Progress Towards ATOMDB 2.0

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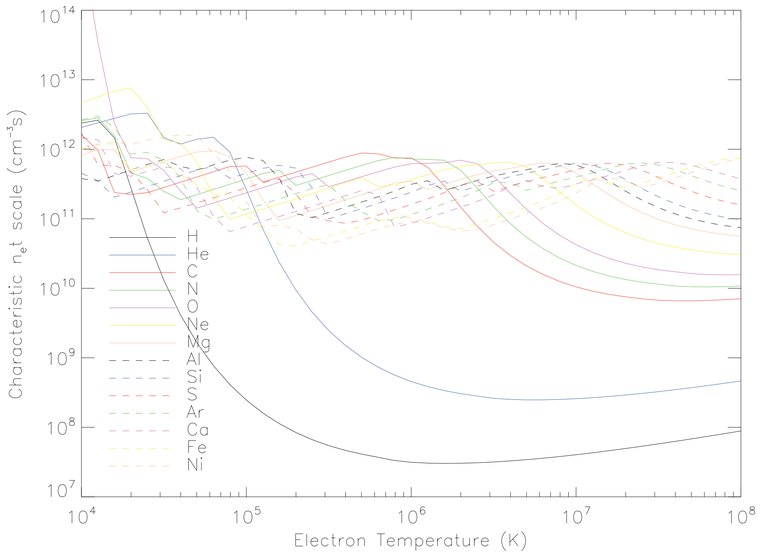
Abstract

ATOMDB (http://www.atomdb.org) is a collection of atomic data for use in X-ray astrophysical spectroscopy. The database includes both raw atomic rates along with the calculated X-ray spectrum from a collisional plasma over a range of temperatures and densities. The current version of ATOMDB is v1.3.2. We have been working on an update that will contain: (1) ionization and recombination rates for all ions, (2) many more transitions from higher n levels, (3) a new calculation of collisional rates for all ions of astrophysical interest in the hydrogenic and helium-like isosequence, and (4) updated wavelengths taken from the ongoing EBIT measurements at LLNL. We will report on progress to date with this effort, and our plans for the future.

How Fast Does A Shocked Plasma Return To Equilibrium?

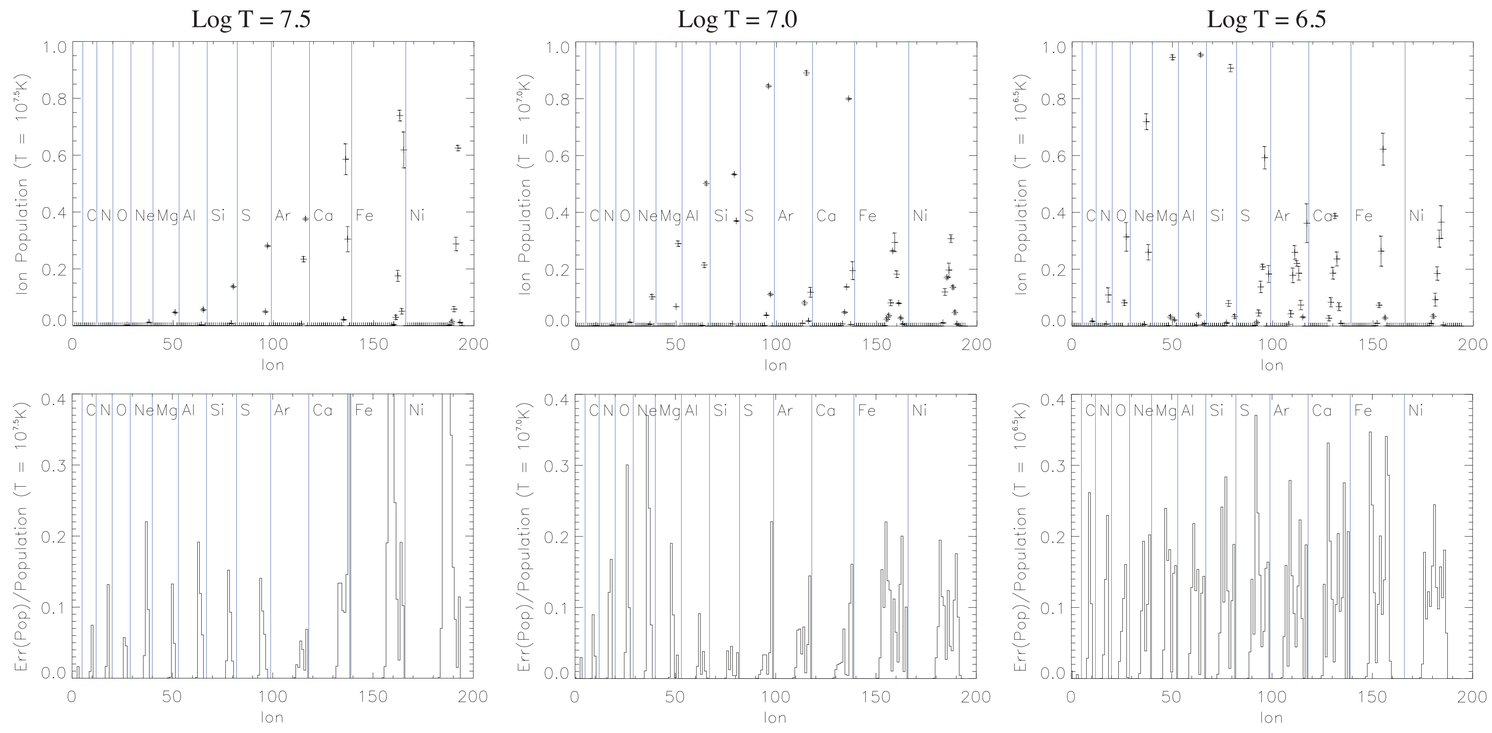
This commonly asked question can be answered using the simple figure shown below, which plots the maximum exponental decay "fluences" for all astrophysically important atoms. Fluence is a convenient quantity defined as $n_e t$, and used because all ionization and recombination rates scale with electron density n_e. The derivation of this quantity arises from the eigenvector method of solution to the problem of an ionizing plasma first described by Hughes & Helfand (1985)

In general the evolution of an ionizing (or recombining) element Z in a constant electron temperature is given by a coupled set of Z+1 first order differential equations. However, by casting these equations in matrix form, imposing conservation of the total ion population, and then finding the eigenvectors of this matrix, the coupled Z+1 equations become Z uncoupled first order differential equations. The solution is simply Z separate exponentials, with the time constant given by the eigenvalues of the rate matrix. The largest of these eigenvalues, then, gives the scale of slowest return to equilibrium independent of the initial conditions. Therefore, this result holds for an ionizing, a recombining, or even a plasma whose initial conditions are entirely random. Note that this does not specify which individual ion stage returns to equilibrium the slowest; in the eigenvector form, the ion stages are mixed and cannot be separated.



A First Step Towards Understanding Error Propogation in ATOMDB's Atomic Rates

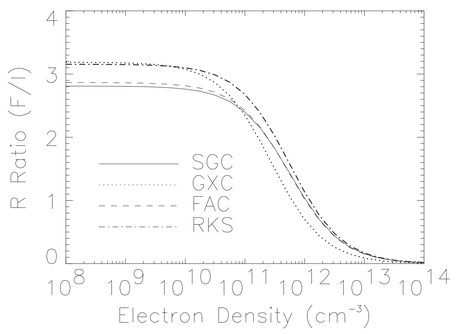
X-ray astrophysical plasma models all suffer from an inherent difficulty – the underlying atomic rates may be complete (if done by theoretical calculation) or they may be accurate within measured errors (if experimental), but rarely are they both. A commonly cited 'error' in theoretical calculations (keeping in mind that in this case, 'error' refers to inadequacies in the assumed theoretical model, and not true 'errors' in the experimental sense) is 'about 30%'. Here we show how a uniformly distributed 30% error in ionization and recombination rates would propagate into the calculated ion populations in thermal equilibrium at three X-ray temperatures. As can be seen, the resulting error tends to be on the same scale (~30%) at the peak although in some cases it can be larger. A more realistic error model might include increasing errors near threshold, or considering correlated errors for particular isosequences; this work is in progress.



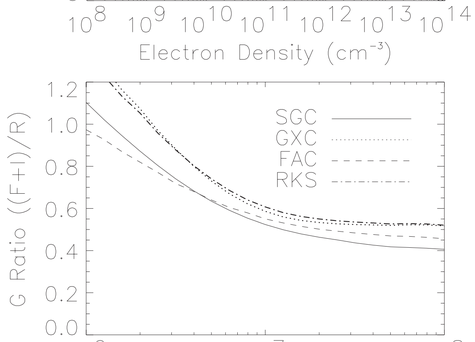
Improving Atomic Rates for the Helium Isosequence

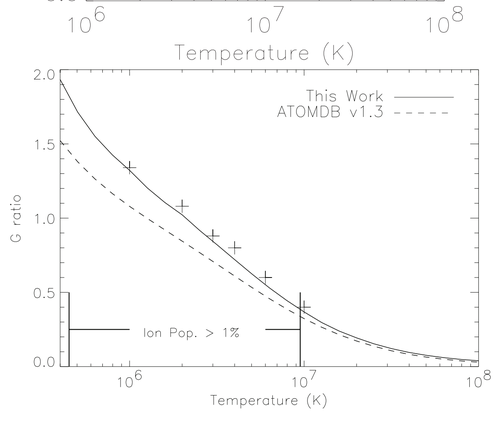
Emission lines from ions in the helium isosequence dominate collisional X-ray spectra and along with the hydrogen isosequence provide most of the diagnostics available at the moderate CCD resolution and even at grating resolution. Despite their importance, the only complete set of published collisional excitation rates for these ions comes from distorted wave calculations done by Sampson and collaborators in the 1980s. We have therefore begun a program to calculate new rates using the R-Matrix approach up to the n=5 levels (after which the R-Matrix method becomes inefficient) and supplementing these with Distorted Wave calculations up to n=10-12 (using M. F. Gu's FAC code). Although the changes in the line ratios as a result of these new calculations are not huge (see figures below), they do exceed the current measurement errors possible with Chandra and XMM/Newton. Although we have begun with Ne IX (see Chen et al 2006), we intend to expand these calculations to cover all the astrophysically important atoms, and eventually to cover all elements up to Z=30.

The R ratio (=F/I) calculated using the original Sampson, Goett & Clark (SGC) rates, the rates from Chen et al (200X; GXC), a FAC code calculation done by the author using levels up to n=10 (FAC), and a separate R-Matrix calculation done by the author using the Belfast/Strathclyde R-Matrix code (RKS), a completely independent code from that of GXC. Note that at low densities the SGC and FAC codes (both of which use the DW approach) underestimate the R ratio, a problem which has been noted in the literature (Testa et al 200X).



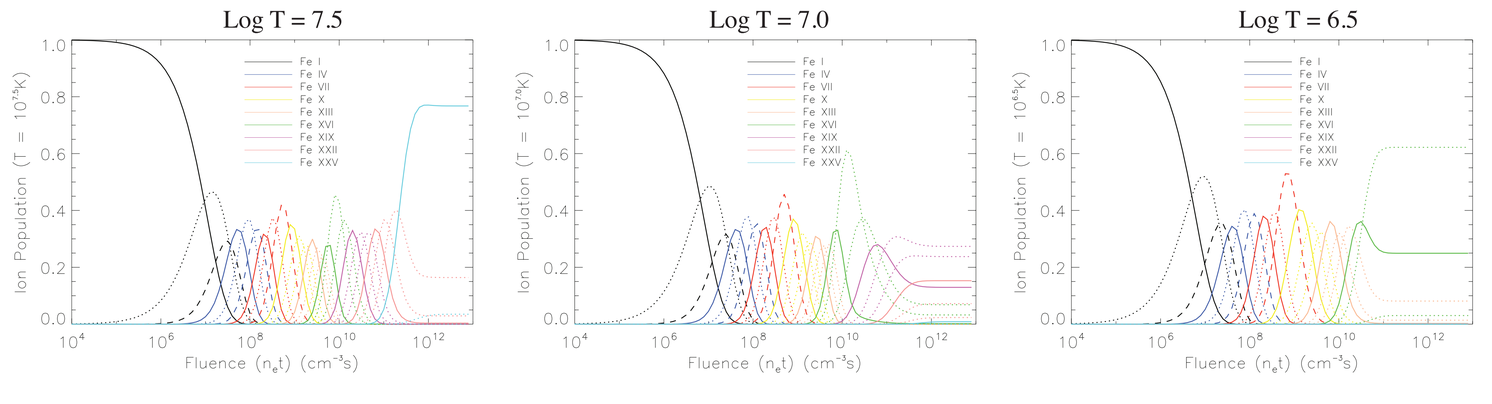
The G ratio





ATOMDB and APEC: Now fully NEI-compatible!

A long-standing problem with APEC was the lack of directly-calculated non-equilibrium models; instead, APEC used pre-calculated tables of ion populations as a function of temperature, ignoring the known density effects due to dielectronic recombination due to a lack of available data. However, thanks to an ongoing collaboration with Dr. Nigel Badnell and the ADAS group at the University of Strathclyde, we now have access to density dependent and level-separated dielectronic and radiative recombination rates (as used in Bryans et al 2006). In addition, there have been two new collections of ionization rates (Dere 2007 and Mattioli 2007) using the latest experimental measurements. Therefore, we have gone ahead an implemented a direct calculation of ion population into the APEC code, along with an implementation of the eigenvector solution to the case of a constant electron temperature but otherwise non-equilibrium plasma. Results for initially pure atomic iron held at three different electron temperatures are shown below, using the atomic rates from Mazzotta et al (1998) since these rates are already available in ATOMDB format. However, the strict separation of code and data enforced by the ATOMDB project means that once these new results from Badnell, Bryans, Dere, and Mattioli have been formatted, they can be easily swapped in and out to test their effects on the results, and to test error propagation as well.



Future Plans for ATOMDB

Despite the best intentions of the many laboratory astrophysics teams working today, the problem of connecting the most recent atomic rate measurements and theoretical calculations with the observational "end user" remains. Although observers should of course remain up-to-date on atomic physics issues affecting their results, this is only one of many different problems that can affect their results, and so is often (or perhaps more accurately, 'nearly always') left for someone else to worry about. At the same time, data producers have a similar difficulty regarding how to release their data in a form that will be both available and useful to other users – ideally, without losing its heritage in a melange of other rates so that the work is rarely cited. *Unfortunately, there are no 'silver bullets' to solve this problem – but progress is possible!*

The PIs of upcoming X-ray missions such as Spectrum-X Gamma, NEXT, and Constellation-X are well-aware of this problem, although none have the funding (yet) to address it. However, the ATOMDB team intends to begin work on this problem now, with the goal of getting long-term support from operating missions. Our plan is to work within the framework of the highly successful HEASARC, which already provides long-term storage and access to data for all X-ray missions dating back to the origin of the field. We intend to use the same approach to store atomic data relevant to X-ray astrophysics within the HEASARC. This will entail defining standard formats for atomic data, along with code libraries in C, FORTRAN, and other languages to help write such formats and other codes to convert from existing formats such as that used by the ADAS team.

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