AtomDB v3.1.0 Release Details

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1 Document Scope

This document outlines the changes between AtomDB v3.0.9 and 3.1.0. It is not comprehensive, and a publication will follow. It is designed as a quick reference to answer initial questions. This document will be updated with any questions which arise. It will also track updates to further subversions (e.g. 3.1.1, 3.1.2...)

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2 Getting the Files/Installation

There are multiple ways to use the AtomDB data files, depending on your use case. For most people, the important files are the equilibrium emissivity files (apec_line.fits, apec_coco.fits), non-equilibrium emissivity files (apec_nei_line.fits, apec_nei_comp.fits) and the eigenvector files (atomdb_eigen.fits).

The first pair of these provide the emissivity in photons cm^3 s^{-1} for lines and continuum (the latter in photons cm^3 s^{-1} keV^{-1}) for each element, assuming an equilibrium ionization balance and the solar photosphere abundances of Anders & Grevesse 1989. The second pair contains the same thing, but without any ionization balance (effectively assuming every ion has a fraction of 1; the emissivity it then multiplied by the appropriate ionization balance). The eigenvector files contain the equilibrium ionization balance for all the elements on a 1201 temperature grid from 10^4 <T < 10^9K grid, and the eigenvectors required to calculate non-equilibrium ionization balance solutions (see Smith and Hughes 2001).

- **To download these files directly (e.g. to use them in XSPEC/Sherpa etc)**
  - Note: these instructions refer to version 3.1.0. For other versions, change the 3.1.0 as appropriate
  - visit www.atomdb.org/download.php

- Within XSPEC, you set the equilibrium files using: xset APECROOT /path/to/files
  Note that you do not include the "_line.fits" at the end, so xset APECROOT /home/afoster/atomdb/apec_v3.1.0 will refer to the files /home/afoster/atomdb/apec_v3.1.0_line.fits and /home/afoster/atomdb/apec_v3.1.0_coco.fits
- xset NEIAPECROOT sets the non-equilibrium emissivity files
- The eigenvector file is slightly more complicated. You unzip it and then copy to $HEADAS/../spectral/modelData/ . Then the NEIVERS command chooses which files to use, using the part **after** "eigen_v". So eigen_v3.1.0.fits is loaded with xset NEIVERS 3.1.0

- **To use within pyAtomDB**
  - Download using pyatomdb by updating to the latest version (1.0.0) and issuing the command pyatomdb.util.switch_version('3.1.0')

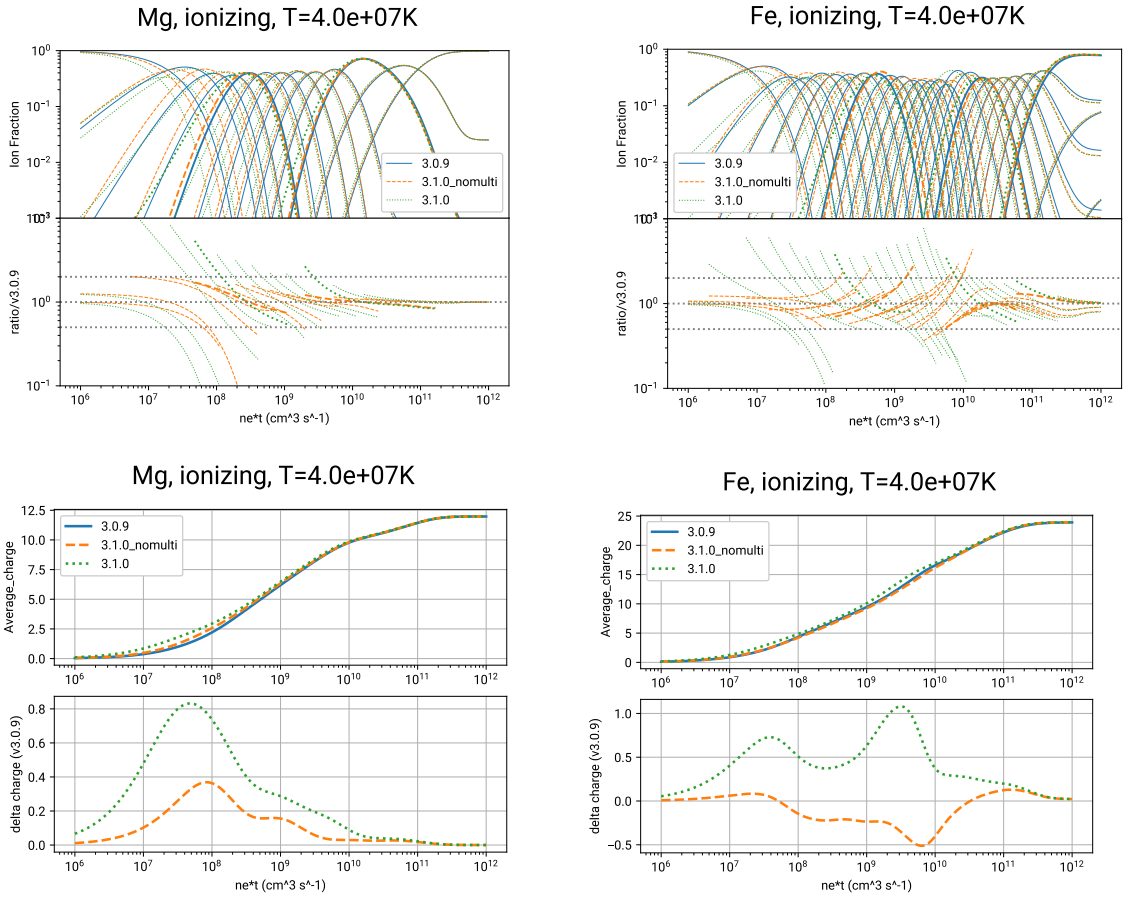

*Figure 1: Ionizing Mg and Fe with the old and new ionization balances included. The closed shell ions (He- Ne- and Ar-like) are highlighted with thicker lines. Bottom plots show the mean charge, sum(q * f(q)). Data in th*

3 What's New

3.1 AtomDB 3.1.0

Ionization Rates

We have made two changes to the ionization rates. The first is inclusion of the Urdampilleta et al 2017 rates for single ionization and excitation-autoionization, which is an update from the Bryans 2009/Dere 2007 data set used before. For more details, see Urdampilleta's paper. This data is taken from SPEX and therefore the ionization and recombination rates should now be equivalent.

The second change in the inclusion of the multiple ionization rate coefficients for electron collisions from Hahn et al 2016. This data includes coefficients for up to 7 times ionization, depending on the ion in question. In general, this data makes no difference for equilibrium plasma, but for ionizing plasma the differences can be quite significant. To enable comparison of the difference this makes, we have included sets of eigenvector files with (the default) and without the multiple ionization rates, which are available on the website download page.

Figure 1 shows the effect of these new ionization rates on Mg and Fe at T=40MK (~4keV). The graph is a little hard to read, but in general, at equilibrium there is little difference between the with and without multiple ionization data, but lower timescales have more significant differences. In the iron case, the differences are an entire ionization stage in this scenario. When fitting, the expected change is that the timescale will adjust to

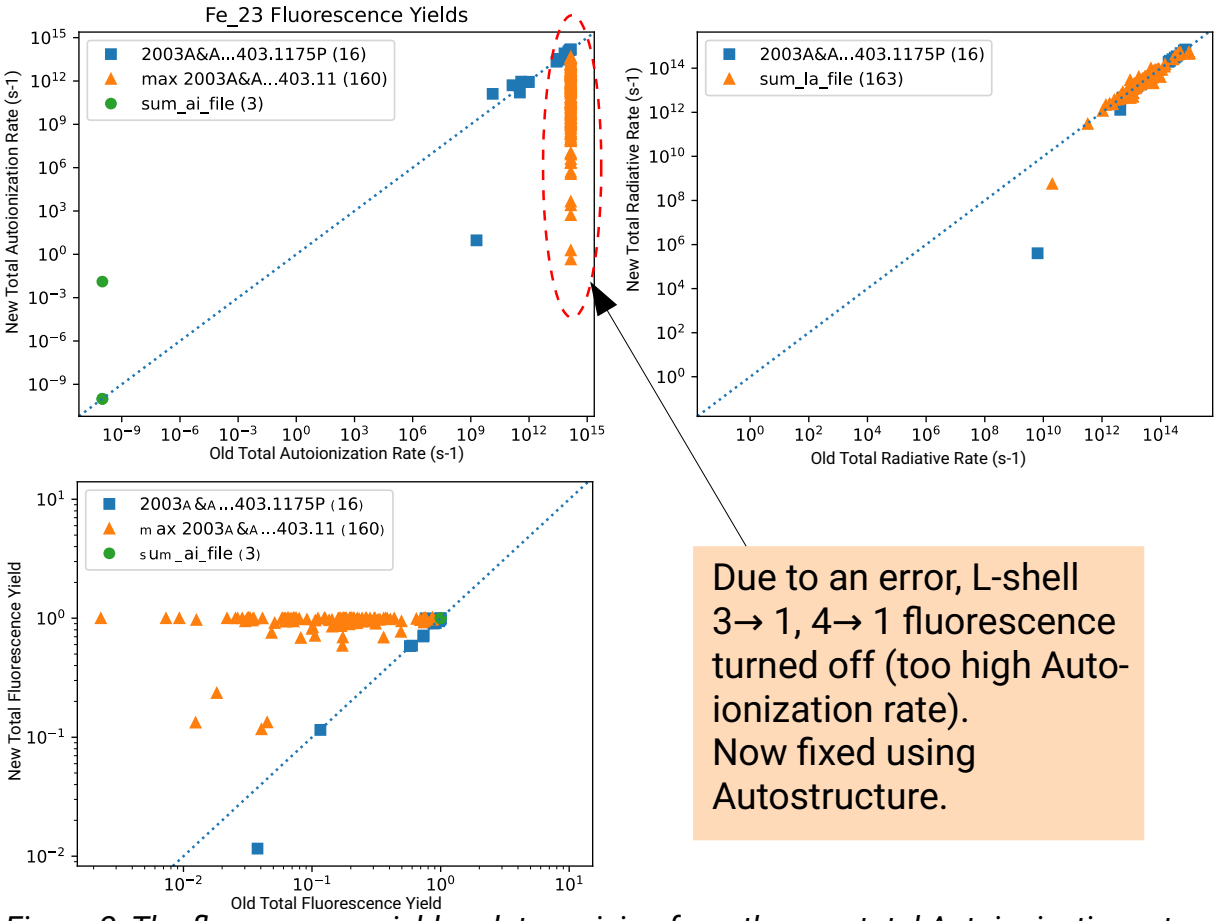

Figure 2: The fluorescence yield updates arising from the new total Autoionization rates replace erroneus ones (orange triangles). These are for Li-like Fe.

compensate: a 10-20% increase in n_e*t will create a similar ionization balance as before. However, this will not be the same between all elements and the effect increases with increasing temperature, so there will be some variation here.

DR Satellite Lines/Inner Shell excitation lines

In AtomDB, satellite lines are calculated separately from the corresponding inner shell excitation transitions which can also create them, as the data come from different sources and they are driven by different ion populations. Therefore they are discussed together here. For the purposes of this documents, we refer to these as satellites when the come from recombination, and inner shell lines at other times, even though they are often the same transition.

The previous release of AtomDB used data from Safranova and Vainstein, from various publications, for the n=2 satellites of H- and He-like ions, up the n=5 shell. (e.g. 1s 2p 5f → $1s^2$ 5f). For the Fe L-shell this was topped up by calculations from Jacobs.

Inner shell fluorescence yields, consisting of the radiative transition probability, total radiative width, and total

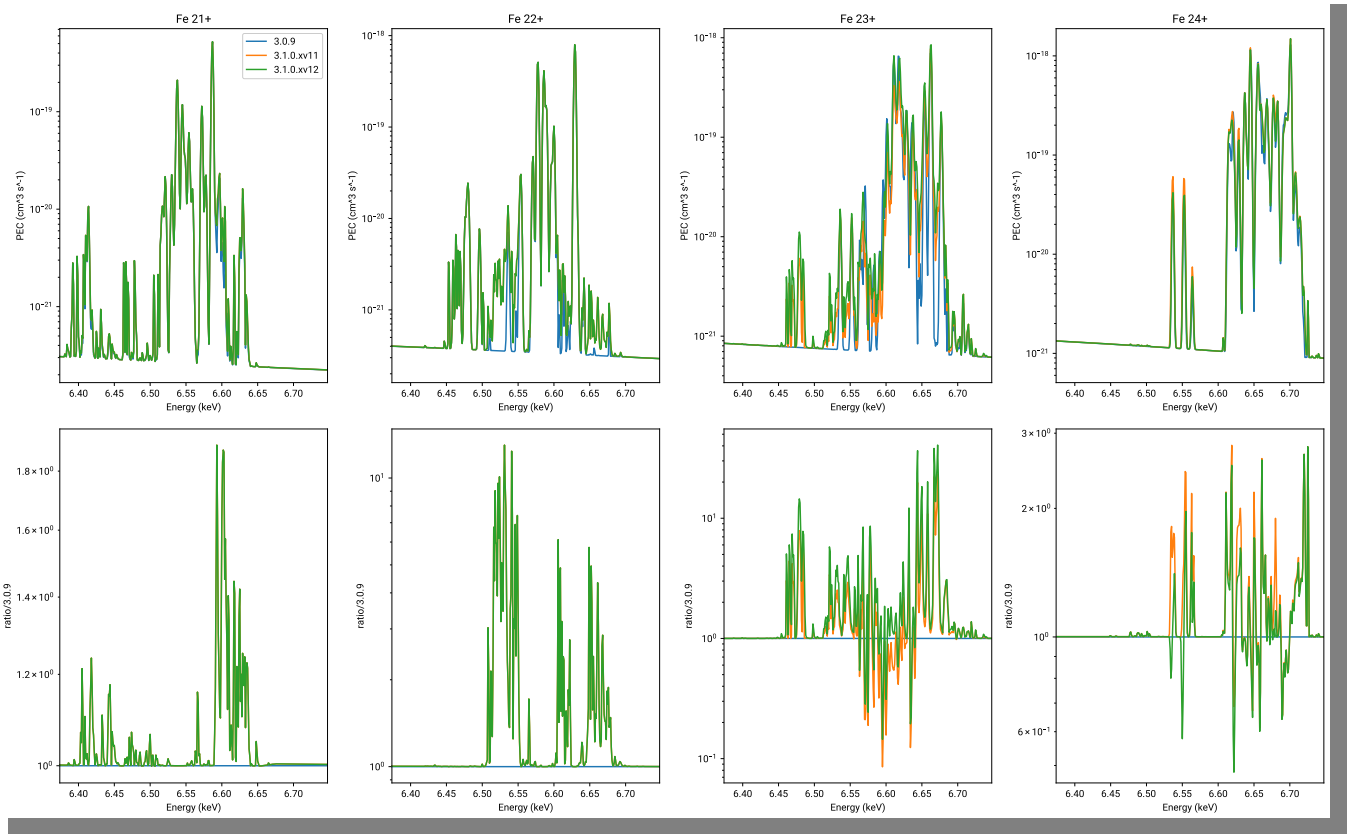

Figure 3: The PEC spectrum of individual Fe ions in a kT=1.5keV plasma. The orange spectrum is an intermediate one, but comparing the green and the blue provides a strong indication of the differences between the data sets.

auger width, were included from the Palmieri group of papers for all K- and L-shell ions, for K shell vacancies from promotion to the L shell (e.g. $1s^2\ 2s^2\ 2p^5$ → $1s^1\ 2s^2\ 2p^6$).

Similarly, they were include for all M shell ions for K→ M shell excitation (e.g. $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^3$ → $1s^1\ 2s^2\ 2p^6\ 3s^2\ 3p^4$) from the same source.

FAC was used to calculate excitation to all of these levels through excitation and inner shell ionization of the previous state. This was also done for the higher n vacancies, in the n=2 and n=3 shells of all ions, with excitation up to n=4, for all ions of all elements down to neutral.

Bugfix – Autoionization of doubly excited levels

However, a glitch was introduced which means for most levels with an inner shell vacancy excited above the valence n shell (eg 1s 3p 5p), where the data was not corrected to literature values, resulting in the autoionization rates being over-estimated, effectively turning off this emission. This affected ions from Fe^{16+} to Fe^{24+}. For most ions, therefore, the Kα emission was modeled correctly, but some of the weaker Kα and Kβ components were suppressed by possibly a factor of two. However, for the Lithium-like state, the issue was significantly worse, and the Kβ and Kγ lines were completely turned off. Figure 2 shows the issue here for Li-like ions, populated by inner shell ionization/excitation. The yields are far too small for the orange levels.

Improvement – Dielectronic Satellite lines

We have used the Autostructure code to calculate excitation up to n=4, n'=15 for DR satellite lines of H-, He-, Li- and like ions (all elements, not just Fe). This has led to a much more comprehensive set of lines in the emission spectra, as well as improvements to wavelengths. Initial comparisons with existing data suggest moderate changes to existing lines, but significant additional emission.

Improvement – Inner Shell Excitation

We have also used Autostructure to calculate inner shell excitation to these lines, using the distorted wave method. This has provided the excitation component of this line emission. Often, due to low fluorescence yields, this is not significant, but the emission at high n should not be ignored. The effects of this and the satellite lines can be seen in Figure 3.

Data Format – Continuum Files

With the release of version 3.1, we have changed the data format of the Continuum emission files. The change is that the Continuum and PseudoContinuum are now variable length arrays of floats (E → PE, in FITS notation). See Figure 4 for an example. Because of the way variable length arrays are handled between astropy and numpy, this required re-writing sections of the PyAtomDB spectrum.py module to suit. Make sure to update PyAtomDB if you are having issues. XSPEC handles these files without changes.

Z	mJ	N_Cont	E_Cont	Continuum	Cont_Err	N_Pseudo	E_Pseudo	Pseudo	Pseudo_Err
1J	1J	1J	77E	77E	77E	1J	55E	55E	55E

Z	mJ	N_Cont	E_Cont	Continuum	Cont_Err	N_Pseudo	E_Pseudo	Pseudo	Pseudo_Err
1J	1J	1J	PE(66)	PE(66)	PE(66)	1J	PE(58)	PE(58)	PE(58)

Figure 4: The HDU header for (top) v3.0.9 and (bottom) v3.1.2 continuum HDUs in the _coco.fits and _cont.fits files. The exact length of each will vary from HDU to HDU.

Note that if you have updated and are still having issues in PyAtomDB, you may need to delete any cached spectral pickle files so they can be re-made and function correctly:

```
rm $ATOMDB/spec*pkl
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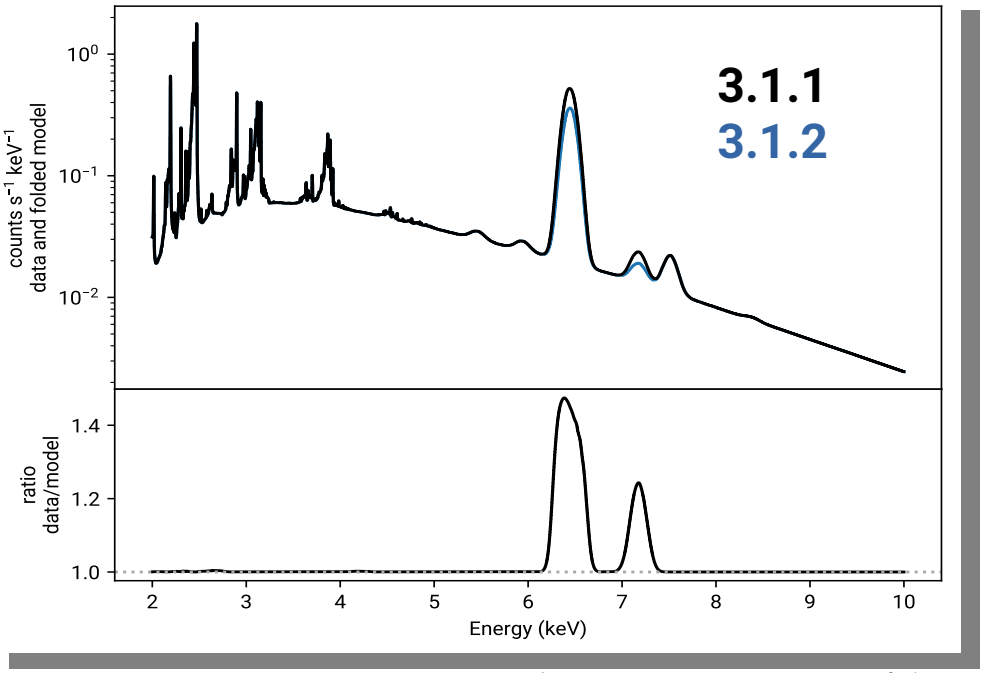

Figure 5: Model based on Kepler's SNR, (kT=4.7keV, tau=3.7e9cm^{-3}s) showing the effect of the updated M shell data.

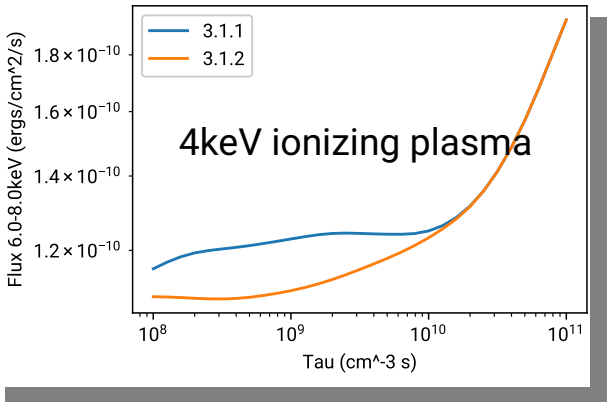

Figure 6: The Flux in the 6-8keV range, showing that the new data is not relevant $n_e t$ < 1e10cm^{-3}s plasma.

3.2 AtomDB 3.1.1

This release is a bugfix release. When packaging the datasets, some of the neutral ions at temperatures above 10^8K produced continua with NaNs present. This was due to the electron-ion bremsstrahlung calculation, which should return zero for these ions, being triggered and returning a NaN instead of zeros.

This bug affected very hot, ionizing plasma (T>10^8K) which have a very short ionizing timescale ($n_e t < 10^9$cm^{-3}s), otherwise neutral ions are not significantly present. If you were affected by the bug, XSPEC and PyAtomDB would have returned no spectra, if your models continued to successfully run then you are unaffected.

3.3 AtomDB 3.1.2

This release is an amendment to the inner shell (Kα & Kβ) lines of M shell Fe ions (Fe^{6+} to Fe^{17+}, excluding Fe^{16+}). The Spontaneous emission (Einstein A) coefficients were taken from the literature values of the Palmeri group, but had been doubled when added to our database. These lines have now been amended and fixed. This mostly affects relatively young plasma, as shown in Figure 5 and Figure 6.

3.4 AtomDB 3.1.3

This is a bugfix to 3.1.2. There was a packaging issue which led to an error in the Argon pseudocontinuum for the equilibrium file. Two points on the pseudocontinuum curve were given at the same energy for the kT=8.617keV entry. Apec models in XSPEC with a temperature between 7.68 and 8.14keV will have been affected. Non-equilibrium models are unaffected. In XSPEC, the issue manifests as a bin with infinite (or zero) flux, which leads to the fit statistic being a “NaN”. If you have not observed this behaviour you are likely unaffected.

In addition, the continuum units were mislabeled in the FITS files, these have been reset to ‘photons cm^3 s-1 keV-1’.