Some Ionization and Recombination Data Needs for Cosmic Atomic Plasmas

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Abstract.
Cosmic atomic plasmas can be divided into two broad classes: electron ionized and photoionized. Electron-ionized plasmas are formed in objects such as the sun and other stars, supernova remnants, galaxies, and the intercluster medium in clusters of galaxies. Photoionized plasmas are formed in objects such as planetary nebulae, H II regions, X-ray binaries, and active galactic nuclei. Understanding the spectral and thermal properties of these objects requires an accurate knowledge of the ionization level of the gas. This in turn depends on a reliable understanding of the underlying ionization and recombination processes which determine the ionization balance. Here we review some of the various atomic collision processes which determine the charge state distribution in a cosmic atomic plasma and briefly discuss some of the recent theoretical and experimental advances in generating the needed atomic data. We close by describing the relevant atomic data needs for the near future.

Keywords: elementary processes in cosmic atomic plasmas, electron impact ionization, electron-ion recombination, collisionally-ionized plasmas, photoionized plasmas, ionization balance calculations
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I. INTRODUCTION

Astrophysics drives much of the study into atomic processes in plamas. This is because spectral observations can be used to infer properties of the cosmos. In fact, in many cases spectroscopy is the only way to do this; and even in cases where imaging or timing observations are possible, plasma properties such as abundances, temperatures, and densities are only accessible through spectroscopy. To do all this this we must improve our knowledge of atomic physics in plasmas to the point where discrepancies between observations and models tell us something about the astrophysics of the observed sources and cannot be attributed to errors in the atomic data used in the models.

In this review we focus on the atomic data needed to calculate the ionization structure of cosmic plasmas. Specifically we will highlight some of the various ionization and recombination data needed for the different types of cosmic objects encountered. The rest of this paper is organized as follows: In Sec. II we discuss the two classes of atomic plasmas encountered in astrophysics: electron-ionized (sometimes called collisionally-ionized) and photoionized. This section also discusses the atomic data needed to calculate the ionization balance for each class of plasma. Section III reviews the current status of electron impact ionization (EII) data used in astrophysics. Recent advances in the dielectronic recombination (DR) data used by astrophysicists are reviewed in Sec. IV. Section V presents recent changes in fractional ionic abundance calculations

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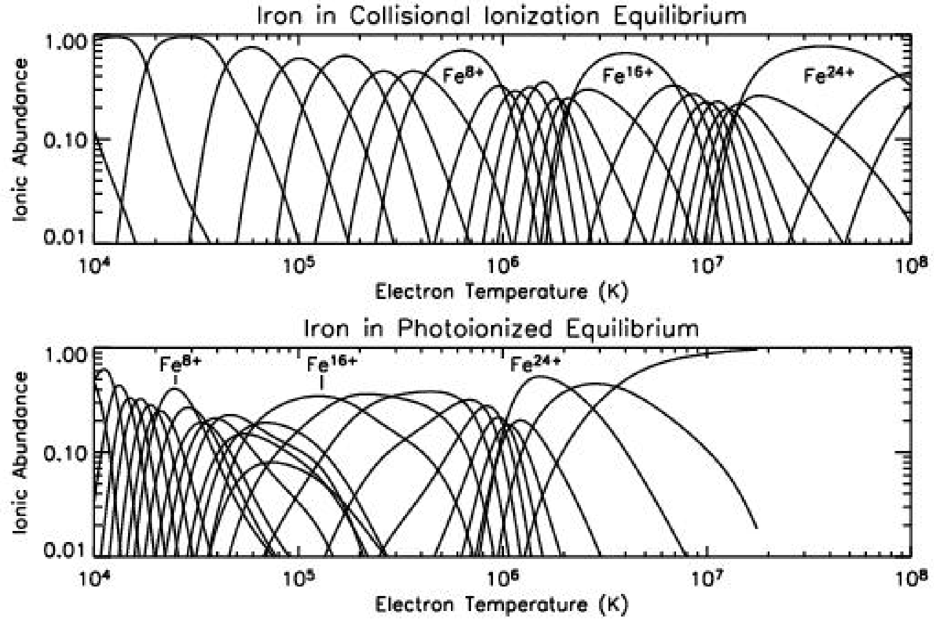

FIGURE 1. Calculated fractional ionic abundances for Fe. The top plot shows the results for collisional ionization equilibrium (CIE) [1]. The bottom plot gives the results for photoionization equilibrium (PIE) of gas with cosmic abundances illuminated by a 10 keV bremmstrahlung ionizing spectrum [4].

due to improvements in the DR and radiative recombination (RR) data available. Results are presented for collisional ionization equilibrium (CIE) and photoionization equilibrium (PIE). Lastly, Sec. VI lists remaining ionization and recombination data needed for modeling cosmic atomic plasmas.

II. TYPES OF COSMIC ATOMIC PLASMAS

Cosmic atomic plasmas can be divided into two broad classes: electron-ionized and photoionized. Electron-ionized plasmas are formed in objects such as the sun and other stars, supernova remnants, galaxies, and the intercluster medium in clusters of galaxies. Photoionized plasmas are formed in objects such as planetary nebulae, H II regions, X-ray binaries, and active galactic nuclei (AGNs).

In electron-ionized gas, the ionization structure at low densities is a function solely of the electron temperature. In CIE, a given ion forms at an electron temperature roughly half that of the ionization potential for that ion (cf., Fig 1). As a result the dominant electron-ion recombination mechanism for most ions is high temperature DR [1]. For temperatures of $\sim 10^4$ K, where significant abundances of H^{0+} and He^{0+} can exist, charge transfer can be an important ionization and recombination process involving systems up to four-times ionized [2]. In some cases EII leading to multiple electron loss can be important. This is particularly true for EII of inner shells leading to the Auger emission of multiple electrons [3].

For photoionized gas, the ionization structure is determined by a number of factors including the shape of the ionizing spectrum, the metallicity of the gas, additional heating and cooling mechanisms, etc. [4, 5]. In PIE, a given ion forms at an electron temperature roughly one-twentieth that of the ionization potential for that ion (cf., Fig 1). As a result, the dominant electron-ion recombination for most ions is low temperature DR [4, 5]. Charge transfer with H^{0+} and He^{0+} can be an important ionization and recombination mechanism for systems up to four-times ionized [6]. Photoionization of innershell electrons and and subsequent Auger emission can also be important [7, 8, 9, 10].

III. ELECTRON IMPACT IONIZATION (EII)

EII can occur through either direct ionization or indirect processes such as excitation-autoionization (EA). Direct ionization is a non-resonant process in which an incident electron transfers energy to a bound electron of the ion, promoting it to the continuum. EA occurs when an incident electron collisionally excites an ion to a state that then decays by autoionization rather than radiative decay and can enhance ionization cross sections by a factor of five or more over direct ionization for ions with certain electron configurations, such as those with one or two valence electrons.

There has been no significant updating of the EII database for astrophysics since 1992. Astrophysicists use the recommended data of Arnaud and Rothenflug [2] for H, He, C, N, O, Ne, Na, Mg, Al, Si, S, Ar, Ca, and Ni, and of Arnaud and Raymond [11] for Fe. The other important set of recommended EII data are those from The Queen's University of Belfast group [12, 13] for elements from H up to and including Ni. The recommended EII data from each group are based on basically the same theoretical and experimental results. Yet surprisingly the recommended rate coefficients are in poor agreement. Differences of up to a factor of 2-3 as has been noted by Kato et al. [14] and Savin [15].

There are a number of challenges to generating reliable EII data. On the experimental side, EII measurement are typically carried out using ion beams of unknown metastable fractions. The resulting lack of unambiguous benchmark measurements has complicated comparison with theory. On the theory side, the infinite number of final states has made the problem computationally challenging. These two difficulties are part of the reason why there has been no significant improvement to the EII database in the last ~ 15 years.

Recently, there have been several promising advances in laboratory studies of EII. Loch et al. [16] measured EII and DR of C^{2+} and used the DR measurements in combination with DR theory to infer the ion beam metastable fraction. Here we refer to the charge of the initial system before ionization or recombination. Fogle et al. [17] have used a gas attenuation cell to directly measure the metastable fraction of their ion beams. With this approach they have carried out EII measurements for C^{2+}, N^{3+}, and O^{4+}. These laboratory advances have also been accompanied by theoretical advances which are discussed in more detail in Refs. [16, 17] and references therein.

IV. DIELECTRONIC RECOMBINATION (DR)

DR is a two-step recombination process that begins when a free electron approaches an ion, collisionally excites a bound electron of the ion and is simultaneously captured into a Rydberg level. The intermediate state, formed by simultaneous excitation and capture, may autoionize. The DR process is complete when the intermediate state emits a photon which reduces the total energy of the recombined ion to below its ionization limit.

Conservation of energy requires that for DR to go forward $E_k = \Delta E - E_b$. Here E_k is the kinetic energy of the incident electron, ΔE the excitation energy of the initially bound electron in the presence of the captured electron, and E_b the binding energy released when the incident electron is captured onto the excited ion. Because ΔE and E_b are quantized, DR is a resonant process. High temperature DR is important in CIE and typically occurs for $E_k \sim \Delta E$. Low temperature DR is important in PIE and typically occurs for $E_k \ll \Delta E$.

Reliable theoretical DR rate coefficients have been a challenge for many years [18], but recently there have been significant advances in DR theory. Modern calculations now exist for K-shell, L-shell, and Na-like ions for all elements from H through Zn [19, 20, 21]. K-shell ions have been extensively benchmarked using EBITs and storage rings and agreement between experiment and theory is typically $\sim 20\%$ [18].

For L-shell ions, there have also been major improvements in DR theory. For high temperature DR theory and experiment agree to within $\sim 35\%$ for the few systems studied. However, the situation is rather mixed for low temperature DR. Difficulties in atomic structure calculations limit the accuracy of DR resonance energies for center-of-mass collision energies $\lesssim 1-3$ eV (see Bryans et al. [1] for a more detailed discussion). Uncertainties in theoretical resonance energies can lead to factors of 2 or more errors in the calculated rate coefficients. Laboratory measurements are often the only reliable way to generate accurate low temperature DR rate coefficients (e.g., [23]). The bottom line is that for L-shell DR in general, little experimental work exists for B-, C-, N-, O-, F-, and Ne-like ions and that theoretical DR rate coefficients for temperatures $\lesssim 3 \times 10^4$ K must be used with caution whether they are for collisionally-ionized or photoionized plasmas.

For ions with an open M-shell, DR theory is even more challenging than for L-shell ions. For example, for Fe^{13+} and Fe^{14+} modern theory does a poor job of predicting DR resonance energies and strengths for collision energies $\lesssim 20$ eV [24, 25]. This is especially an issue for low temperature DR. For these cases, difference of up to a factor of two are found between experimentally-derived and theoretical DR rate coefficients [24]. A significant amount of experimental and theoretical work remains to generate reliable DR data for M-shell ions of all cosmically abundance elements.

Reliable DR data for Fe M-shell ions are particularly important for analyzing spectra from AGN warm absorbers. Recent *Chandra* and *XMM-Newton* satellite observations of these sources have detected absorption between 15-17 Å due to Fe M-shell ions [26, 27]. The blend of numerous absorption lines, due mainly to $2p-3d$ photoexcitation, form an unresolved transition array (UTA). The shape, central wavelength, and equivalent width of the UTA can be used to diagnose the properties of these AGN warm absorbers [28].

AGN models, however, which fit absorption features from second and third row elements are unable to reproduce correctly the observed UTAs. The models appear to predict too high an ionization level for iron. Netzer et al. [29] attribute this to an underestimate of the low temperature DR rate coefficients for Fe M-shell ions. Subsequent modeling studies support this hypothesis [30, 31].

These errors in the DR data used should not be surprising. The data used are nearly 20 years old, calculated when computational power was a small fraction of what it is now. Additionally the M-shell DR data had been calculated with a focus on high temperature plasmas [11, 32]. Moreover, underestimated low temperature DR rate coefficients should have been expected based on experimental work predating the observations [33, 34].

Communication between the astrophysics and atomic physics communities is sometimes poor. But issues like this have strengthened some of the ties between the two fields. As a result, in the last couple of years there has been a concerted experimental and theoretical effort to generate reliable DR data for Fe M-shell ions [24, 25, 35, 36].

V. IONIZATION EQUILIBRIUM CALCULATIONS

Plasmas encountered in astrophysics are often optically-thin, low-density, dust-free, and in steady-state. Under these conditions, ionization and recombination balance one another and the fractional ionic abundances can readily be calculated. But the accuracy of these ionization equilibrium calculations is determined by the reliability of the ionzation and recombination used in the models. Hence the recent publication of state-of-the-art DR data [19, 20, 21] and RR data [37, 38] for K-shell, L-shell, and Na-like ions of all elements from H through to Zn represents a significant advance.

Bryans et al. [1] used these modern DR and RR data to generate new CIE results for H through Zn. The solid curve in Fig. 2 shows their fractional ionic abundances for Fe using the data of Badnell and colleagues [19, 38]. Similar results are found using the data of Gu [20, 21, 37]. The dashed curve in Fig. 2 show the results for Fe from Mazzotta et al. [39] which represented the state-of-the-art for CIE calculations until their work was superceded by that of Bryans et al.

Significant differences are found between the results of Bryans et al. [1] and those of Mazzotta et al. [39]. Peak fractional abundances for the various elements differ by up to 60%. At 0.1 fractional ionic abundances, differences between the two datasets of up to a factor of 5 are found. At 0.01, these differences can grow to a factor of 11. The temperature of peak formation shifts for some ions by up to 20%. Lastly, ions with particularly large differences include Mg, Al, Ca, Fe, Co, and Ni.

The new DR and RR data of Badnell and colleagues have also been incorporated into CLOUDY, a commonly used code for modeling photionized gas [4]. The solid curve in Fig. 3 shows the calculated PIE fractional abundances for Fe in a gas of cosmic abundances illuminated by a 10 keV bremmstrahlung ionizing spectrum. The dashed curve shows the same results but using the old recommended DR and RR data of Mazzotta et al. [39]. As can be readily seen, differences for some charge states can approach a factor of 50.

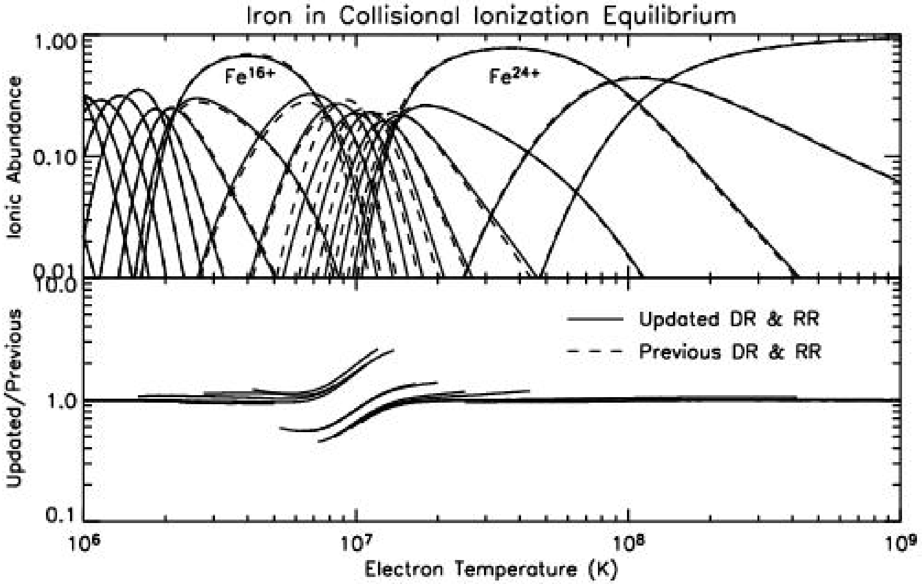

FIGURE 2. Calculated fractional ionic abundance for Fe in CIE [1]. The *solid curves* in the top plot shows the results using the state-of-the-art DR and RR data of Badnell et al. [19] and Badnell [38], respectively. The *dashed curves* use the previously recommended DR and RR data of Mazzotta et al. [39]. The bottom plot shows the ratio of the new to old fractional ionic abundances for abundances > 0.01. Little to no differences are seen in the ratio for charge states of Mg-like or less highly ionized as modern electron-ion recombination data for these isoelectronic sequences are only now becoming available (e.g., [35, 38]) and have yet to be incorporated into the models.

VI. REMAINING ATOMIC DATA NEEDS

The current oustanding data needs for calculating the ionization balance of collisionally-ionized and photoionized cosmic atomic plasmas can be summarized succinctly:

- EII data for K-, L-, and M-shell ions.
- DR for L- and M-shell ions.
- Improved atomic structure calculations for reliable low temperature DR data.
- RR for M-shell ions.
- Photoionization cross sections.
- Innershell ionization/Auger yields.
- CT data for H^{0+} and He^{0+} with systems ionized ≤ 4 times.

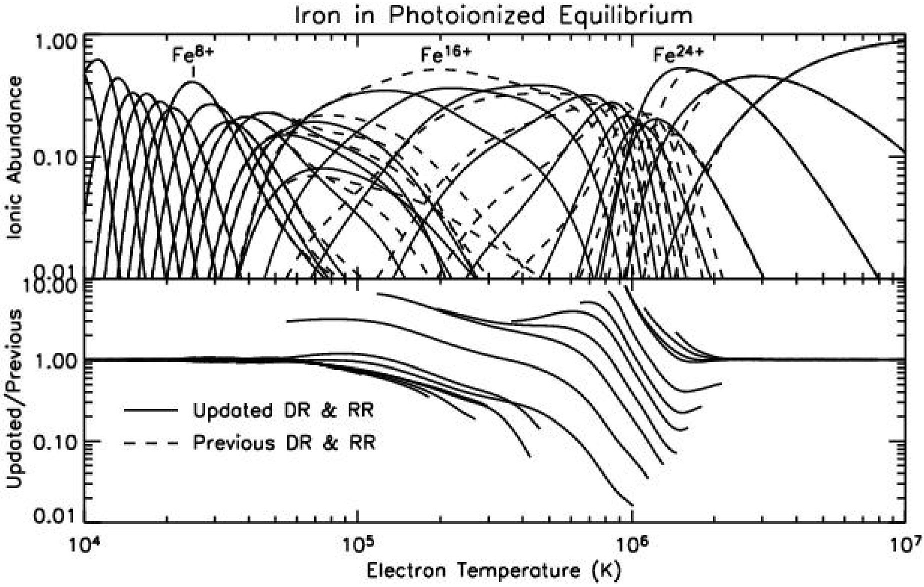

FIGURE 3. Calculated fractional ionic abundance for Fe in PIE as described in Fig. 1. The *solid curves* in the top plot shows the results using the state-of-the-art DR and RR data of Badnell et al. [19] and Badnell [38], respectively. The *dashed curves* use the previously recommended DR and RR data of Mazzotta et al. [39]. The bottom plot show the ratio of the new to old fractional ionic abundances for abundances > 0.01. Little to no differences are seen in the ratio for charge states Mg-like or less highly ionized as modern electron-ion recombination data for these isoelectronic sequences are only now becoming available (e.g., [35, 38]) and have yet to be incorporated into the models.

Here we have focused on the first three of these points. But significant improvements are still needed for much of the ionization and recombination data used in astrophysics. We propose that these data be generated with an aim for an accuracy of $\lesssim 35\%$ to match that of the best experimental and theoretical work.

Note added in manuscript.–After this paper was submitted, a re-evaluation and updating of the EII data base was published by Dere [40]. We plan to incorporate these new EII data into our CIE model [1] and will present the results elsewhere.

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