Cloudy in the microcalorimeter era: improved energies for Kα transitions

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ABSTRACT

X-ray missions with microcalorimeter technology will resolve spectral features with unprecedented detail. In this work, we improve the H-like Kα energies for elements between 6 ≤ Z ≤ 30 for the release version of the spectral simulation code Cloudy to match laboratory energies. We update the ionization potential (I_{ion}) for these elements and add a fourth-order polynomial to the level energy difference. This brings the release version of Cloudy into a near-perfect agreement with NIST. The updated energies are ~15-4000 times more precise than that of the current release version of Cloudy (C17.02). These new changes will be a part of the next update to the release version, C17.03.

Keywords: High resolution Spectroscopy — X-ray astronomy

INTRODUCTION

Cloudy (Ferland et al. 2017) has long predicted intensities of X-ray lines due to its need to do physical simulations of a non-equilibrium plasma. The original design for one and two-electron species took advantage of scaling relationships along iso-electronic sequences. A series of papers, part of Ryan Porter’s thesis, reporting on this development include Porter et al. (2005) and Porter et al. (2012) on optical emission from He I and Porter & Ferland (2007) on X-ray emission from O VII. While the physics remains close to state of the art, the level energies and line wavelengths derived in the older work had largely sufficient accuracy for the then-operational optical observatories and X-ray missions but not future missions.

The available spectroscopic resolution has increased dramatically with the advent of microcalorimeter missions like Hitomi and the upcoming missions XRISM and Athena. We are now extending Cloudy to meet the spectroscopic challenges of such missions as part of Priyanka Chakraborty’s thesis. The first papers focused on two-electron Fe Kα emission. Chakraborty et al. (2020a) discussed line interlocking and Resonant Auger Destruction (Ross et al. 1978; Band et al. 1990; Ross et al. 1996; Liedahl 2005), and electron scattering escape (ESE) in the Fe XXV Kα complex. Chakraborty et al. (2020b) discussed the Case A to B transition in H- and He-like iron. These atomic processes are very sensitive to line wavelengths due to line overlap with nearby satellites (Mehdipour et al. 2015; Chakraborty et al. 2020a) and require precise energies. This development is a work in progress and will be part of a future release of Cloudy. In the meantime, we have improved the treatment of levels and line energies in the release version of Cloudy, as described below. These improvements will be part of the C17.03 release in late 2020.

RESULTS

The previous versions of Cloudy, through to C17.02, used ionization potentials (I_{ion}) derived by Verner et al. (1996) with four significant digits. Level energies were then derived from the following equation:

$$I_n = I_{ion}/n^2$$

(1)

and the Kα energies were calculated from:

$$E_{Kα}^{old} = I_1 - I_2$$

(2)

The I_{ion}’s in equation 1, stored in the ‘phfit.dat’ file in the Cloudy data directory, were used to compute the photoionization cross-sections in Verner et al. (1996). Although these values are reasonably accurate, microcalorimeter
observations require much better precision. We update the $I_{\text{ion}}$’s in ‘phfit.dat’ for H-like ions with those of NIST (Kramida et al. 2018), keeping up to the eighth significant digits. Our updated version of ‘phfit.dat’ will be included in the C17.03 release.

Following this, we generated a fourth-order polynomial for the energy correction ($\Delta E$) for better agreement with the NIST $K\alpha$ energies:

$$\Delta E = 0.1783Z^4 - 1.8313Z^3 + 27.803Z^2 - 208.04Z + 570.59$$

The updated energies ($E_{K\alpha}^{\text{new}}$) for the $K\alpha$ transitions are given by the following equation:

$$E_{K\alpha}^{\text{new}} = E_{K\alpha}^{\text{old}} + \Delta E$$

Figure 1. The absolute value of the difference between NIST and Cloudy Kα energies versus Kα energies for H-like ions of elements between $6 \leq Z \leq 30$. The x-axis on top shows the corresponding atomic numbers (Z). Red triangles show the difference with NIST for the updated Cloudy (C17.03) energies and the old Cloudy energies appearing in C17.02 and before, respectively. The figure also shows the absolute values of the energy accuracy of the current and future X-ray observatories. Refer to the results section for a detailed description.

Figure 1 shows the absolute values of the differences in $K\alpha$ energies between NIST and Cloudy for H-like ions versus $K\alpha$ energies for elements between $6 \leq Z \leq 30$. The red triangles and green circles show the difference with NIST for the updated Cloudy (C17.03) energies and the old Cloudy energies appearing in C17.02 and before, respectively. The figure also shows the absolute values of the energy accuracy of current and future X-ray observatories. The solid and dashed magenta lines represent the energy accuracy of Chandra HEG and MEG, respectively. The solid and dotted

1 https://cxc.harvard.edu/proposer/POG/html/chap8.html
brown lines indicate the accuracy of RGS1 (1st and 2nd order) and RGS2 (1st and 2nd order) onboard XMM-Newton. The solid black and blue lines represent the energy accuracy of XRISM (Ishisaki et al. 2018) and Athena (Barret et al. 2016), respectively. The updated Kα energies in the revised Cloudy release (C17.03) are ∼ 15-4000 times more precise than that of C17.02. This energy precision is also much superior to the energy accuracy of the current and future X-ray instruments. The improved Cloudy energies will therefore be in excellent agreement with the future microcalorimeter observations.

Finally, we created a patch file: ‘H.total.correction.diff’, which includes the changes leading up to the updated Kα energies ($E_{Kα}^{new}$). These changes will be part of C17.03, and are now posted to the Cloudy user group. Updates on the development of Cloudy are posted to its wiki.

The improvement described here is made only for the Kα energies for elements between Carbon (Z=6) and Zinc (Z=30) since it is negligible for lighter elements. The doublet splitting for the 2p levels is not included in this update but is part of the thesis work and will be incorporated into the next major release of Cloudy. This future version will read extensive data files from NIST instead of using the above correction.

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