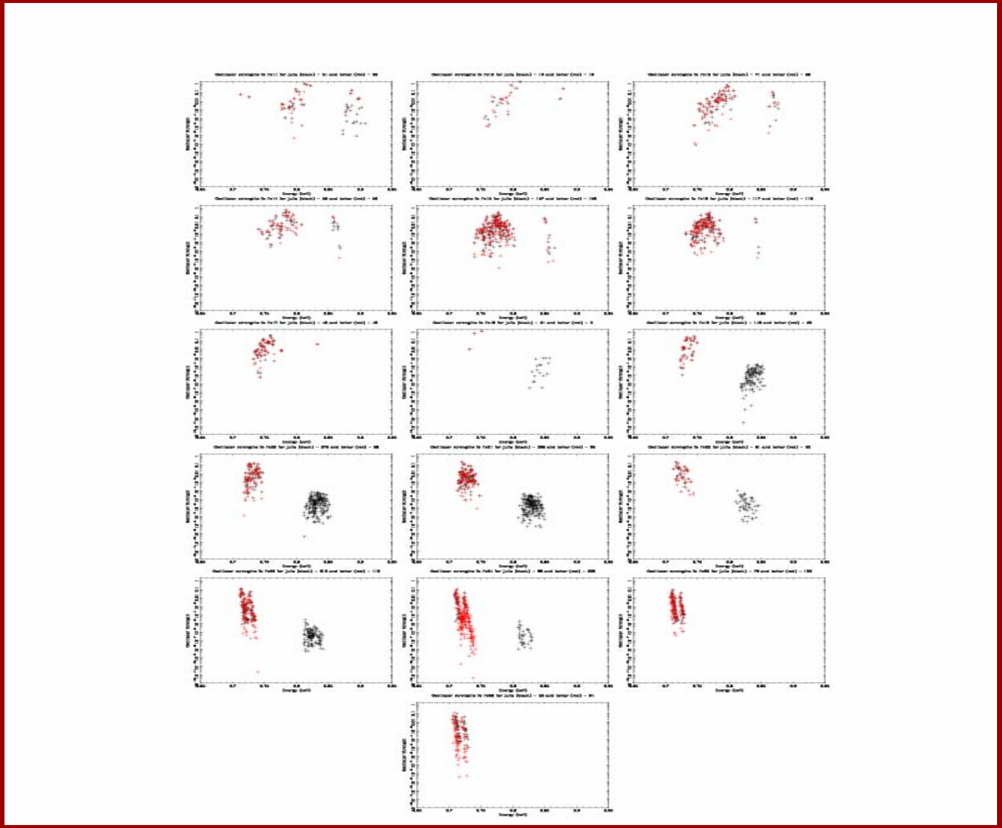
- ❖ Absorption measurements; wavelengths and oscillator strengths
- ❖ Particularly needed:
  Inner-shell lines
- ❖ Ionization balance and line emission measurements are also possible
- ❖ High laboratory densities might still hinder direct application to astrophysics



Bailey, Cohen, Chandler, et al. 2001

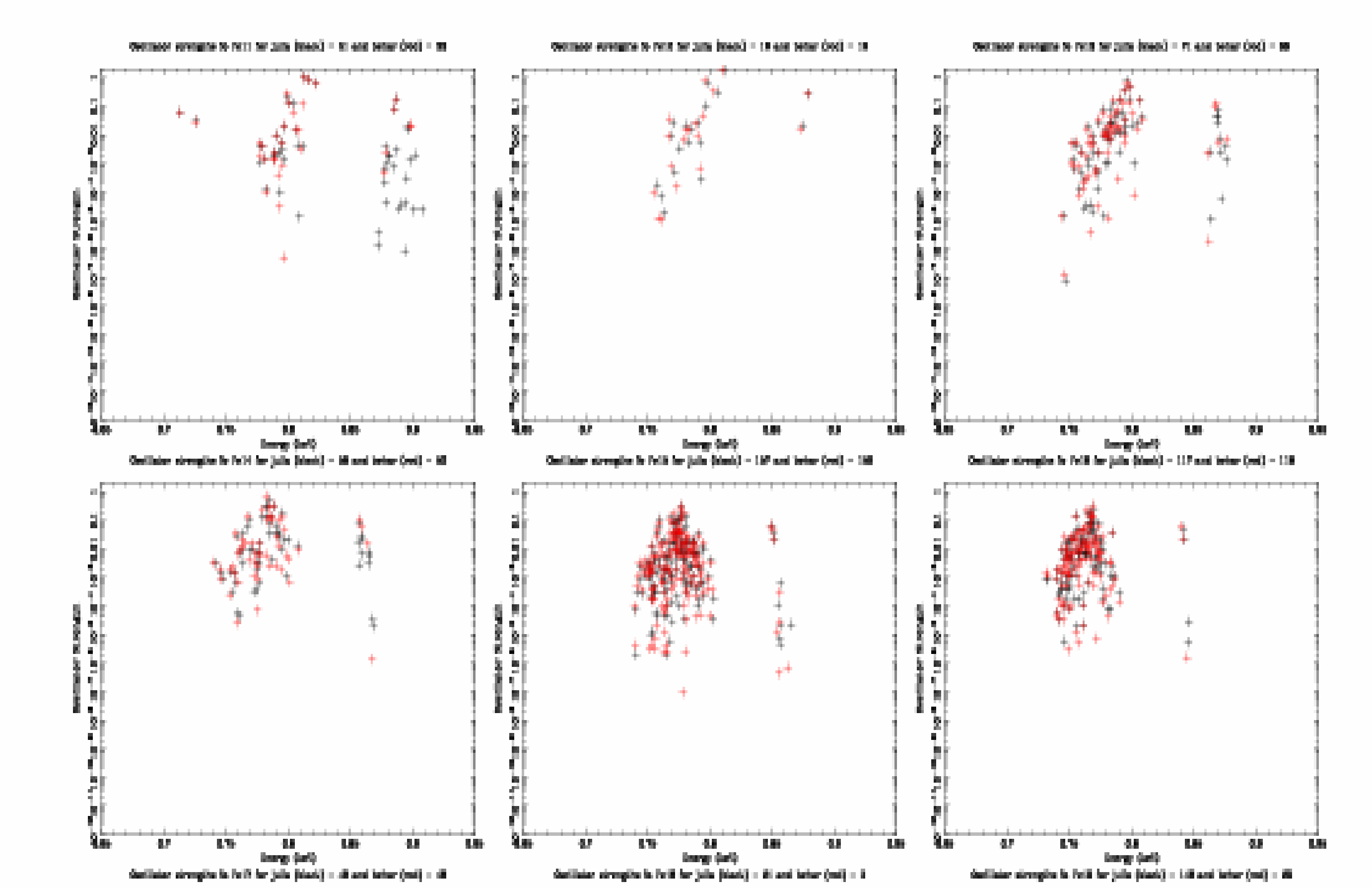
Inner-Shell Absorption (cont.)
Fe M-shell 2p-3d UTA

- Comparison between the HULLAC and FAC atomic codes shows fair agreement in line energies and oscillator strengths for Fe I – Fe XVI



(courtesy of
Adrian Turner)

Fe M-shell 2p-3d UTA (cont.)



courtesy of Adrian Turner

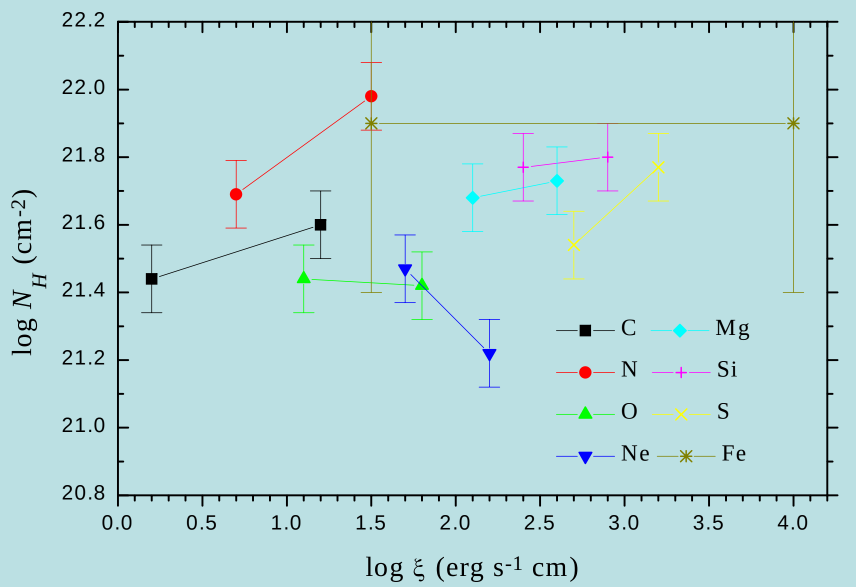
Type II AGN (cont.)
Measuring Elemental Abundances

- Vertical offsets in plot of N_H as a function of the ionization parameter ξ, as deduced from the measured *ionic* column densities N_i , reveal the *relative* elemental abundances

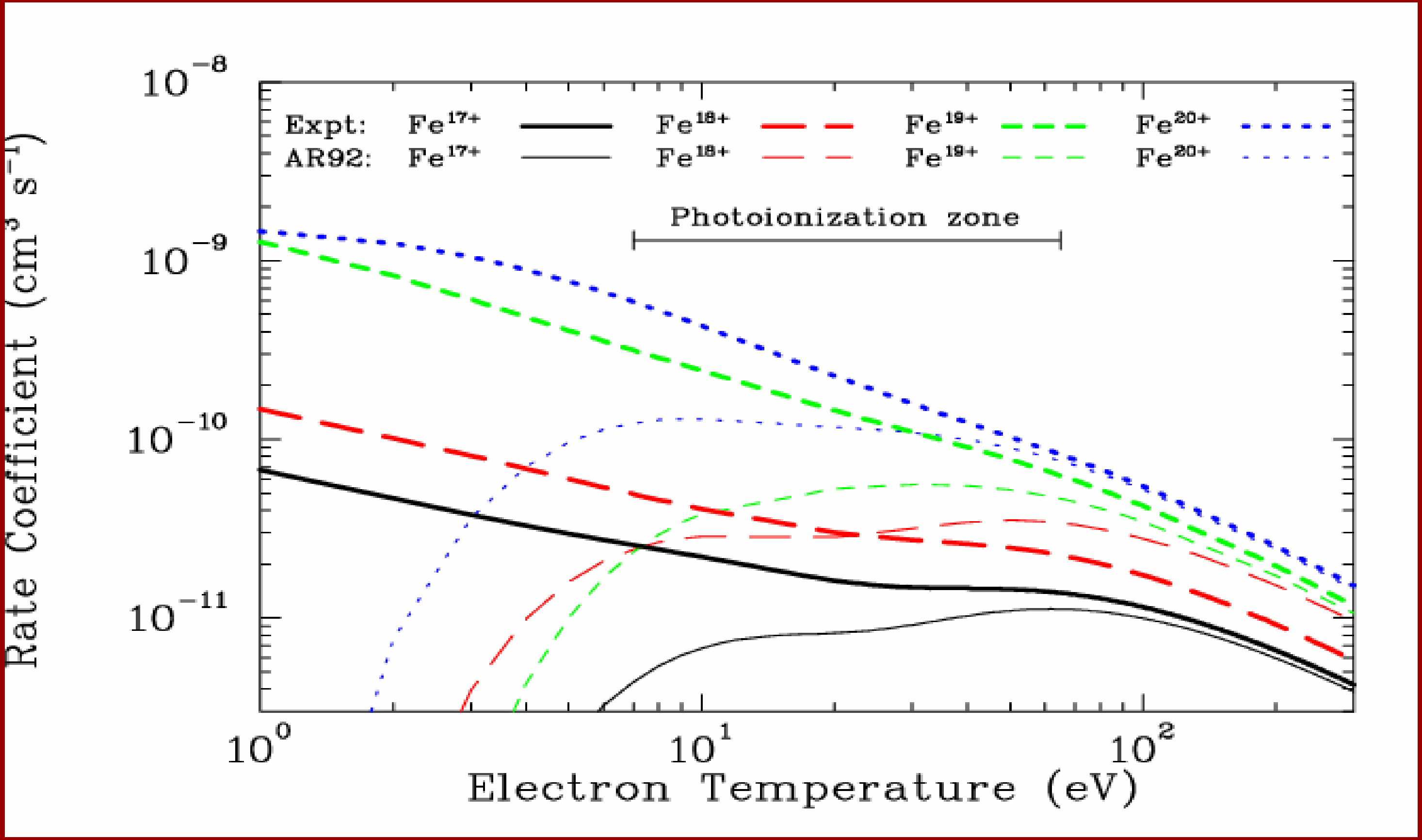
$$N_H = {N_{i,z}} \Big/ f^{+q}(\xi_{\max}) A_Z$$

- Need f^{+q} and ξ_{max}
- Fe-L analysis to be completed (A. Kinkhabwala - tomorrow morning)

NGC 1068; Brinkman, Kaastra, van der Meer et al. 2002



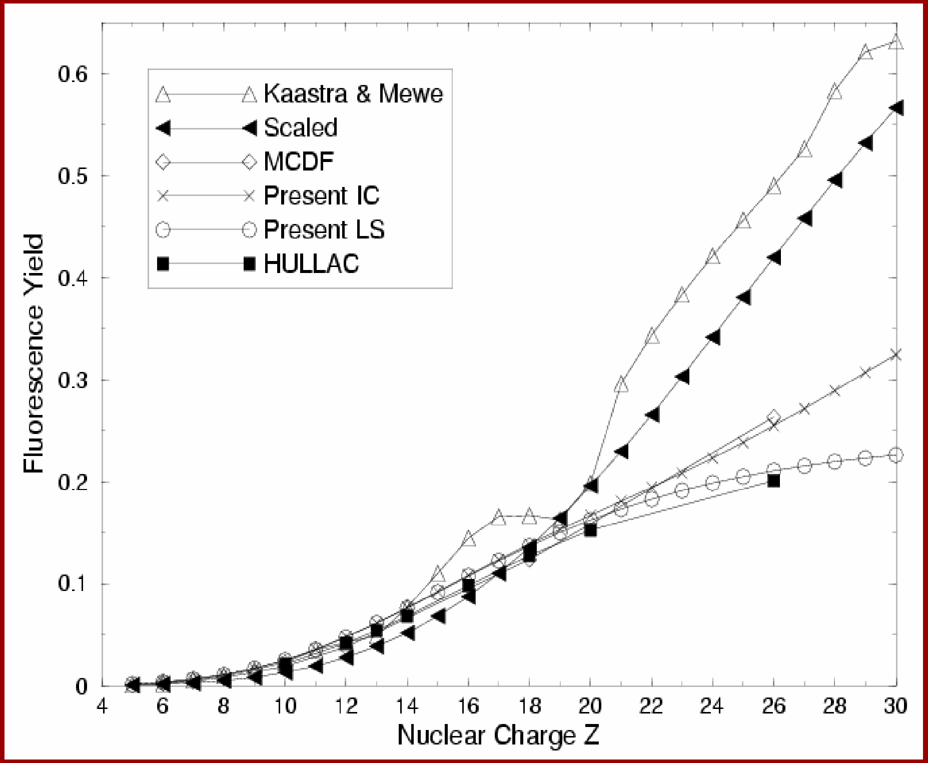
Low-T DR of Fe-L



Courtesy of Daniel Savin

Photoexcitation-Autoionization

- New level-by-level calculations enable re-evaluation of fluorescence yields (Gorczyca, Kodituwakku, Korista et al. 2002)
- Note that effect on ionization balance could be spectrum-dependent and complex



Conclusions

- The acquired high-resolution spectra from *Chandra* and *XMM-Newton* gratings need to be matched with equally high-quality atomic data.

- For x-ray *collisional plasmas*, most of the atomic data are satisfactory, allowing for high precision measurements of EM structures, abundances, densities, and UV effects.
- PLEASE USE SPECIAL CAUTION with 2p-3s LINE INTENSITIES, NON-Fe L-SHELL IONS, and the IONIZATION BALANCE.

- For x-ray *photoionized plasmas*, atomic data allow for sound measurements of outflow velocities, temperatures, column densities, and abundances.
- PLEASE USE SPECIAL CAUTION with
  INNER-SHELL LINE WAVELENGTHS (especially low-Z),
  the IONIZATION BALANCE (density & location),
  and FLUORESCENCE YIELDS.

Questions ?

The Tale of Fe^{16+}: What’s the matter with the 2p-3s lines?

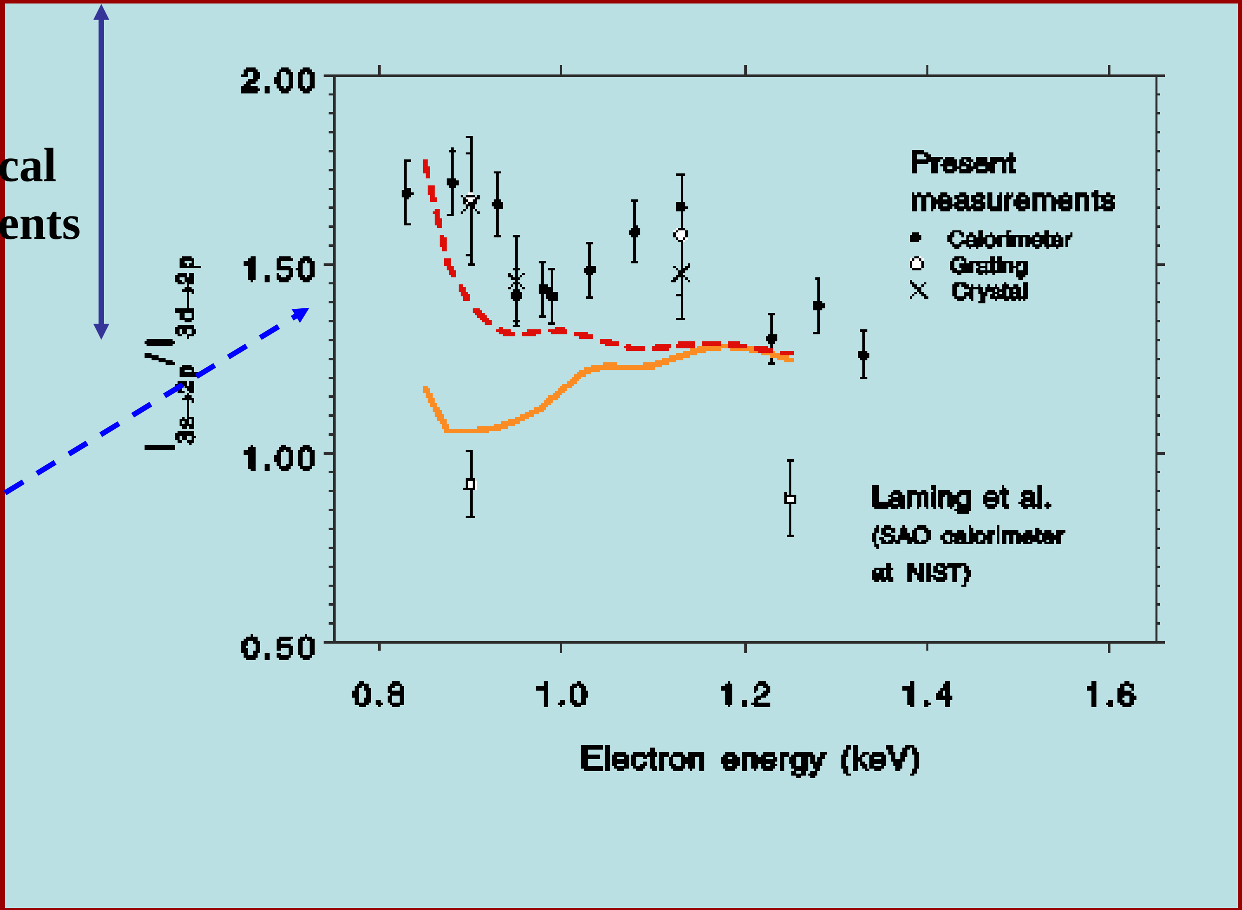
- It was pointed out by Laming et al. that EBIT-NIST measured 2p-3s / 2p-3d line ratios at high energies (> 0.9 keV) are consistent with calculations for direct collisional excitation (DE), while being discrepant with astrophysical observations.
- The agreement with theory seemed to be consistent with the assumption (based on calculations by Chen & Reed, Goldstein et al.) that resonant excitation (RE) is negligible at the high beam energies of EBIT.
- For real (Maxwellian) plasmas, it was shown (Doron & Behar) that DR (and RE) processes enhance the line ratios at high (low) *T*, which could explain most observations.
- New calculations (Chen & Pradhan, Gu) yield higher RE rates, including at high energies.
- Very recent EBIT-LLNL measurements of this ratio by Beiersdorfer et al. give much higher values than those of EBIT-NIST.

The Tale of Fe^{16+}: What’s the matter with the 2p-3s lines?

Low-T_e with RE (D&B)

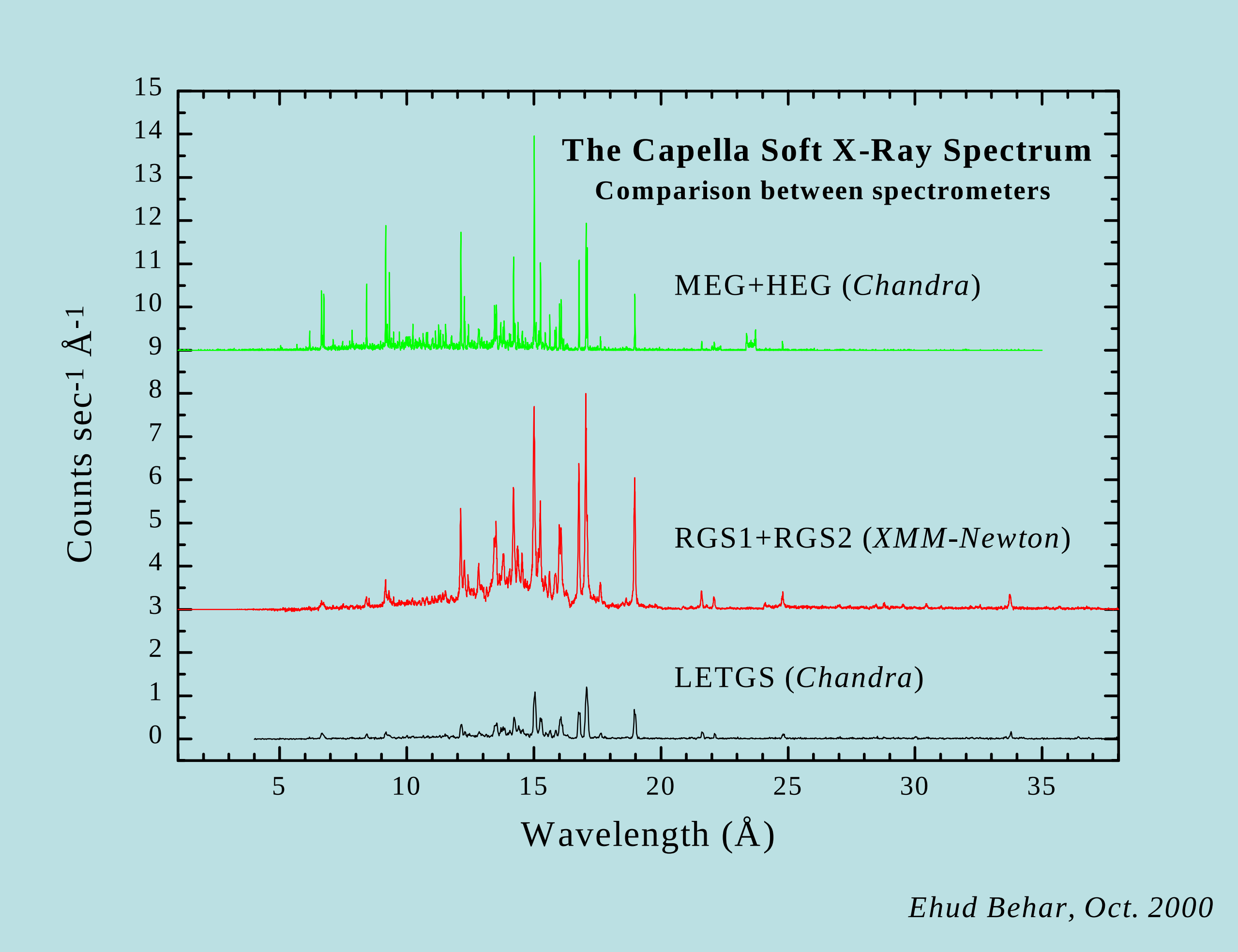
Various astrophysical measurements

High-T_e with DR ~ 40% effect (Doron & Behar)



Beiersdorfer, Behar, Brown et al. 2002

Stellar Coronae (contd.)



QUOTES ON UNCERTAINTIES IN THE Fe L-SHELL

- Kaspi et al. (2000, ApJL 535, L17) on the Seyfert 1 NGC 3783

  "…oscillator strengths for the various iron L-shell lines are not well known and there is no standard published data set."
- Sako et al. (2000, ApJL 535, L17) on the HMXB Vela X-1

  "The exclusion of iron L-shell ions leads to a great simplification in the spectral fit."
- Finoguenov et al. (1999, ApJ 514, 844) on the Galaxy NGC 5846

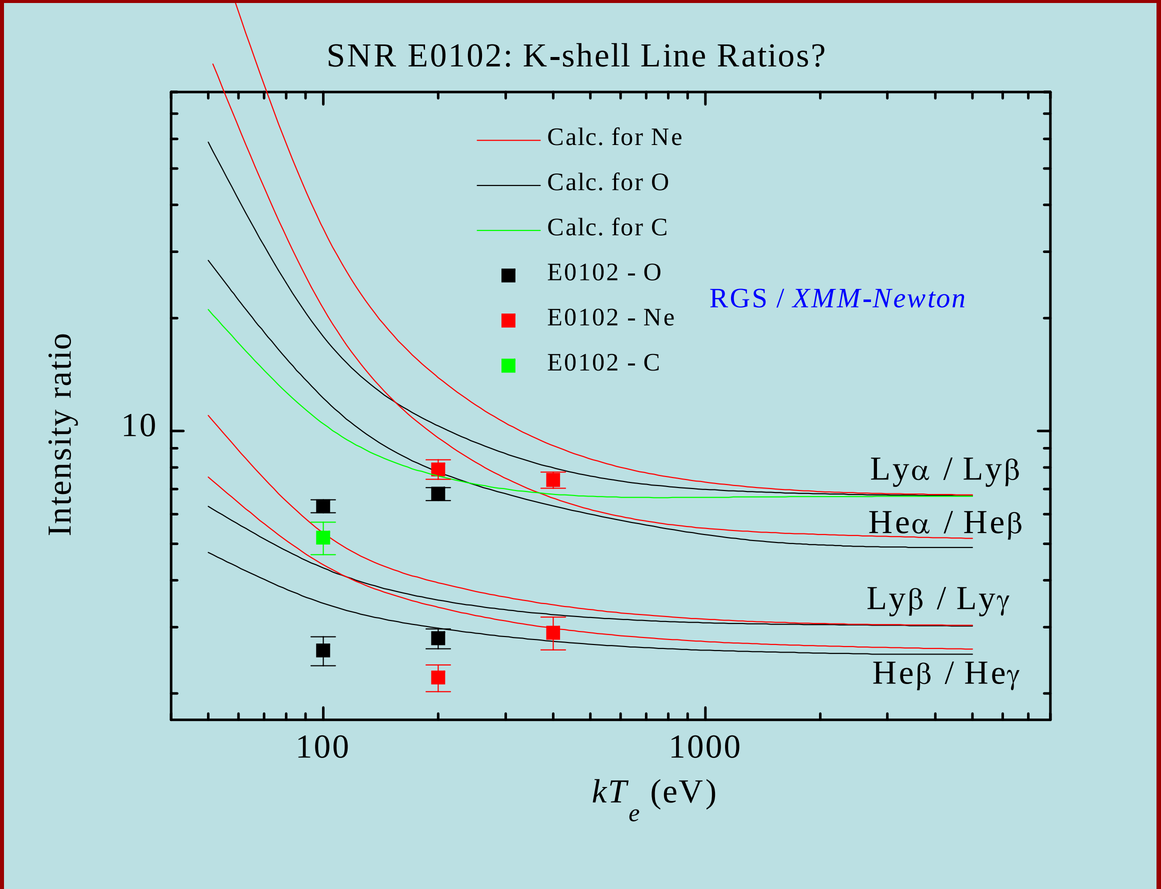
  "…possible uncertainties in the iron L -shell modeling."
- Harrus et al. (1997, ApJ 488, 781) on the SNR W44

  "…although we are wary of this result because of uncertainties in the atomic physics of iron L-shell emission."
- Masai (1997, A&A 324, 410) on X-ray spectral analysis

  "The atomic processes involved with K-lines are less uncertain than those with the L-lines."

- We would like to:
  - Show that there are no uncertainties in the iron-L emission line spectrum
  - Point out a few inaccuracies in the iron-L emission

SNR E0102: Anomalous Lyman Line Ratios?



Rasmussen, Behar, Kahn, et al. 2001