

*Atomic Physics for X-ray  
Astronomy: A Primer*

*Randall K. Smith*

*Chandra X-ray Center*

# Introduction

## Some Simplifications:

- **Atoms only:** Molecules (and dust grains) are only observable in absorption X-ray spectra with difficulty.
- **No nuclear transitions:** By definition these are  $\gamma$ -rays.
- **No three-body transitions:** Except in the densest regions, these are astrophysically unimportant.
- **No metal-metal collisions:** Densities are such that even He-atom collisions are unimportant.
- **No neutral plasmas:** Most X-ray emitting plasmas are at least partially ionized, so  $n_e \approx n_H$

# Important Processes In X-ray Plasmas

- Ionization
  - Electron/Proton Collisions
  - Photoionization
  - Innershell ionization
- Recombination
  - Radiative
  - Dielectronic
  - Charge Exchange
- Excitation/De-excitation
  - Electron/Proton Collisions
  - Photoexcitation
  - Radiative Decay

# Energy Levels

## Grotrian diagram for He-like Fe XXV

Some points to notice:

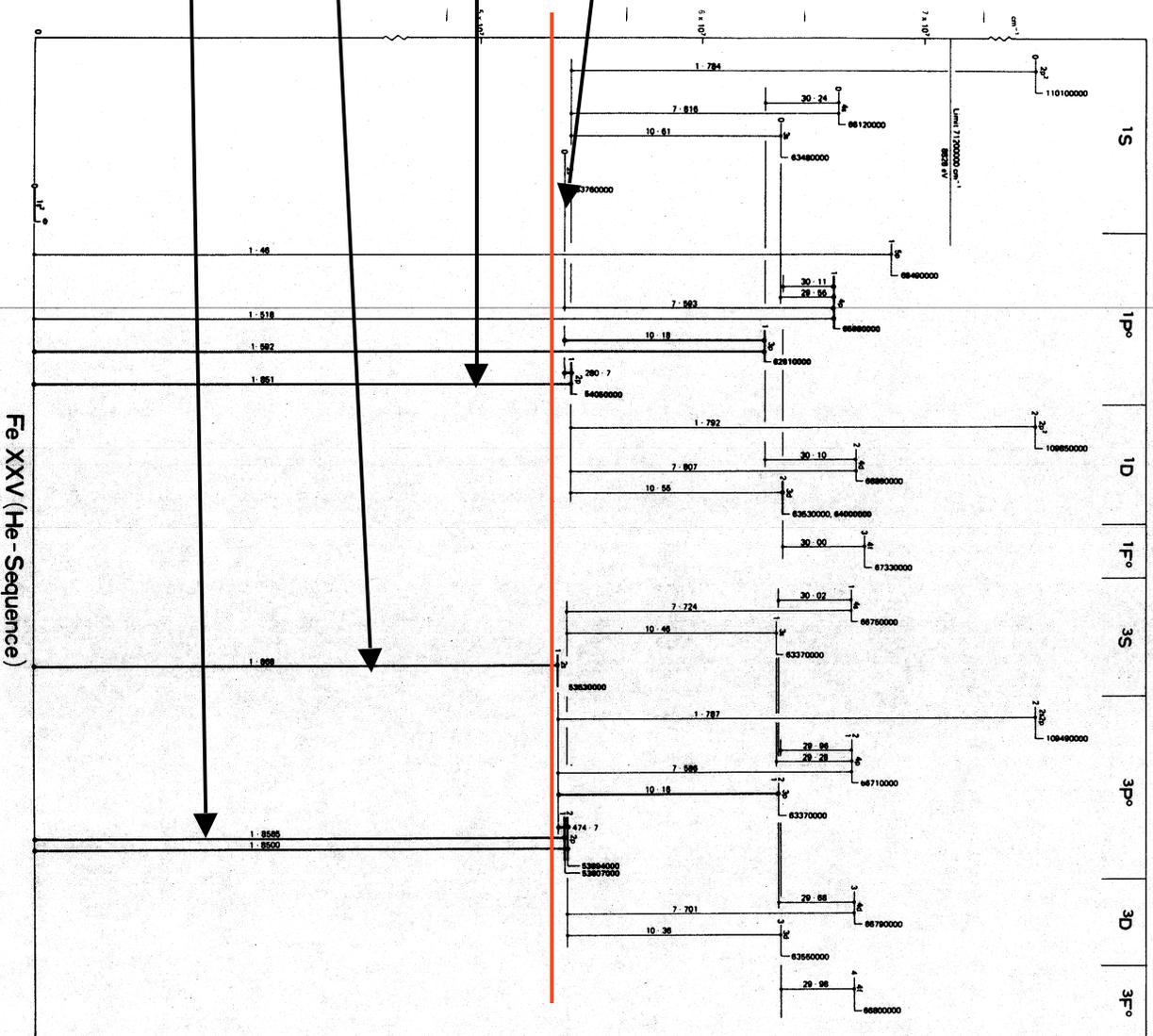
$n = 2$  level

Two-photon

Resonance line

Forbidden line

Intercombination line(s)

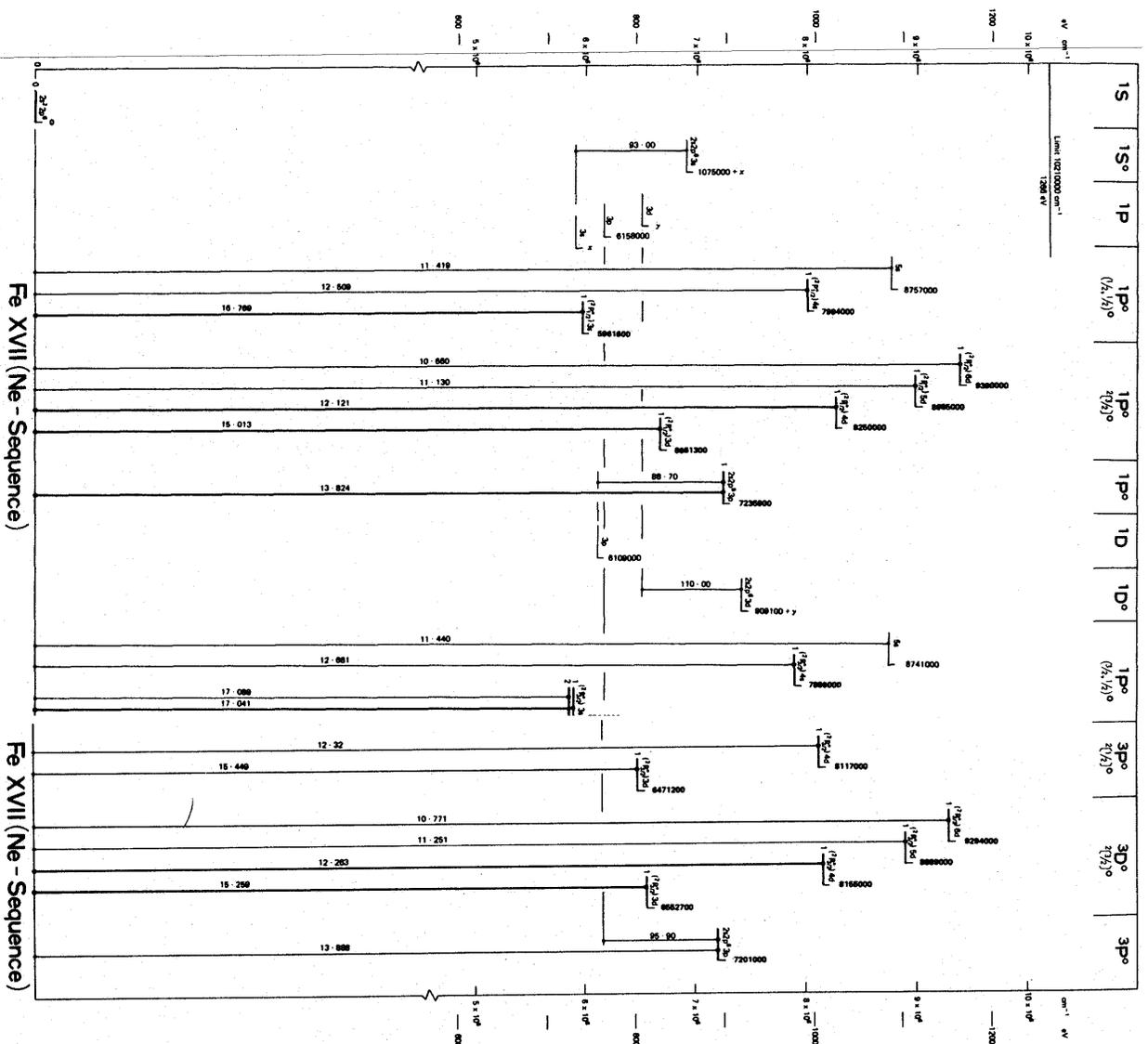


# Energy Levels

Of course, with more complex ions, the diagram becomes more complex.

In many cases, it is impossible to measure all of these levels in the lab.

But the level energies (and thus wavelengths) can be inferred indirectly from other wavelengths.



## Energy Level Descriptions

Energy levels are most frequently given in LS-coupling :

$$n_1 l_1 \quad n_2 l_2 \quad \dots \quad 2S+1 L_J$$

H-like:  $1s \quad {}^2S_{1/2}, 2p \quad {}^2P_{1/2}, 2p \quad {}^2P_{3/2}, 4d \quad {}^2D_{5/2}$

He-like:  $1s^2 \quad {}^1S_0, 1s2p \quad {}^1P_1, 1s2p \quad {}^3P_2, 1s4d \quad {}^3D_3$

However, when atoms become more complex, this simple system breaks down. Sometimes both the core structure and the outer electron structure is given, as in :

O-like:  $1s^2 \quad 2s^2 \quad 2p^4 \quad {}^3P_2, 2s^2 2p^3 ({}^4S) \quad 3s \quad {}^5S_2, 2s^2 2p^3 ({}^2D) \quad 3d \quad {}^1F_3$

## Wavelengths

### How do we identify emission lines?

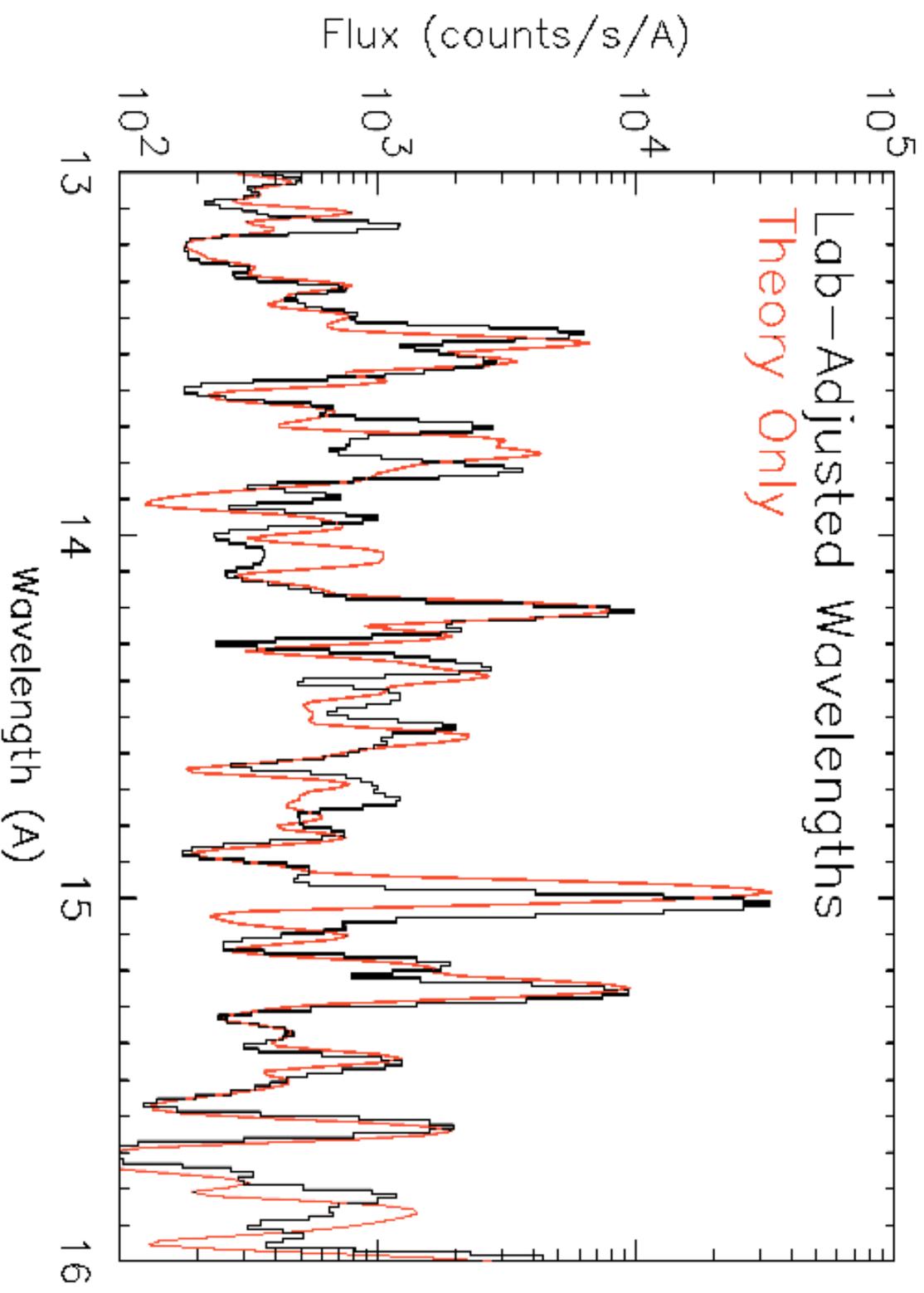
Wavelengths present a difficult problem. Unless the analysis is done line-by-line, there is currently no way to include wavelength errors (even if they are available) automatically.

How good are theoretical wavelengths? It depends on the ion involved, but in general 1% is a reasonable number.

Theoretical wavelengths are derived from the energy levels (the inverse of the lab method, where energy levels are derived from the measured wavelengths). It is possible to adjust theoretical energy levels to match lab wavelengths and thus improve all the wavelengths, measured or not.

## Wavelengths

Laboratory measurements are necessary!



## Electron/Proton Collisions

Inherently, electron/proton collisional excitation is a three (or more) body process, although it does not appear to be:



Of course, the ion I actually has at least 1 electron, and likely more. As a result, the atomic calculations of the cross section for these processes are non-trivial and subject to significant errors (30% is common).

## Electron/Proton Collisions

Usually, the cross section is written as a dimensionless quantity called the “collision strength” (which is a function of energy, as well as lower energy level  $i$  and upper energy level  $j$ ):

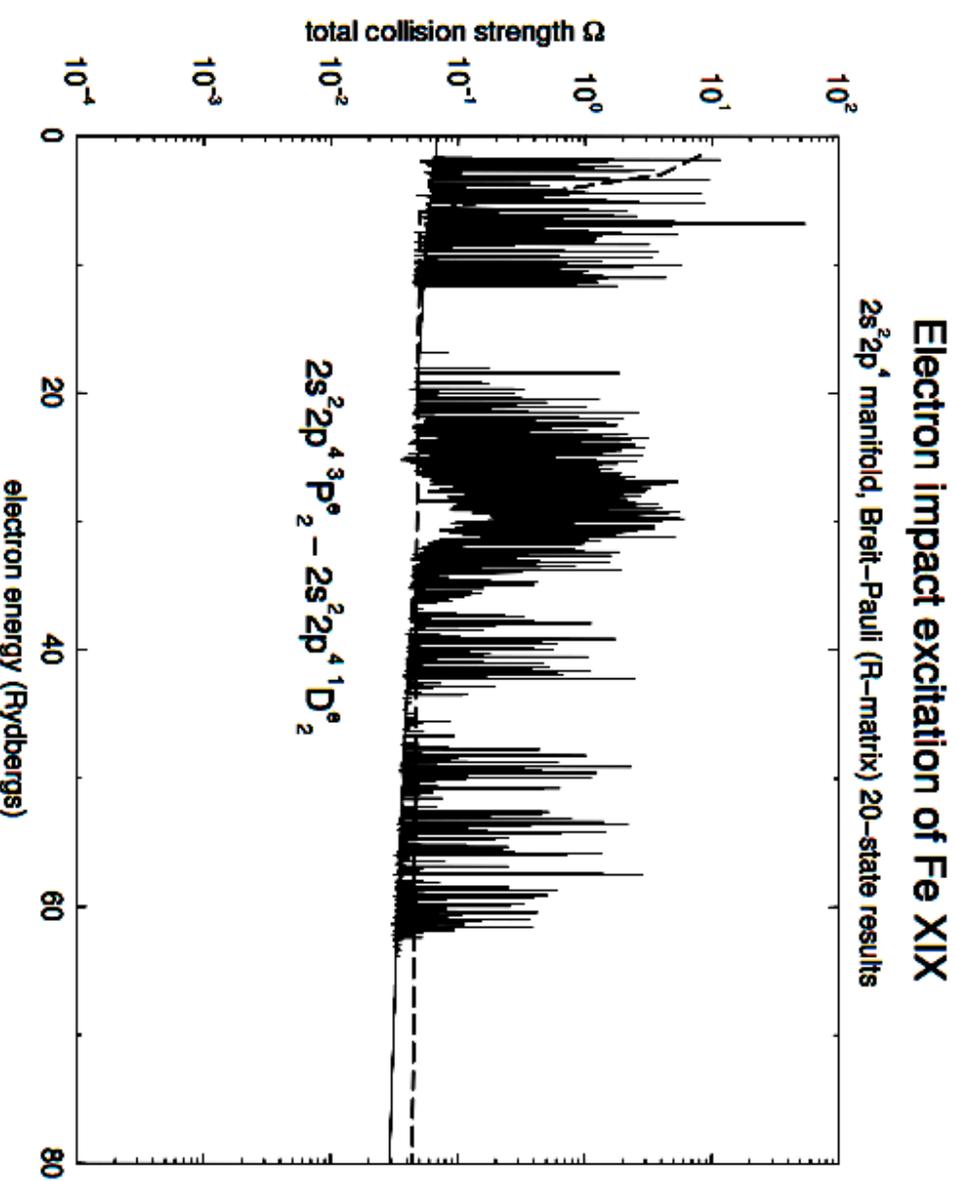
$$\Omega_{ij} = \frac{4\pi\omega_i}{\lambda^2} Q(i \rightarrow j)$$

This can be (and usually is) integrated assuming a Maxwellian velocity (*i.e.*, energy) distribution:

$$\Upsilon(T) = \int_0^\infty \Omega_{ij} \exp\left(-\frac{\Delta E_{ij}}{kT}\right) d\left(\frac{\Delta E_{ij}}{kT}\right)$$

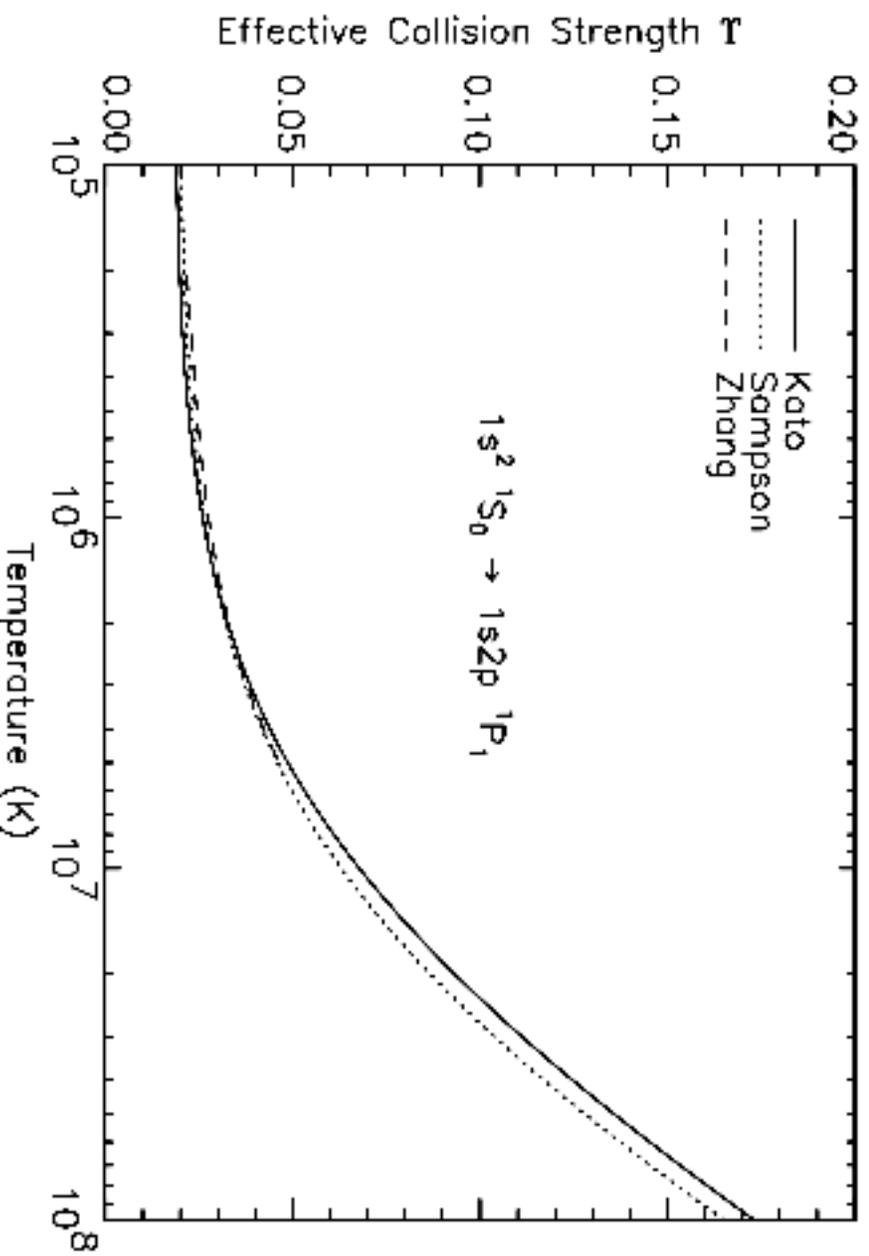
## Electron/Proton Collisions

Shown here is a calculated excitation collision strength for Fe XIX, using two different methods :



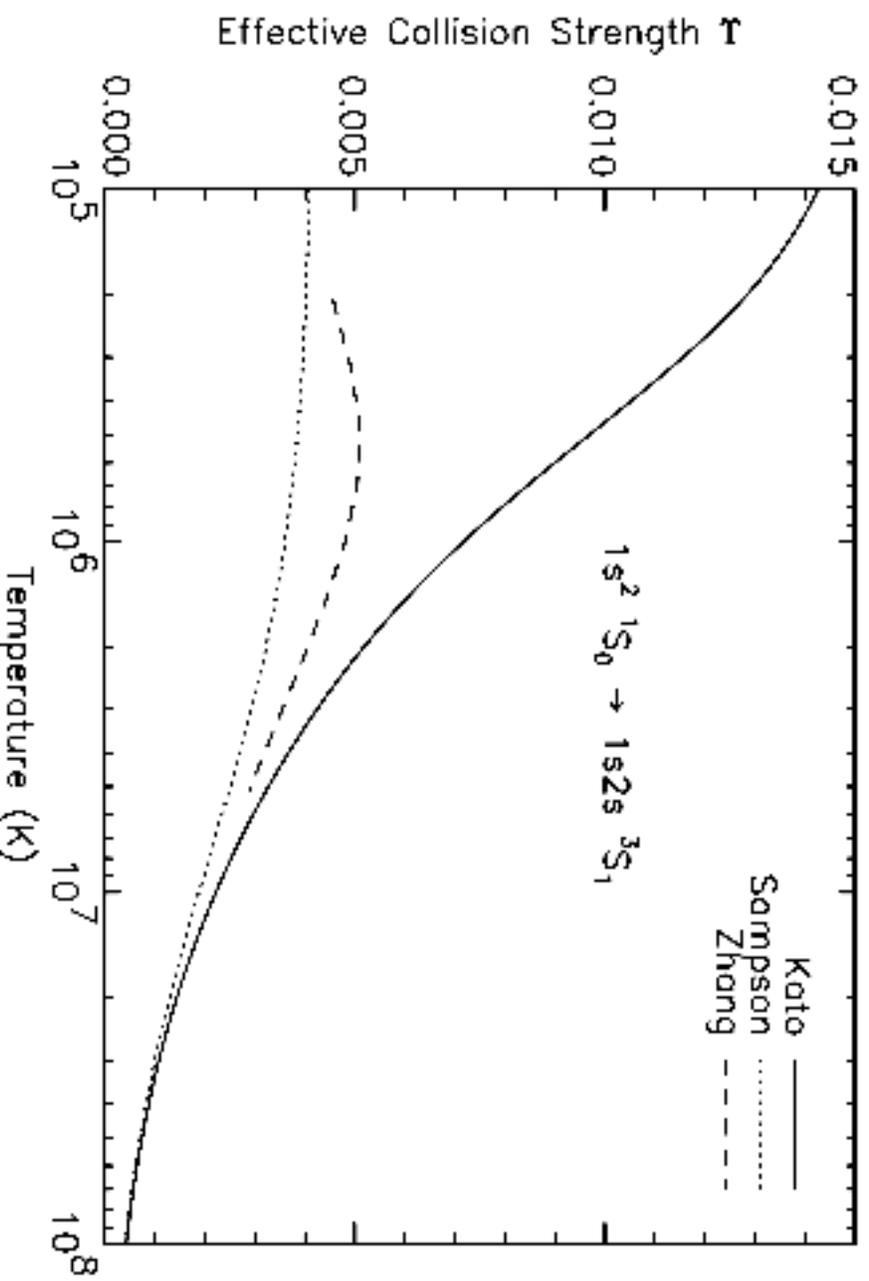
## Electron/Proton Collisions

Resonances such as those shown in the previous calculations may be significant or not, depending upon the “type” of transition. For resonance (allowed) transitions, ironically, resonances are not particularly important:



## Electron/Proton Collisions

Resonances (which occur near the transition energy, and thus are more important at lower temperatures) are more important for forbidden transitions:



## Electron/Proton Collisions

Just what **is** a resonance, in this terminology? It refers to a specific energy where the excitation cross section is enhanced. This is commonly due to some autoionizing level that is briefly populated by the colliding electron:



The electron excites the ion into a doubly-excited state, but then detaches itself before any further decay happens, leaving the ion in a singly-excited state. It is therefore a more important process for forbidden levels, where decay times are larger.

## Electron/Proton Collisions

Conveniently, there are some high-energy extrapolations for electron collisions. Burgess & Tully (1992) compiled these results:

- Electric Dipole:  $\sigma(E \rightarrow \infty) = c \ln(E)$
- Multipole:  $\sigma(E \rightarrow \infty) = c$
- Spin-change:  $\sigma(E \rightarrow \infty) = c / E^2$

This particular feature of atomic physics has been used by the Chianti group in fitting collision strengths, guaranteeing proper extrapolations to high energy.

## Electron/Proton Collisions

**And now for some words on Proton collisions.**

In equilibrium, since protons are 1836x more massive than electrons, their speed will be  $\sim 43x$  slower than that of electrons. As a result, the collision rate  $\langle n \langle v \rangle \rangle$  for protons will be much lower. In addition, protons are positively charged, as are ions, so that also means small impact parameter (high momentum transfer) collisions are suppressed.

As a result, proton collisions can *usually* be ignored - except for low-lying transitions within an ion's ground state, which can be excited by proton collisions.

## Radiative Transitions

Transition rates (a/k/a “Einstein A values”) are not as important in X-ray spectroscopy as they are in other fields, since only a subset of X-ray plasmas are photoionized.

Transition rates for allowed X-ray transitions are large; typical values are  $10^{10}$  -  $10^{14}$  s<sup>-1</sup>. In general, the rates increase with proton number Z.

Forbidden transitions can have *much* smaller values; the O VII  $1s2s\ ^3S_1 \rightarrow 1s^2\ ^1S_0$  transition is only  $\sim 1000$  s<sup>-1</sup>.

Transition rate data are available on WebGUIDE:

<http://obsvis.harvard.edu/WebGUIDE>

## Charge Exchange

Charge exchange is a process where an atom gives up an electron to a nearby ion, usually into an excited state.

In an astronomical context, the neutral ion is almost always hydrogen (helium is the only other real possibility), and that limits the importance of charge exchange to those regions where neutral hydrogen coexists with X-ray-emitting gas.

An example of such a region is the solar wind, which has plenty of highly ionized carbon and oxygen. This can charge exchange with neutral hydrogen in the solar system and lead to possibly significant emission. At low temperatures ( $kT < 50$  eV) charge exchange may also significantly affect the ionization balance.

## Inner-shell Excitation

Electrons from an “inner” shell may be collisionally excited as well. In some cases this is unremarkable; in Fe XIX,



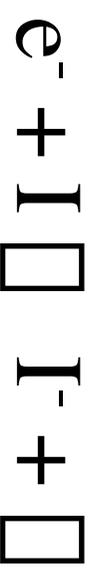
could be called a innershell excitation. It decays with a 106.3 Å photon but it isn't incredibly significant. However, some transitions are more important:



This excitation in Li-like ions creates a photon called the  $q$  line, which appears between the resonance and forbidden lines in the same ion's He-like system. Seeing this line shows that there is a noticeable amount of Li-like ion in the plasma.

## Radiative Recombination

Radiative recombination occurs when an electron collides with an ion and becomes bound, emitting a photon in the process:



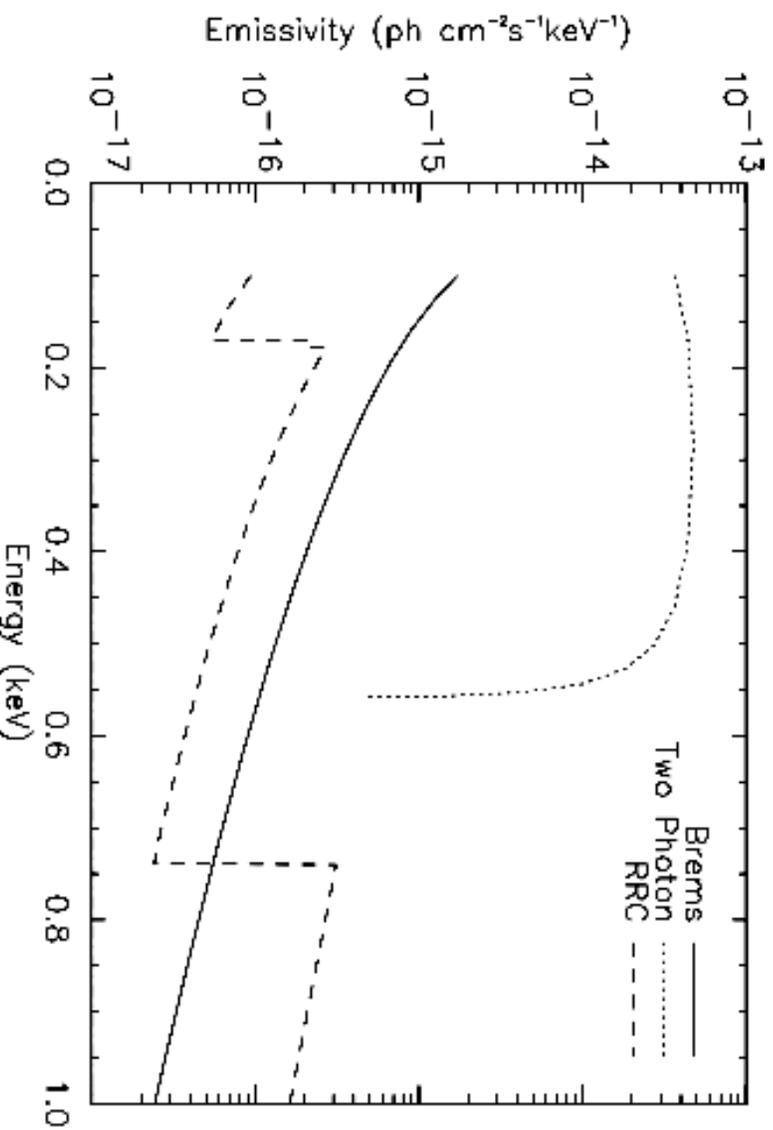
Consider the energy balance in this interaction. Even if the electron has zero velocity, it has a certain binding energy  $E_i$  in the  $I^-$  ion. So the emitted photon has a minimum energy  $E_i$ , plus whatever energy the electron had to begin with.

This process creates a continuum of emission, bounded at one end, called the **Radiative Recombination Continuum (RRC)**.

# Radiative Recombination

In many cases the RRC is weak, but it is an excellent diagnostic if it can be measured. The power emitted per keV is:

$$\frac{dP}{dV d\omega} = \frac{dP}{dE} = n_e n_{Zj+1} E_\gamma \sigma^{rec}(E_e) n_e \frac{f(\nu) d\nu}{dE_\gamma} \quad \text{Tucker \& Gould 1966}$$



Sample  
O VII  
(collisional)  
continuum

## Dielectronic Recombination

When an ion recombines dielectronically, two electrons are involved. The first electron recombines and is bound to the atom. Unlike RR, where the energy balance is maintained via an emitted photon, in DR a second electron is excited as well, putting the ion in a “doubly-excited” or “autoionizing” state.

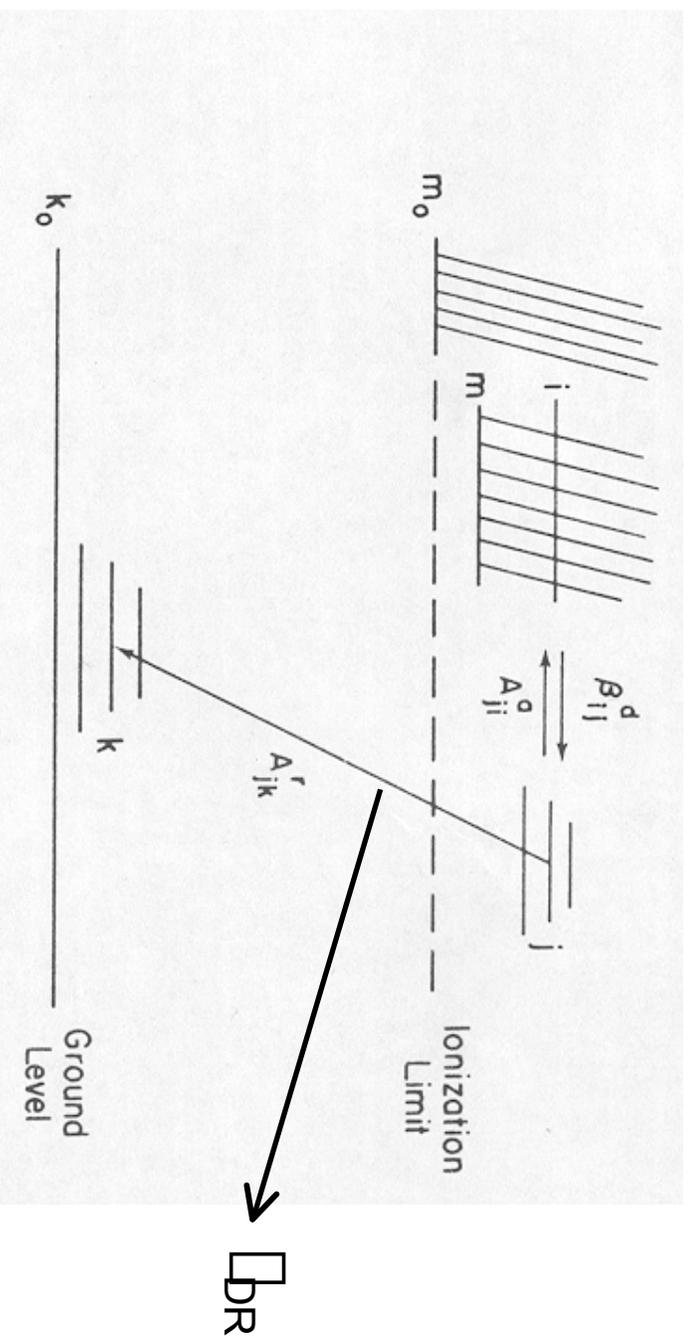
From there, it may ionize (resulting in either an elastic collision, or resonant excitation) or it may radiate, “relaxing” into a singly-excited state which then radiates as well.

Mathematically:



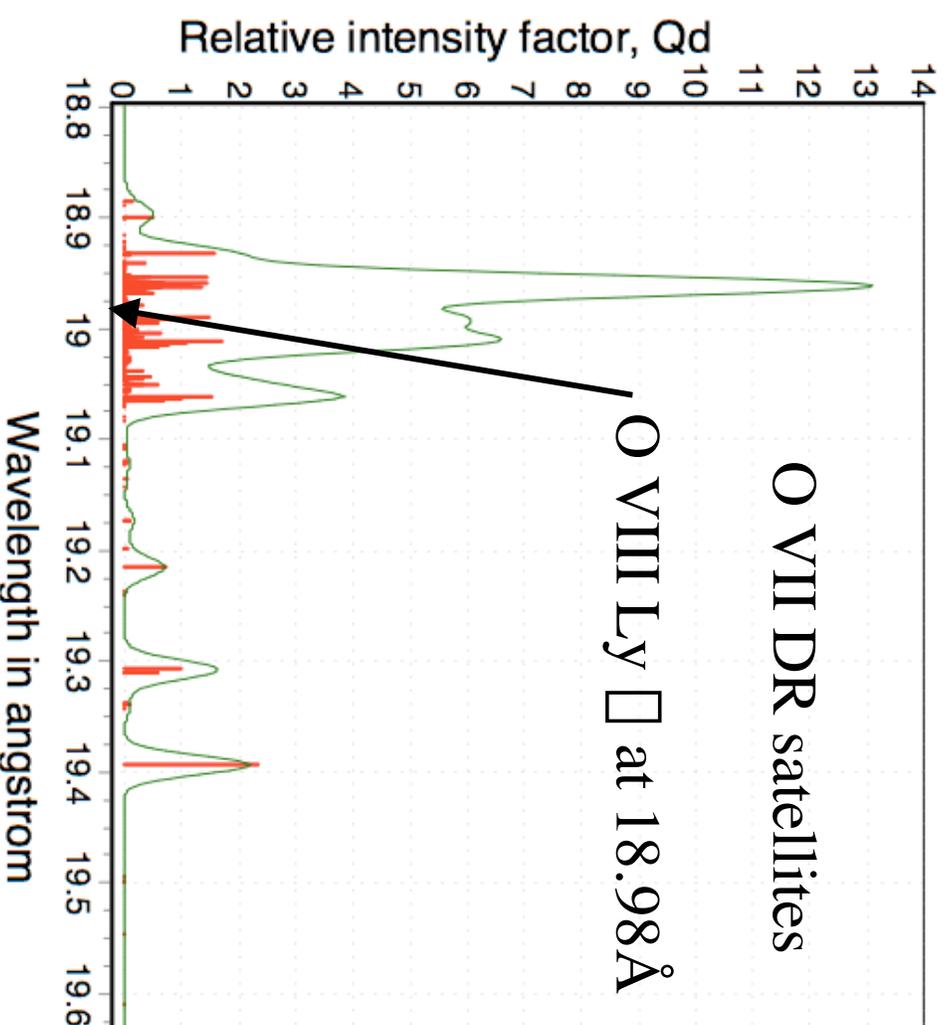
# Dielectronic Recombination

DR is a *resonant* process; the incoming electron must have an energy that matches that of the doubly-excited level, otherwise no transition will occur.



## Dielectronic Recombination

Photons emitted from the doubly-excited state are usually called “DR Satellite lines” because they are transitions made in the presence of an additional electron, so are shifted slightly to the red.



## Dielectronic Recombination

The dielectronic recombination rate for any given transition in a Maxwellian plasma is simply:

$$\text{Rate}_{\text{DR}} = n_{\text{I}^+} n_{\text{e}} Q_{\text{d}} \exp(-E_{\text{exc}}/kT) / g_{\text{l}}$$

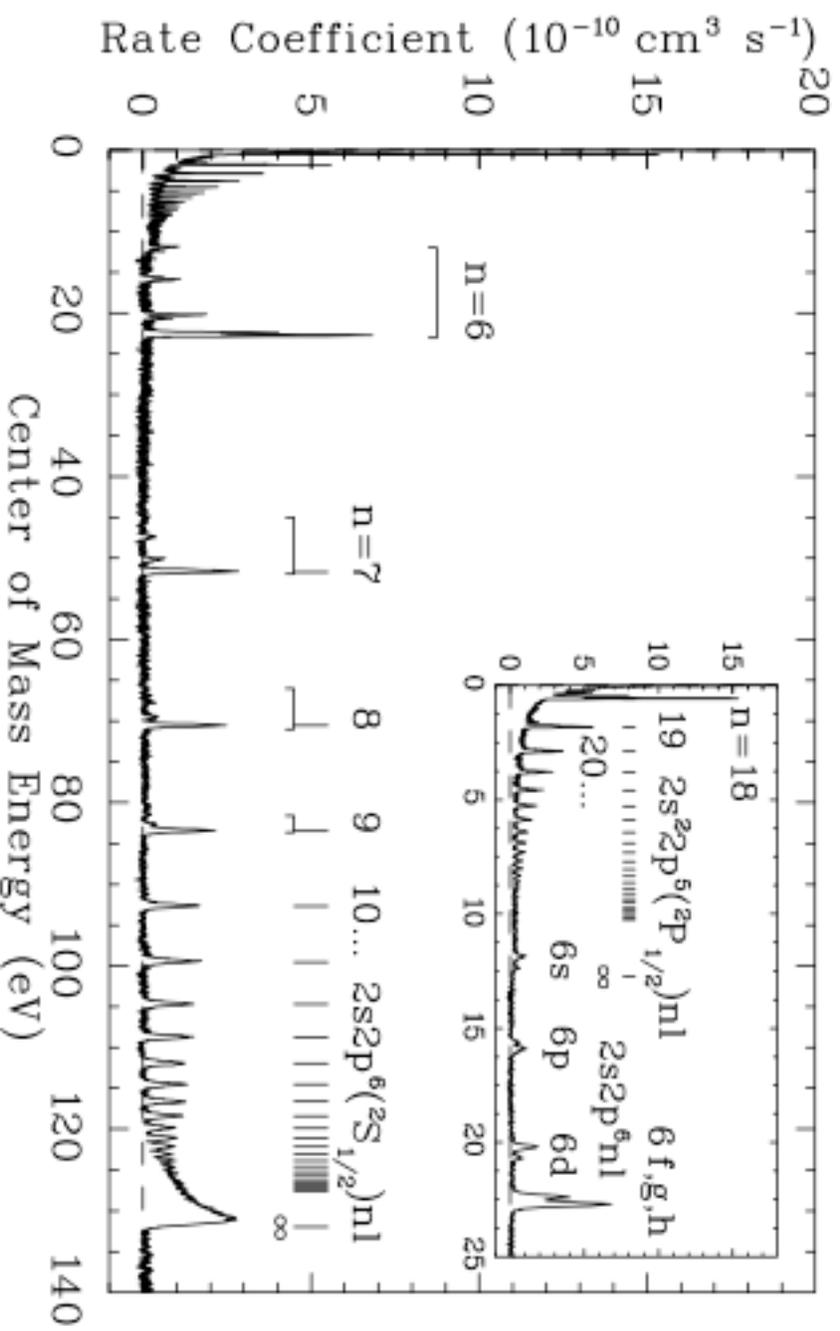
The two terms of note are  $Q_{\text{d}}$ , the total intensity, and  $E_{\text{exc}}$ , the excitation energy for the transition.

□  $n = 0$  DR transitions are those where the excited electron does not change principle quantum number  $n$ . As a result, its excitation energy will be very small.

□  $n = 1$  DR transitions are those where the excited electron does change principle quantum number  $n$ . As a result, its excitation energy will be large, on order the ionization energy.

## Dielectronic Recombination

Here is a laboratory measurement of  $\sigma_{n=0}$  DR on Fe XVIII (from Savin *et al.* 1999). Note the *resonances*, which are evident all the way down to 1 eV, despite the large ionization energy of Fe XVIII:



# Ionization

Ionization is a relatively simple process, with three main channels:



Photoionization and collisional ionization have been measured in the lab and theoretical calculations are relatively straightforward, so little attention is paid to them now.

## Inner-shell ionization

Innershell ionization is more exciting. Usually in the X-ray regime, it refers to a K-shell (a/k/a 1s electron) being removed.

At this point, the ion is very unstable. It will either emit a photon (radiatively stabilize) or an electron, called an Auger electron. If the ion has been photoionized, this is also called a “photoelectron” and the number of electrons emitted the “photoelectric yield”

Whether a photon or an electron is emitted depends upon chance and the ion involved. As  $Z$  increases, the probability of a photon being emitted increases; for iron, it is  $\sim 30\%$ . For oxygen, it is  $\sim 1\%$ .

Innershell ionization of Fe I - Fe XVI tends to emit a 6.4 keV photon, commonly called the “cold” or “neutral” iron line.

## Two Photon Transitions

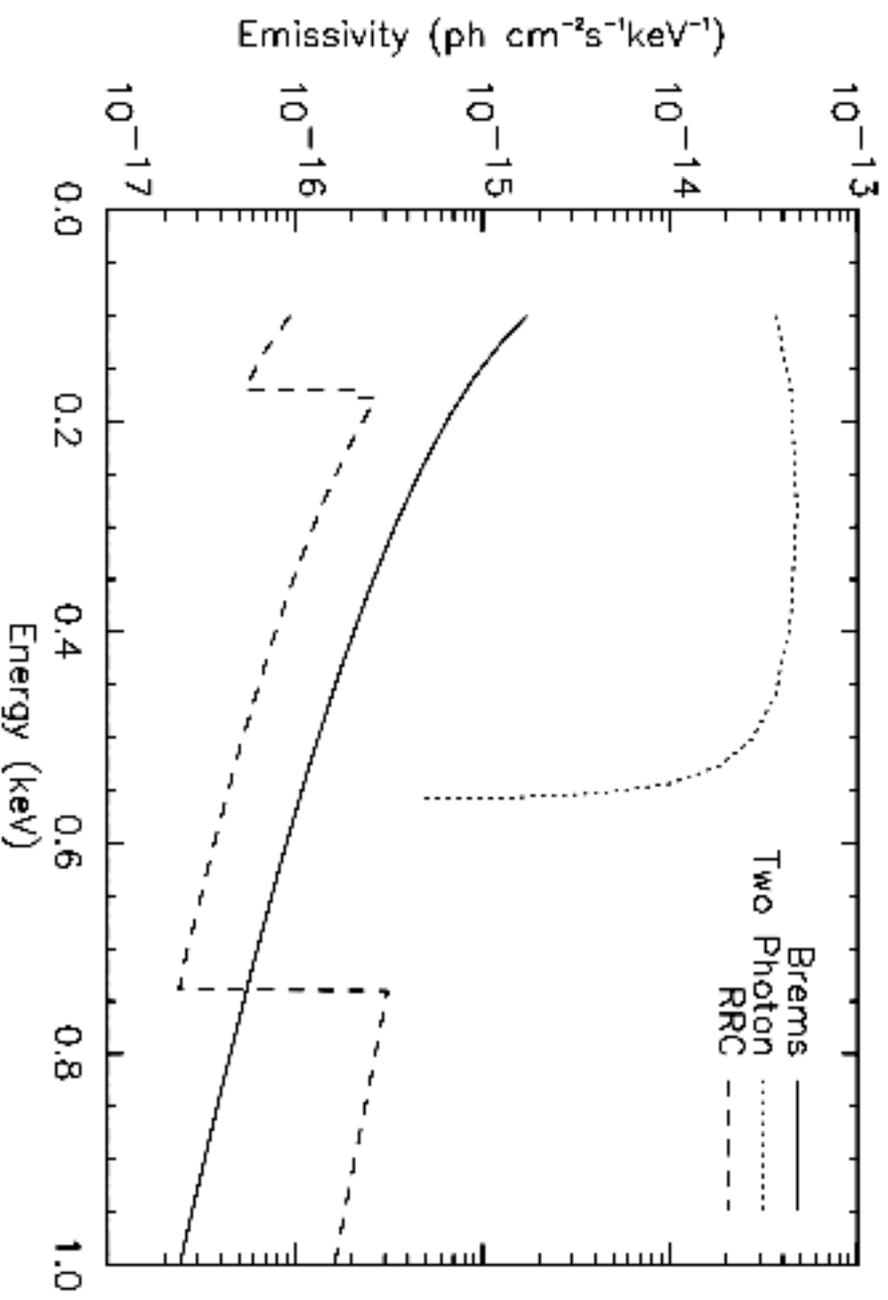
Some transitions are absolutely forbidden, and as a result transition via the so-called “two-photon” transition. The only two of importance for X-ray astronomy are:



Curious fact: The A values for these transition in Oxygen are 8425 and  $2.31 \times 10^6/s$ . The A value for the O VII “forbidden” transition is 1044/s! There is a two-photon transition from the forbidden level, but its A value is  $\ll 1/s$ .

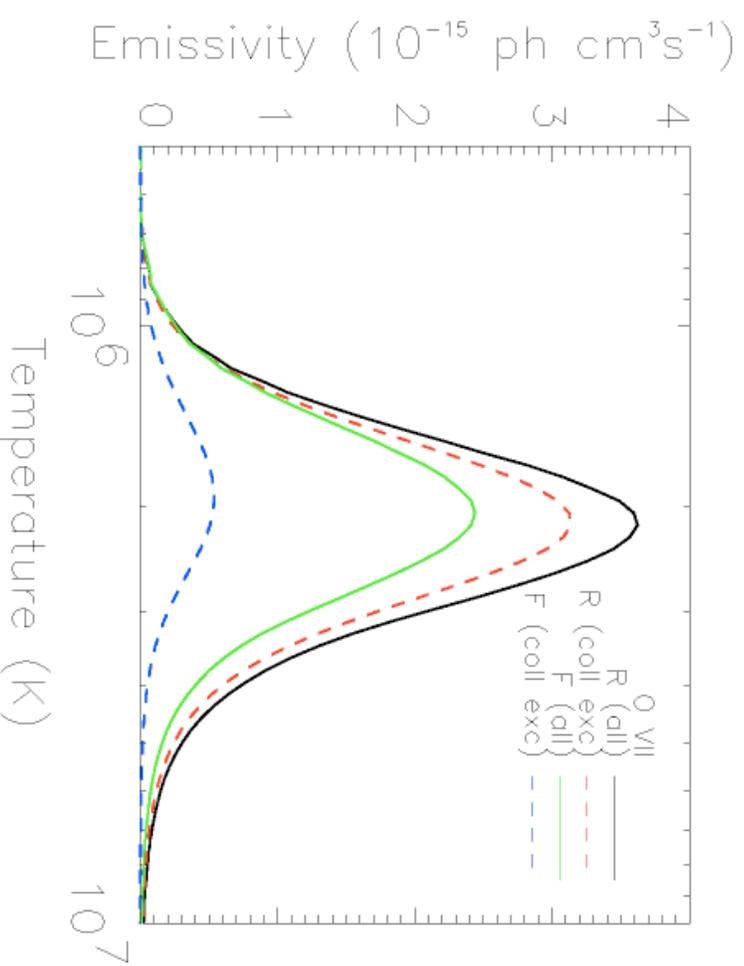
## Two Photon Transitions

The O VII two-photon transition :  $1s2s\ ^1S_0 \rightarrow 1s^2\ ^1S_0$



## Error Estimates

This is much easier for some transitions than others.  
The resonance line of O VII ( $1s2p\ 1P_1 \rightarrow 1s^2\ 1S_0$ ) is dominated by collisional excitation:



But the forbidden line of O VII ( $1s2s\ 3S_1 \rightarrow 1s^2\ 1S_0$ ) is **not** dominated by collisional excitation.

## Conclusions

### Basic Atomic Physics (for X-ray plasmas)

- Ionization (mostly easy)
  - Electron/Proton Collisions (i.e., “collisional plasma”)
  - Photoionization (i.e., “photoionized plasma”)
  - Innershell ionization (can emit photons)
- Recombination (harder)
  - Radiative (emits temperature-dependent continuum)
  - Dielectronic (dominates recombination; satellite lines)
  - Charge EXchange (comets; plasmas with neutral H)
- Excitation/De-excitation (harder)
  - Electron/Proton Collisions (resonances)
  - Photoexcitation (A values matter here)
  - Radiative Decay (emits observable photons!)