

The propagation of uncertainties in atomic data through collisional-radiative models

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Outline

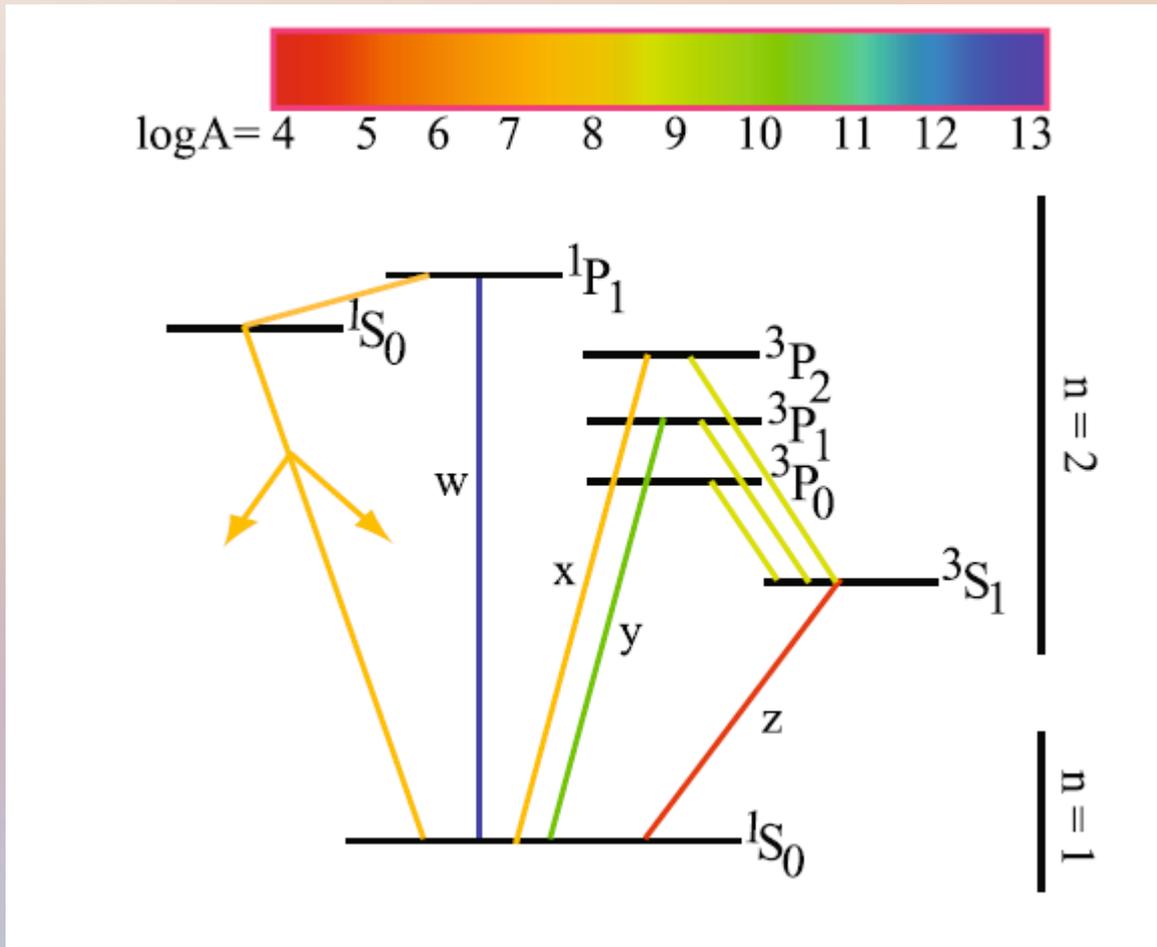
- The importance of having uncertainties on theoretical atomic data.
- The propagation of uncertainties through modeling codes.
- Our procedure for assigning uncertainties
 - Baseline uncertainties
 - Method sensitivity uncertainties
- O^{6+} results
- Future work

The importance of uncertainty estimates on fundamental atomic data

- The modeling community has been requesting for quite some time that atomic databases have an uncertainties associated with the data.
- This has been done for some processes, e.g. the NIST letter codes for spontaneous emission coefficients.
- However, for collision data there are very few systematic assessments of the uncertainties in theoretical data.

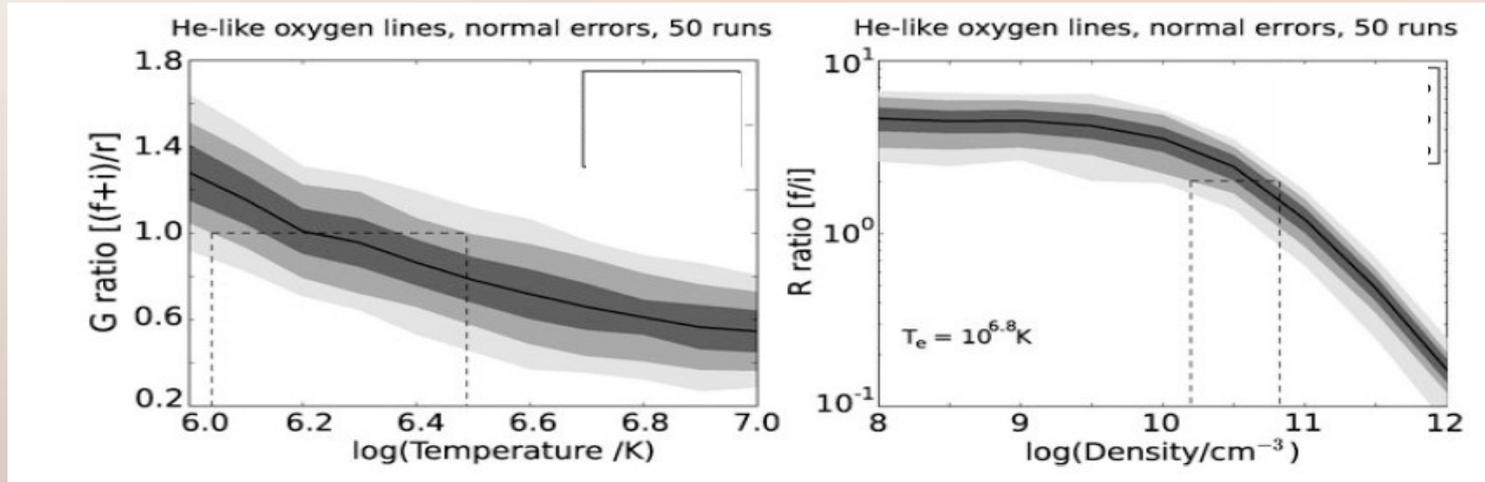
He-like line ratio diagnostics

O⁶⁺ example

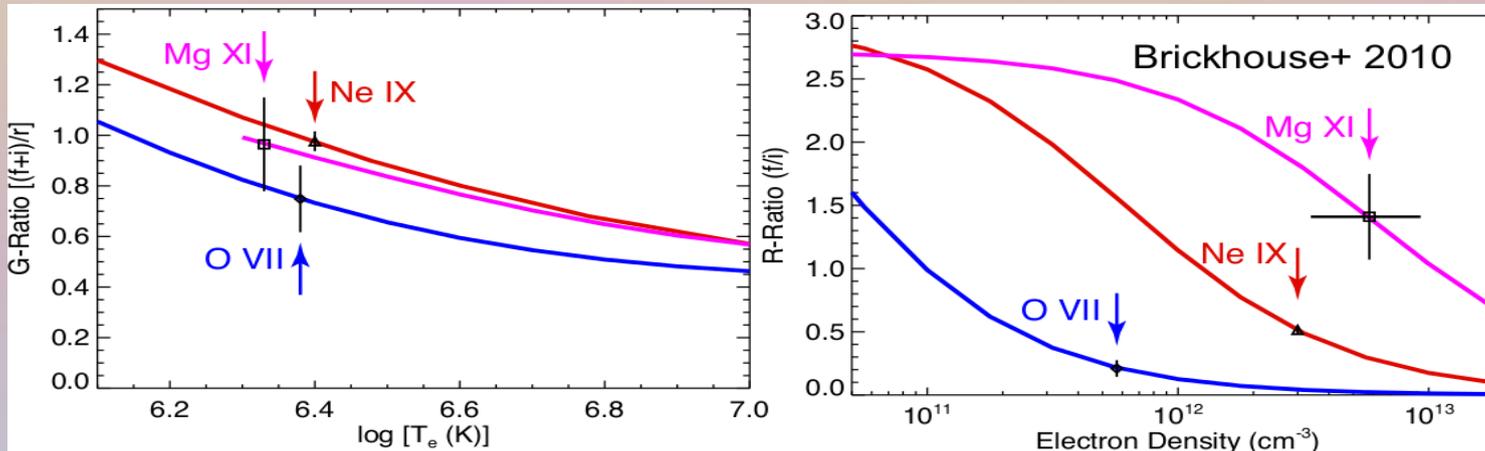


- The ratio of the $(X+Y+Z)/W$ is T_e dependent for $N_e < 1 \times 10^7 \text{ cm}^{-3}$.
- The ratio of the $Z/(X+Y)$ is density dependent.

Examples



Taken from
Foster et al.
*Space Science
Review* **157** : 135
(2010)



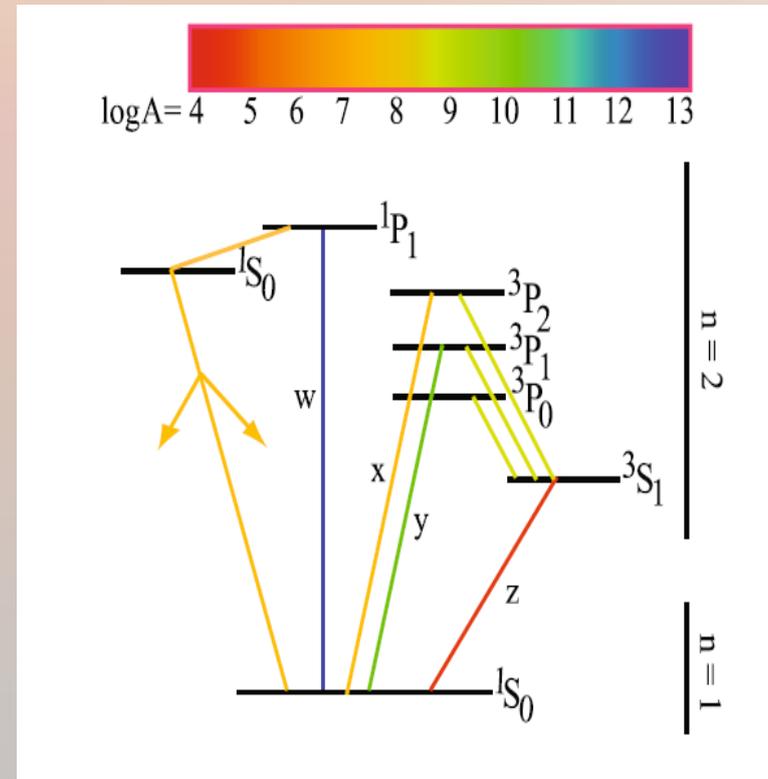
Taken from
Brickhouse et al.
ApJ **710** : 1835
(2010)

Uncertainties

- So what atomic processes should be considered?
 - Whatever the dominant ones are for the particular plasma.
 - We will be focusing on *electron-impact excitation, ionization and recombination*.
 - We will concentrate on uncertainties on *theoretical* data.
 - The principles outlined could be used for other processes such as charge exchange, photo-rates, proton collisions.
- What general properties should the uncertainty have?
 - It should reflect the dominant source of uncertainty.
 - It should have the right behavior with energy, temperature and process type.
 - The uncertainties could, in principle, be correlated.

Collisional-radiative modeling

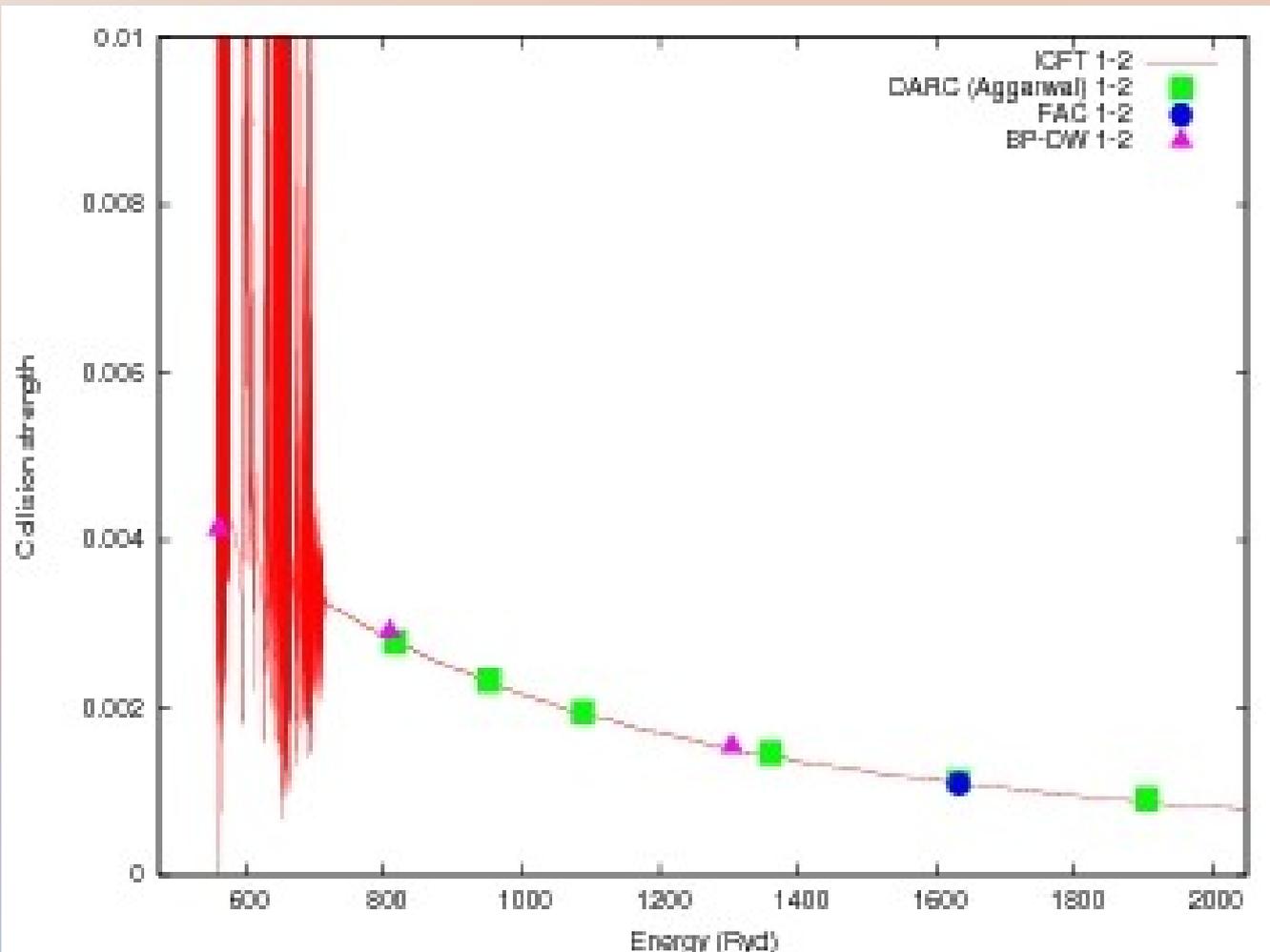
- The collisional-radiative equations solve for the excited populations.
 - They balance all of the excitation, de-excitation, radiative, ionization and recombination rate coefficients.
- Two commonly produced quantities are
 - Photon emissivity coefficients
 - Generalized ionization and recombination rate coefficients.
- There are three density regimes:
 - Coronal
 - Collisional-radiative
 - LTE



Approach for generating uncertainties

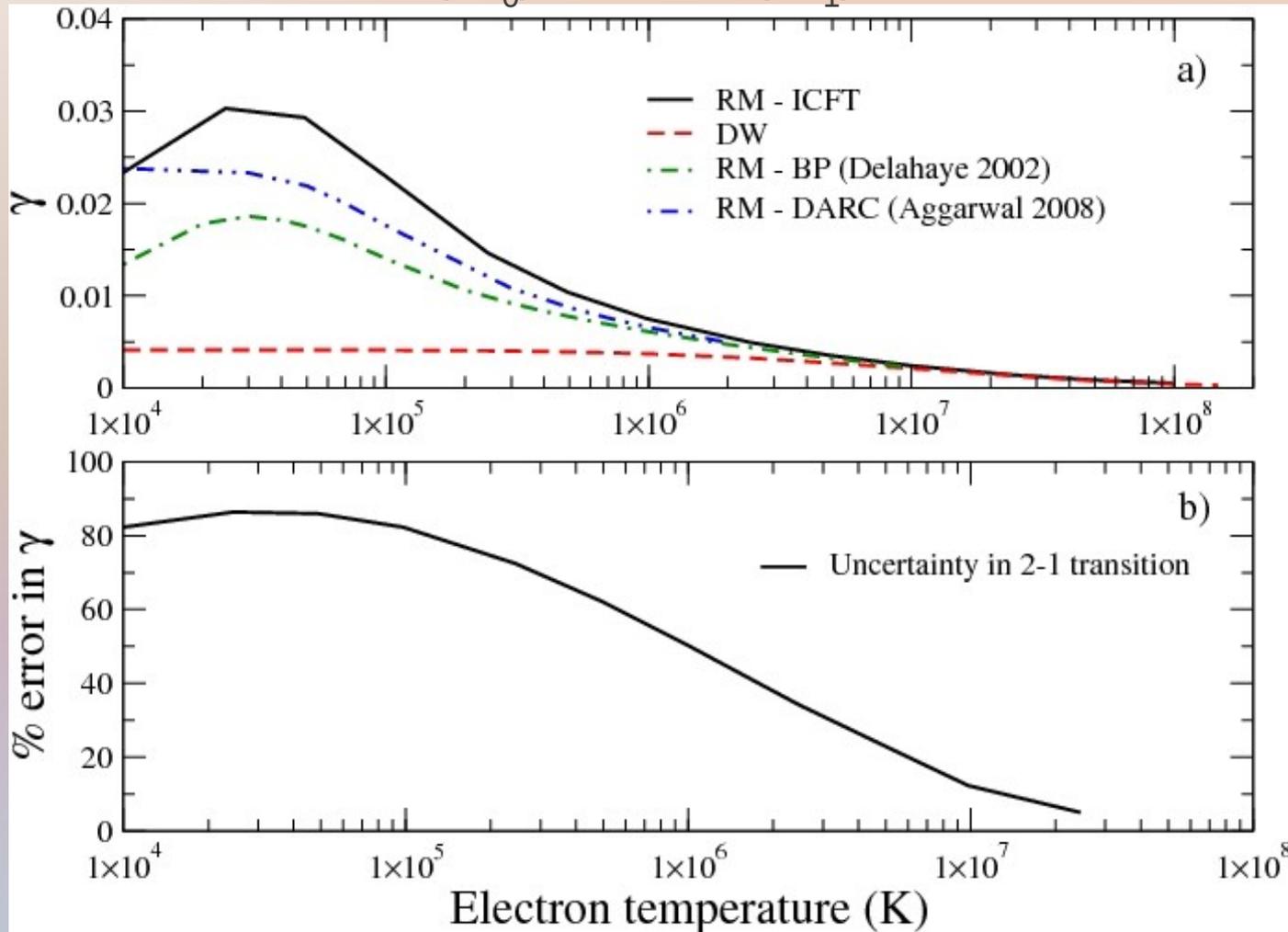
- We consider moderate to highly charged ions and have a recommended dataset that consists of
 - DW data for ionization and recombination, R-matrix data for excitation.
- We have a two-tiered approach to generating uncertainties.
 - ***Baseline uncertainties***
 - A generous estimate of the uncertainties that should encompass most of the currently available data in the databases.
 - We also want uncertainties that have the correct temperature and n-shell behavior.
 - ***Method sensitivity***
 - Represents the variation within a chosen method
 - Provides a tighter constraint on the uncertainty.

Baseline uncertainties on electron impact excitation data for O^{6+}



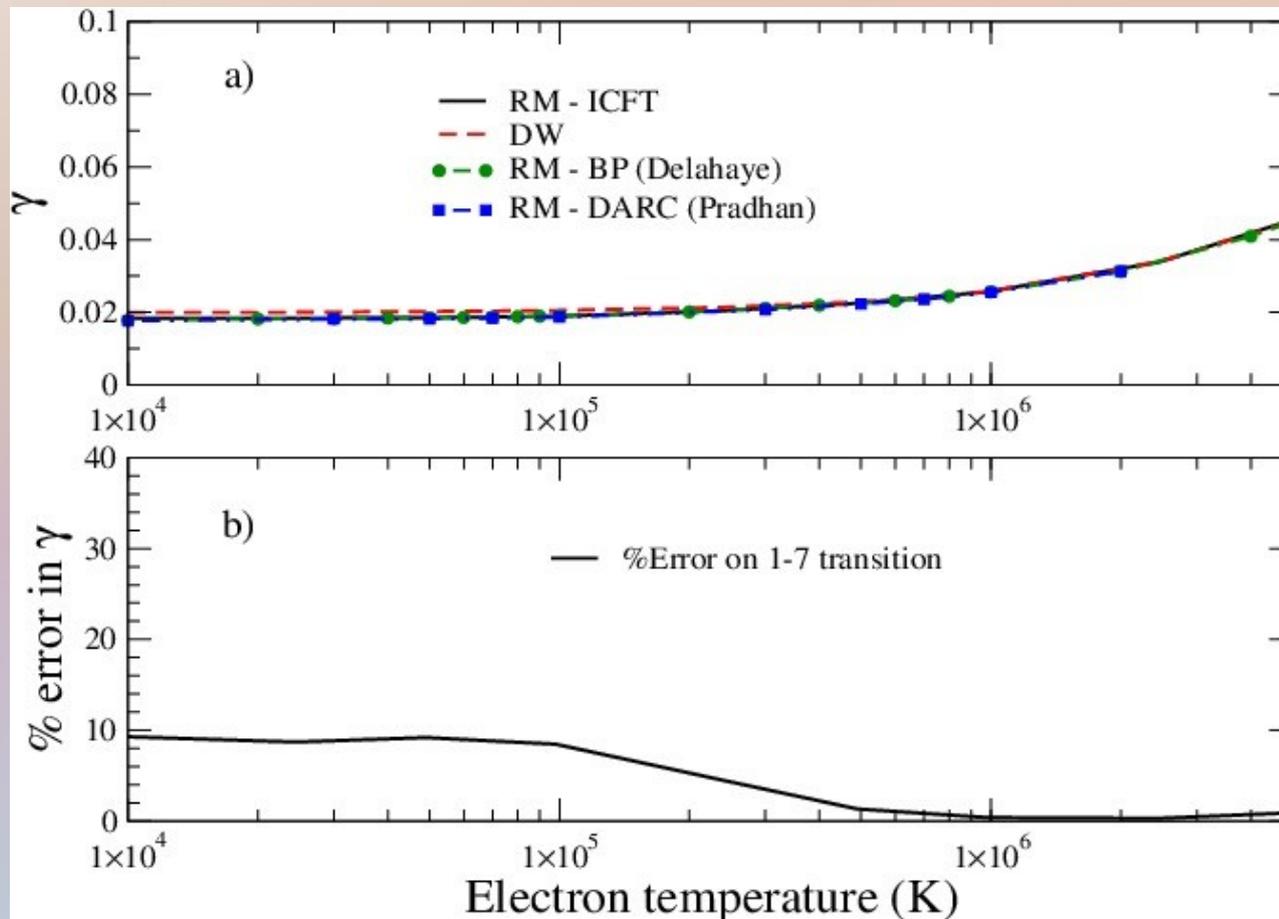
- A quick scan of the literature shows
 - Two recent R-matrix calculations.
 - One DW calculation.
- They all agree very well for the background cross section.
- The dominant source of error is in the resonance contribution.

Effective collision strengths - forbidden transition



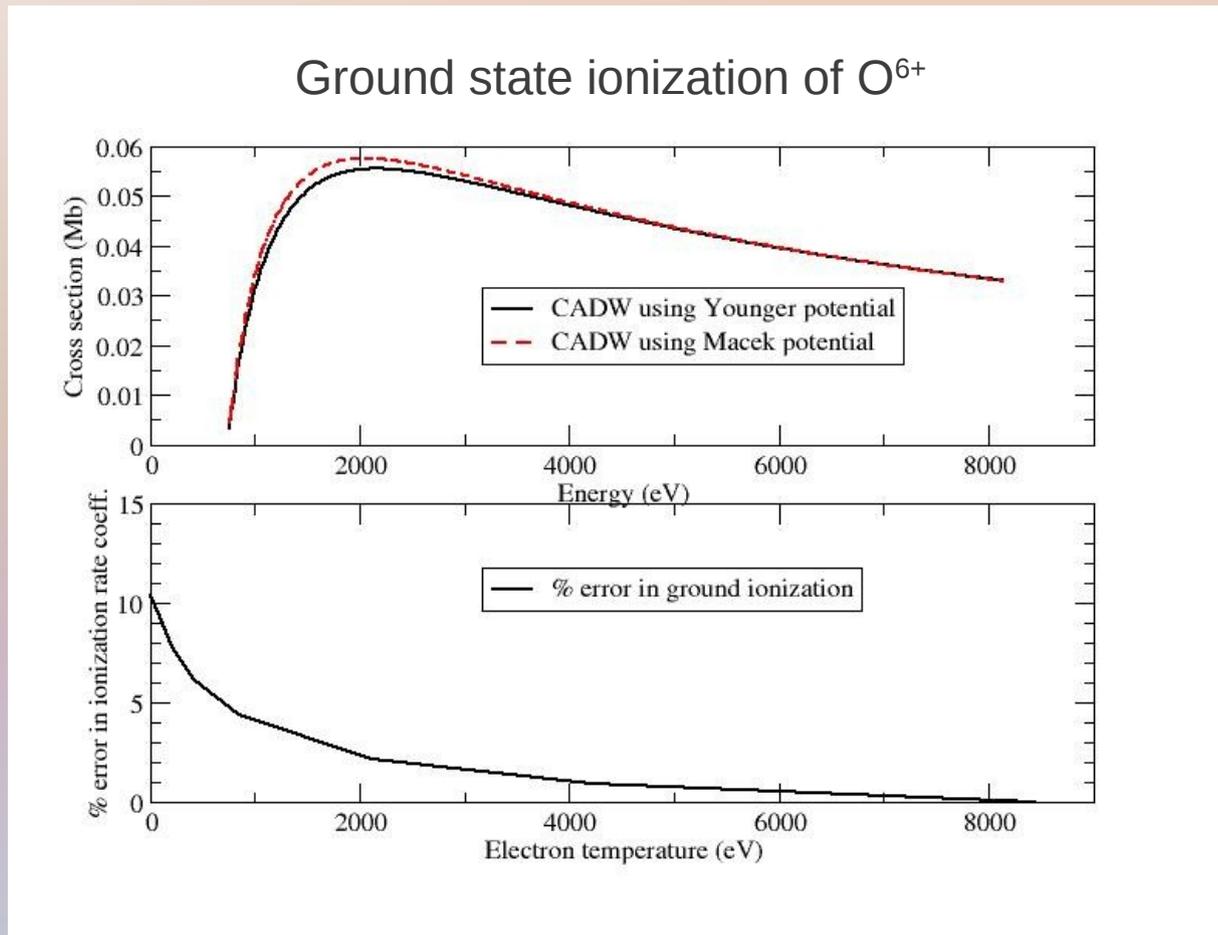
- Our baseline uncertainty data for excitation is the difference between the RM and DW upsilons.
- The uncertainty decreases with increasing temperature.

Effective collision strengths - allowed transition



- Note that the uncertainties are very small for the resonance line.
- The uncertainties decrease with increasing temperature.

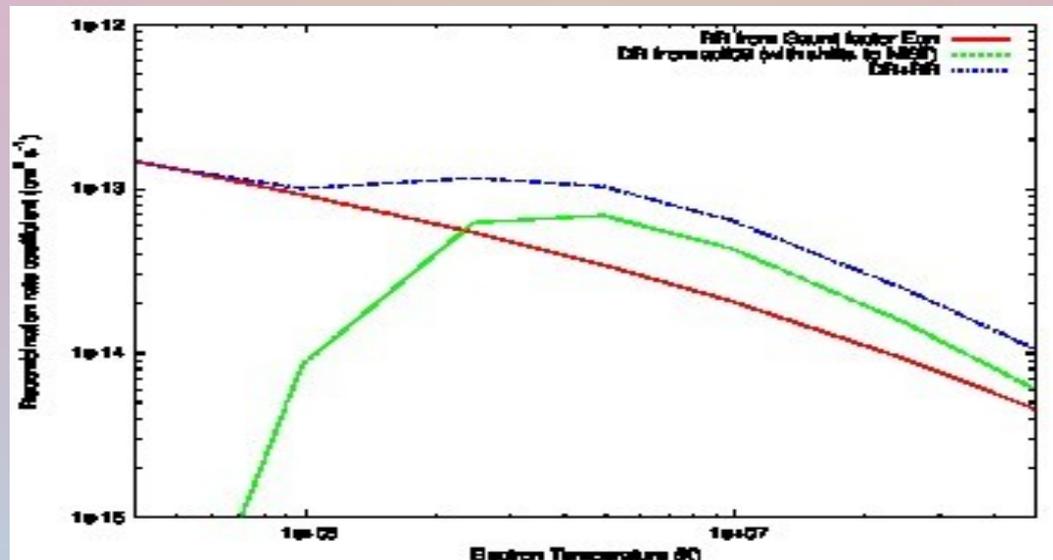
Uncertainties on ionization cross sections



- We took the difference between a Post and Prior scattering potential calculations.
 - Has an appropriate energy scaling and n-shell scaling
- We calculated level-resolved data for the first 4 n-shells.

Uncertainties in recombination

- The uncertainty in the DR rate coefficient is due to the sensitivity to resonance positions and heights. The difference between our default core excited structure and NIST values gives an indication of our energy uncertainty.
 - Thus our baseline uncertainty is the difference between two DW AUTOSTRUCTURE calculations. One with and one without shifts to NIST core excited energies.
- The uncertainty in the RR data is the difference between a Gaunt factor calculation of ADAS and a DW calculation from AUTOSTRUCTURE.



Propagating these uncertainties through a collisional-radiative model

- Generate correlated sets of random numbers in an appropriate distribution.
- Solve the collisional-radiative (CR) equations with a Monte-Carlo approach keeping track of the statistics of important output parameters (relative populations, ionization/recombination rates, and emissivities) and their raw data.
- Determine the average values and uncertainties for the output data and, importantly, the distribution of each quantity about its average.
- Perform another Monte-Carlo calculation using the output distributions to determine fractional abundances, emissivities or line ratios.

Baseline Studies

- Uncertainty is quantified as the difference between different theoretical approaches
- Representative of differences in the literature
- Quickly provides a generous uncertainty on an atomic dataset, while providing the correct temperature and density trends of more elaborate calculations.
- May not reflect the tighter constrained uncertainties derived from more elaborate calculations.
- Fundamental atomic structure and collisional rates remain uncorrelated.

Sensitivity Studies

- Uncertainty is determined from the sensitivity of the calculation to key input parameters.
- Can produce fully correlated uncertainties.
- The objective choice of variation in the input parameters that reflects meaningful physical values remains difficult
- Does not determine the absolute uncertainty between methods.
- More time and resource intensive.

Guides choices made in more elaborate models

Reassess the quality of the baseline rates and confirm baseline uncertainty range.

Monte-Carlo Collisional Radiative Modeling

Emissivities

Uncertainties

Monte-Carlo line ratio diagnostics

Effective ionization and recombination

Uncertainties

Monte-Carlo ionization balance

Uncertainties on Te and Ne

Uncertainties on abundances and ionization age

ATA: Oct

Distribution functions for input atomic data

- We initially used Gaussian distributions with the standard deviation provided by the uncertainty value.
- We changed this to a log-normal distribution to ensure that there were no negative values.

$$f(x_i) = \frac{1}{\sqrt{2\pi\sigma_i^2}} e^{-\frac{(x_i - \mu_i)^2}{2\sigma_i^2}}$$

The density function for the log-normal distribution takes a similar form:

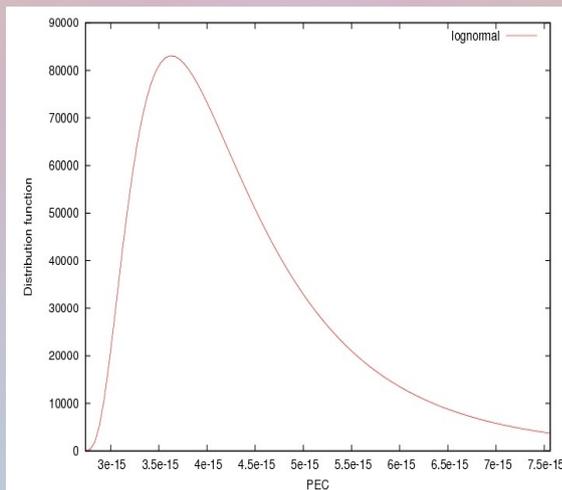
$$f(x_i) = \frac{1}{\sqrt{2\pi s_i^2 x_i^2}} e^{-\frac{(\ln x_i - m_i)^2}{2s_i^2}}. \quad (\text{B.4})$$

where m_i and s_i play the same role as μ_i , σ_i above. The parameters for this distribution can also be determined statistically. It is usually easiest to calculate μ and σ using the formulae above and then convert to m and s using

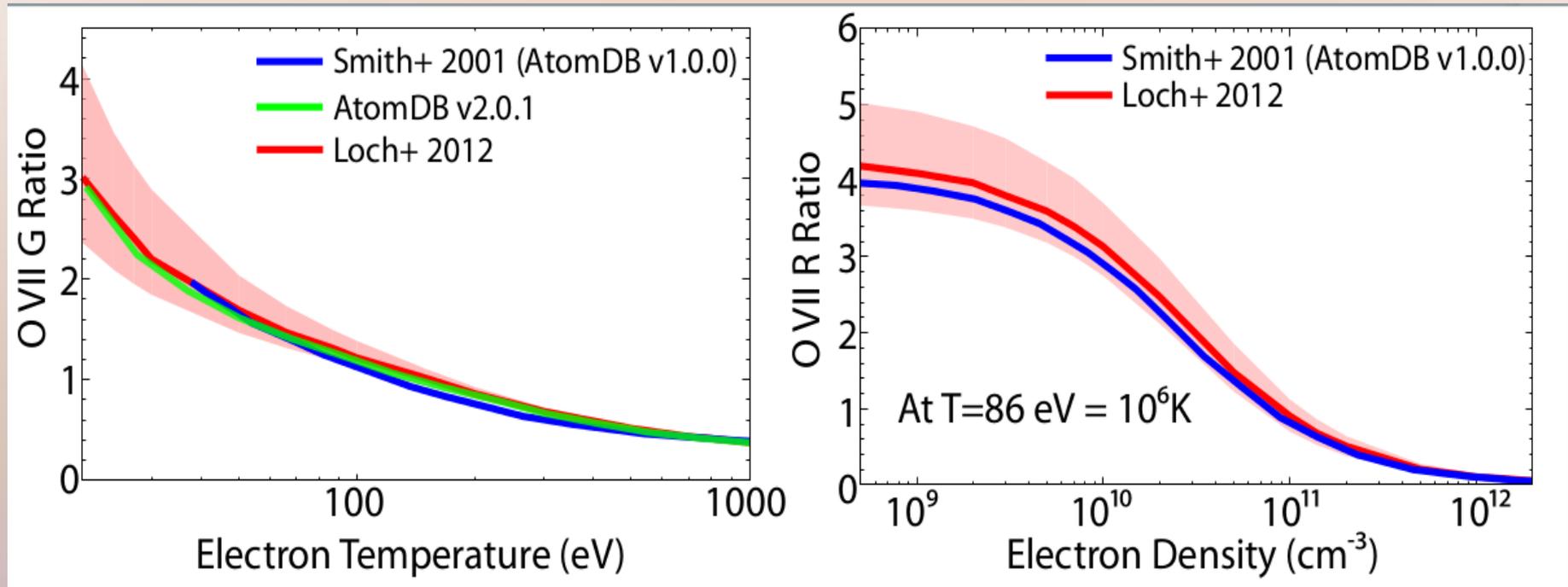
$$s^2 = \ln \left(1 + \frac{\sigma^2}{\mu^2} \right) \quad (\text{B.5})$$

$$m = \ln \mu - \frac{1}{2} \ln \left(1 + \frac{\sigma^2}{\mu^2} \right) \quad (\text{B.6})$$

$$= \ln \mu - \frac{1}{2} s^2. \quad (\text{B.7})$$

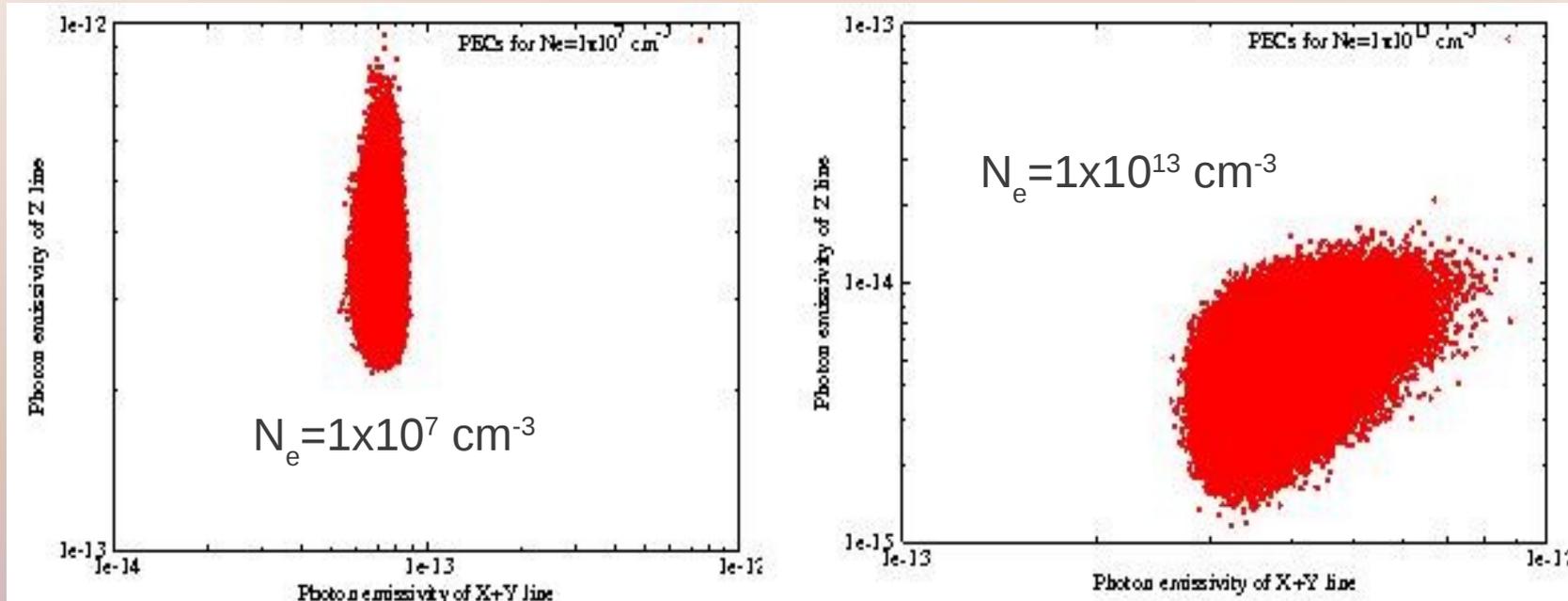


Line ratio results for O⁶⁺



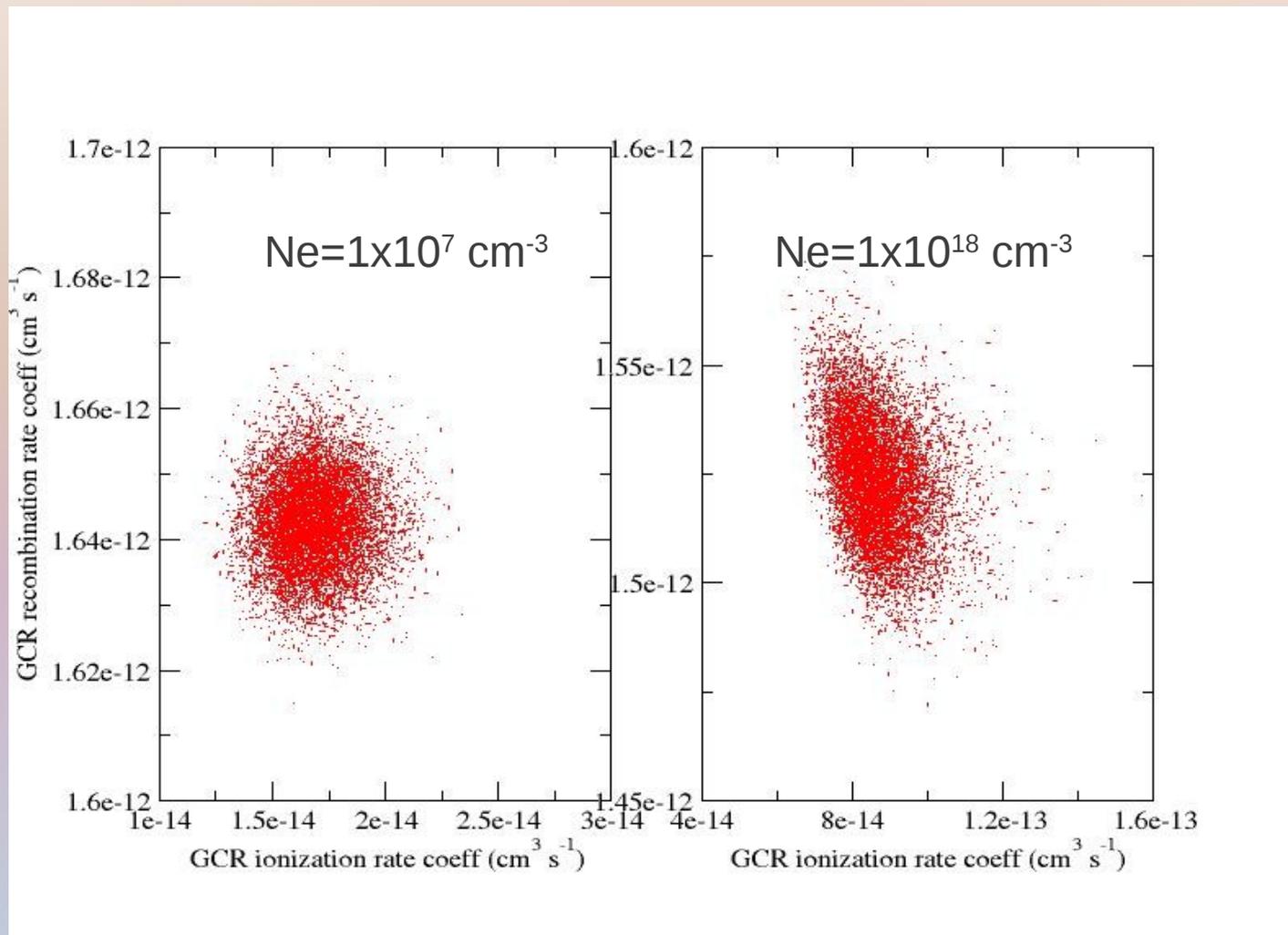
- The uncertainties in the line ratios have the right trends.
- Despite the fact that we are using baseline uncertainties, which are an overestimate, the overall uncertainty is relatively small.
- It has been useful in tracking down differences in different atomic databases.

Correlation in emissivities



- As one increases the density in the R-ratio, the emissivities become correlated.
- This is accounted for in the line ratios shown.
- Note that there is still no correlation in the input atomic data.

Correlation in effective ionization and recombination rate coefficients



Method sensitivity

- Future work will involve developing and refining the method sensitivity approach.
- Our plan is
 - For DR to do a set of Monte-Carlo DR calculations, varying the core excited levels within a range defined by the energy difference with NIST values.
 - For excitation do a set of Monte-Carlo R-matrix calculations, varying the energy mesh in the outer region and the orbital scaling parameters.
 - For ionization do a set of Monte-Carlo DW calculations, varying the orbital wavefunctions.
- Note that this will produce a set of correlated input atomic data, and will give the distribution functions to be used in our collisional-radiative code.

Conclusions

- We have developed an approach to defining baseline uncertainties on moderate to highly charge ions.
- These uncertainties can be propagated through to uncertainties on line intensities, line ratios, fractional abundances etc.
- Work on method sensitivity approaches is continuing.
- If you have an atomic system/diagnostic that you would like to collaborate on, we would be very interested.