CHIANTI: APPLICATION TO X-RAY HIGH RESOLUTION SPECTROSCOPY

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The new Version 4 (released in 2002) of the CHIANTI atomic database and software is briefly described. New atomic calculations for ions important in the X-rays are included, together with proton rates, new relativistic continuum calculations and photoexcitation. The application of CHIANTI atomic data to *Chandra* stellar X-ray spectra is presented, together with comparisons with other spectral codes such as APED and SPEX.

1. Introduction

The definition of an accurate atomic database for the X-ray wavelengths is of great importance to the analysis and interpretation of the high-resolution X-ray spectra that the *Chandra* and *XMM-Newton* satellites are now providing.

CHIANTI is a collaborative project involving the Naval Research Laboratory (Washington DC, USA), the Universities of Florence (Italy) and Cambridge (UK) and the Rutherford Appleton Laboratory (RAL, UK).

The CHIANTI package consists of a critically evaluated set of atomic data and user-friendly software. It has unique features in many respects. The atomic data (energy levels, wavelengths, radiative transition probabilities and excitation data) are stored in ascii files. The wavelengths are based on experimental data. The energy levels are normally obtained from NIST[1] but often supplemented by other laboratory values. Lines for which only theoretical energy levels are available are also provided. The radiative data are taken from published literature and where necessary, supplemented by new calculations. Electron and proton collision strengths, taken from the published literature, are scaled and stored in a compact form, following [2]. All the atomic data in the CHIANTI database have been visually displayed and assessed for accuracy. The original sources are documented in each data file, together with detailed comments. The atomic data are kept up-to-date, and the details of each new release published. The atomic data are also provided directly on the WWW. Note that for some ions CHIANTI provides more up-to-date atomic data than NIST.

CHIANTI also includes a number of ancillary data such as standard differential emission measures DEM, elemental abundance and ionization fraction files, and effective areas of many X-ray instruments.

User guides with explanations and examples are provided. A number of Interactive Data Language (IDL) procedures are also provided as part of the CHIANTI package. These include routines to calculate ion level populations, line intensities, temperature- or density-dependent line intensity ratios. Synthetic spectra, eventually folded through effective areas can be created. A package for DEM calculation is also included. All the IDL routines are user-friendly (many have interactive displays) and have been documented with extensive headers giving detailed descriptions and examples. Modifications to the software are logged in a HISTORY file.

The CHIANTI package is freely available at one of the updated CHIANTI homepages, e.g.: `http://www.chianti.rl.ac.uk/` (RAL, UK) or via SolarSoft, a programming and data analysis environment for the solar physics community: `http://www.lmsal.com/solarsoft/`

Users are just asked to acknowledge CHIANTI appropriately in any relevant publication. If a detailed analysis with particular data is carried out, it would also be appropriate to refer to the paper where the original atomic calculations are presented.

The first version of CHIANTI was released in 1996 and is described in [6]. Since then, 3 other major versions have been published. In version 3.0 [7], the package was extended to the X-rays, by including atomic data for the hydrogen and

[1] `http://physics.nist.gov`

helium isoelectronic sequences, inner-shell transitions and satellite lines. Important ions for the X-rays such as Fe XVII-XXIV were updated with new atomic data. In particular, many new energy levels were identified using the [16] compilation.

CHIANTI data are included (directly or indirectly) in many other spectral codes, such as: XSTAR (HEASARC/GSFC - USA); APED/ATOMDB (CfA, Harvard-Smithsonian - USA); XSPEC (HEASARC/GSFC - USA); PINTofALE (CfA, Harvard-Smithsonian - USA); Arcetri Spectral Code (Italy). Users should check which CHIANTI versions are included in these packages, so they can trace back their results to the original atomic data source.

Version 4 of CHIANTI was released in Sept. 2002 [18]. A major change is the inclusion of proton excitation data, principally for ground configuration levels. The inclusion of proton excitation changes the level balance within the ground, and therefore directly affects the forbidden transitions at the optical and infrared wavelengths, but also indirectly affects X-ray lines, for a number of ions (such as Fe XXI).

Photoexcitation and stimulated emission are also included in v.4 by assuming a blackbody radiation field when solving the level population. Photoexcitation is very important at low densities when its effects become comparable with the other collisional excitation processes, or whenever a strong radiation field is present.

New data (published in 2001 and 2002) for the X-rays have been included in Version 4. In particular, new collisional data from close-coupling calculations for important ions that produce strong lines observed by the *Chandra* and *XMM-Newton* gratings (Fe XIX, Fe XX, Fe XXI, Fe XXII, Fe XXIII). New Fe lines have been identified using the results of [1] based on EBIT laboratory measurements.

The continuum routines have been re-written, including a new relativistic free-free, and new free-bound and two-photon continua. The relativistic thermal bremsstrahlung is based on the analytical fits given by [8], while the free-bound uses the the [10] approximation to calculate the gaunt factors for the photoionization cross-sections.

Users should be aware of what atomic data are included in the database, and also of the approximations used. In particular, it is assumed that the plasma is in steady state, optically thin, collisionally dominated and in ionization equilibrium. Line emissivities are only accurate within certain temperature ranges, as described in the CHIANTI papers that describe each release.

Care should be used when applying the atomic data for plasma diagnostic purposes (see [11] for a review). In particular for any estimates that strongly depend on the ionization fractions, such as emission measures and elemental abundances. In regard to the derivation of the chemical abundances, note that most authors have used (and still use) approximate approaches that sometimes result in large errors [3,5]. In regard to estimates of emission measures and densities, note that a large number of ions exhibit an anomalous behaviour, which is still largely neglected in the literature. When anomalous ions are used (for example as they have been for the past two decades for the studies of active stars transition regions), incorrect results are obtained [4].

CHIANTI will continue to grow and be updated in the future. Planned research areas are: develop procedures that account for non-maxwellian electron distributions and non-ionization equilibrium; refined photoexcitation models; new assessments for the X-rays; inclusion of lines originating from levels $n = 3, 4, 5, 6$. Any contributions and suggestions to the CHIANTI team are welcomed.

2. Direct comparison between widely-used codes and observed X-ray spectra

There are very few published high resolution solar spectra in the 1-50 Å range. Solar spectra such as those of the SOLEX [12] and SMM/FCS [14] spectrometers were excellent in terms of spectral resolution, but had some drawbacks for atomic benchmarking. For example, spectra were recorded by scanning over a wavelength range during solar flares, when line intensities were changing by large factors.

There has been a lot of work with regard to spectral line identifications and wavelengths adjustements. For example, [15] revised identifications and wavelengths of the lines in the MEKAL spectral code. However, much work is still required in terms of line identifications and assesment of the accuracy and completeness of presently-available atomic data. For this, high-resolution, high S/N and well calibrated spectra are needed.

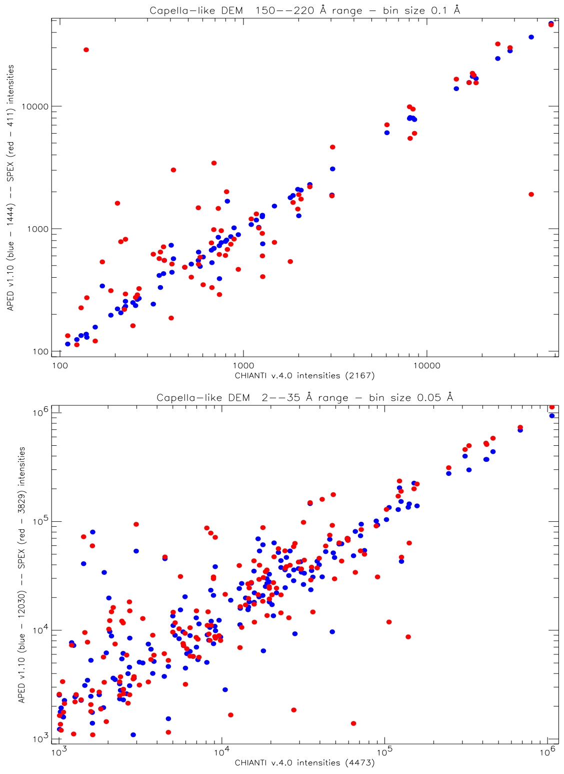

Figure 1. Plots of APED (blue) and SPEX (red) vs. CHIANTI Version 4 line intensities, for an EUV spectral region (top, 150-220 Å) and in the X-rays (bottom, 2-35 Å).

The CHIANTI Version 3 was compared with observed spectra in the 1–50 Å wavelength range in order to test for accuracy and completeness. Paper IV [7] includes a comparative list between CHIANTI-predicted lines and identifications and the observed lines from published high resolution solar spectra. The great majority of X-ray lines are now included in the CHIANTI database. However, there are a number of lines for which radiative data are available, but no collisional data have yet been published. These lines are 'missing' in the CHIANTI database. They are mostly weak lines from Fe XVII-XIX originating from $n = 3, 4, 5, 6$ levels. A list is provided in [7].

Here, we present preliminary results based on benchmarking the atomic data in CHIANTI Version 4 against two solar and stellar high-resolution X-ray spectra. The solar spectrum was recorded on 1980 August 25 in the 5 – 19 Å region by the SMM/FCS in $\simeq$ 18m [14]. The stellar spectrum is a composite of the publicly available *Chandra* HETG Capella spectra extracted by D. Huenemoerder (MIT).

A differential emission measure analysis was performed on the spectra, in order to reproduce the majority of lines.

First, the idea was to compare three different atomic codes, CHIANTI V.4, APED and SPEX. CHIANTI undoubtely has far more accurate and up-to-date atomic data, but the other codes are still widely used by the astrophysical community.

The version 1.10 of the APED atomic database [17], available through XSPEC was used. This version included the entire CHIANTI v.2 database and a collection of other sources for the X-rays, mainly from HULLAC (Hebrew University/Lawrence Livermore Atomic Code) calculations. The version 1.10 of the SPEX [9] code, as available through PintofAle[2] was used. SPEX contains the MEKAL (Mewe-Kaastra-Liedahl) line emissivities of the original Mewe's code [13] with additions of $n = 3, 4$ to $n = 2$ transitions from HULLAC calculations.

A detailed comparison is complex, for many reasons. First of all, because line emissivities are strongly dependent on the temperature, and partially dependent on the density. Second, because the numbers of lines and their wavelengths are different from code to code. A few comaprisons, based on varying the DEM were performed. The largest differences were found when considering peak emission measures at temperatures where Fe XVIII is formed. The DEM derived from the *Chandra* Capella spectra was selected as example here. Line emissivities of the three codes were folded with this DEM distribution, and calculated assuming the same set of parameters, i.e. ionization equilibrium, densities and elemental abundances. The resulting line intensities were then summed into equal bins in wavelengths, for a direct comparison. Obviously, in a few cases the same lines fall in different bins because their wavelengths are different in the codes.

In the EUV, the comparison is satisfactory. For example, in the 150-220 Å region, the deviations between the CHIANTI-predicted intensities and those from SPEX are small (see Fig. 1, top). The APED vs. CHIANTI correlation is almost 1-1, because APED contained almost exclusively

[2] http://heawww.harvard.edu/PINTofALE/-

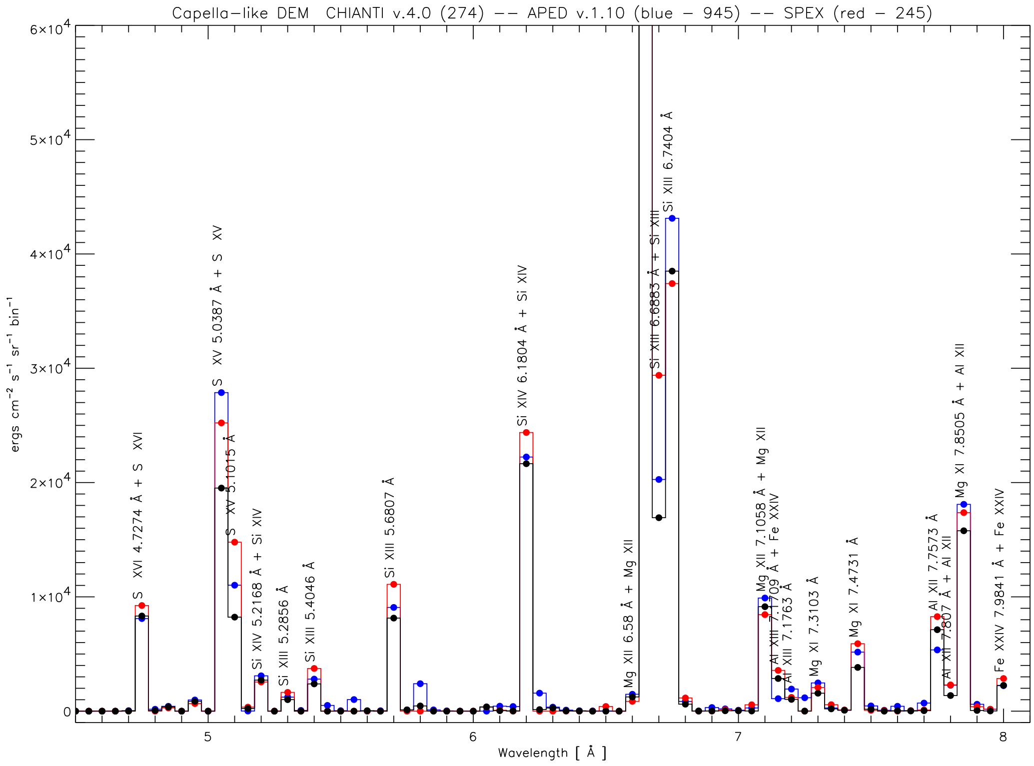

Figure 2. Comparison between APED (blue), SPEX (red), and CHIANTI Version 4 (black) line intensities in the 4-8 Å spectral region. Line identifications are from CHIANTI. Note the good agreement between the codes.

CHIANTI data in this spectral region.

In the X-ray region, larger differences are present, as Fig. 1 (bottom) shows. For the majority of lines, and in particular for the brightest ones, the agreement between the codes is good. For a lot of bins, the disagreements between SPEX and CHIANTI are due to the same 10-30 mÅ wavelength shifts in the MEKAL lines found by [15] and still present in the currently available SPEX (some examples are given below). The differences between CHIANTI and APED are partly due to the fact that APED has a far larger number of lines, including most of the 'missing' CHIANTI lines. Other discrepancies are related to the large differences between the atomic calculations used. Figs. 3,5 show some selected wavelength regions, where the above-mentioned differences are evident.

Finally, after having established in which cases the differences between the various codes are more important, the CHIANTI data have been compared directly with the observations. As a first approximation, CHIANTI simulated spectra have been calculated by convolving the line intensities with gaussian profiles having fixed width. A few sample spectral region are displayed in Figs. 4,6.

For a few regions (as in Fig. 4), the level of accuracy and completeness is good, even down to the weaker lines, where experimental energies (or wavelengths) have not been assigned yet.

For other regions (as in Fig. 6), newly-assigned energy levels and wavelengths are also in good agreement with the observations. However, there is still a considerable number of observed lines for which the disagreement is large. In some of these cases, this is simply due to 'missing' lines. However, a large number of lines still awaits proper identification.

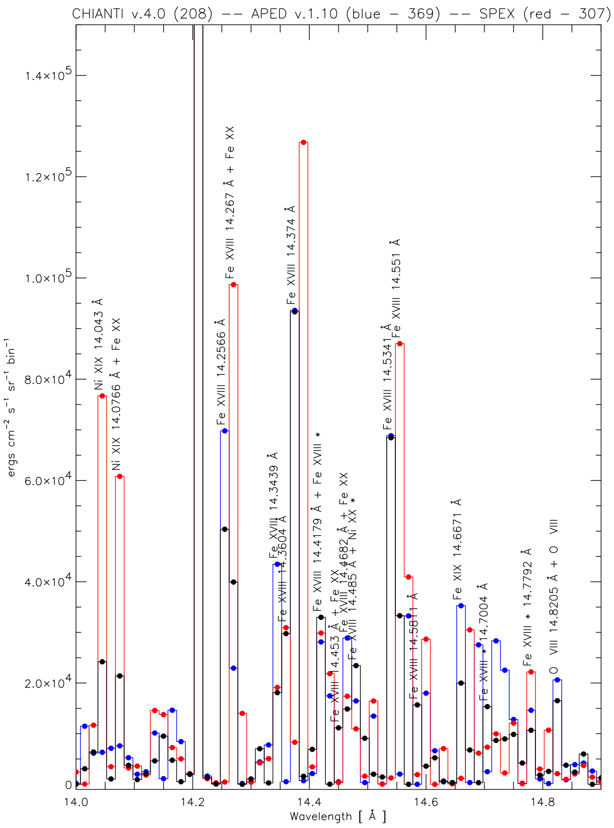

Figure 3. Same as Fig. 2 for the 14-14.9 Å spectral region. Lines marked with an asterisk do not have experimental energy levels. Note the relatively good agreement for most lines. Some of the lines in SPEX are shifted in wavelengths.

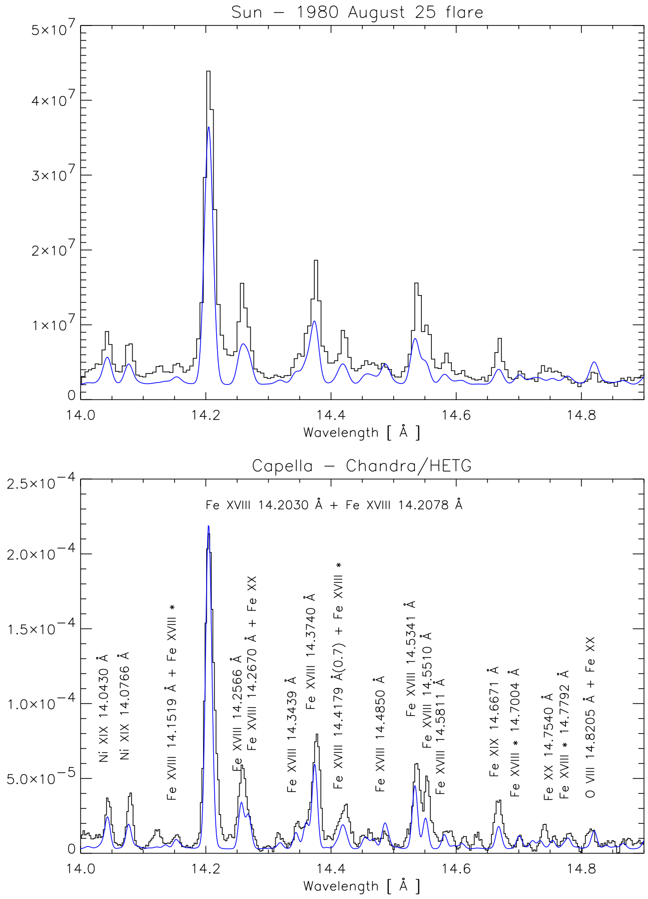

Figure 4. An SMM/FCS solar spectrum (above) and the *Chandra* HETG spectrum of Capella in the 14-14.9 Å region. CHIANTI v.4 simulated spectra are overplotted. Note that most of the lines are identified. Lines marked with an asterisk do not have experimental energy levels.

3. Conclusion

The comparisons between CHIANTI and other spectral codes has shown that for the majority of the brightest lines the agreement is good. The inclusion in CHIANTI version 4 of recent atomic data, in particular for the Fe XVII-XXIV ions, provides a significant improvement in our understanding of the X-ray spectrum. However, there are still many unidentified lines, and lines for which no atomic data are available. The issue of completeness is extremely important, considering that the majority of data taken by *Chandra* and *XMM-Newton* are low-resolution spectra.

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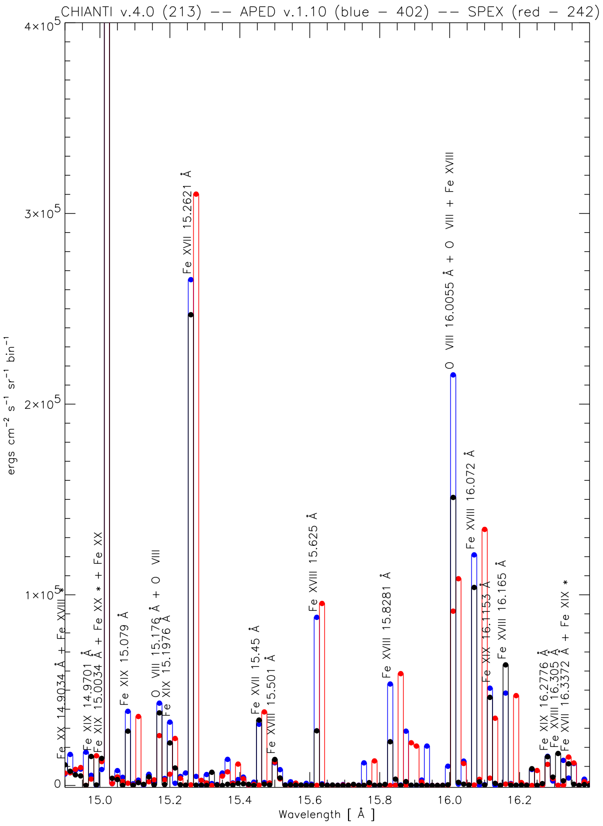

Figure 5. Same as Fig. 2 for the 14.9-16.4 Å spectral region. Some large wavelength shifts in SPEX are evident. SPEX and APED have a few of the lines 'missing' in CHIANTI.

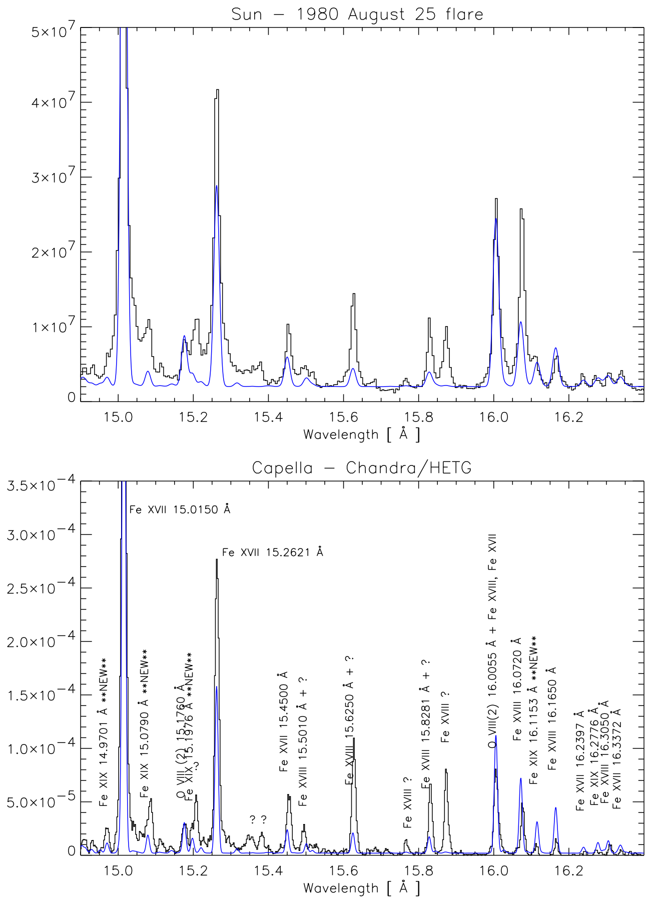

Figure 6. Same as Fig. 4 for the 14.9-16.4 Å spectral region. Lines marked with **NEW** have new experimental wavelengths (and energy levels) assigned in CHIANTI v.4, and have corresponding observed lines. On the other hand, there are many observed lines that are still blends with unidentified lines.

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