NASA LAW, February 14-16, 2006, UNLV, Las Vegas

Collisional Ionization Equilibrium for Optically Thin Plasmas

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ABSTRACT

Reliably interpreting spectra from electron-ionized cosmic plasmas requires accurate ionization balance calculations for the plasma in question. However, much of the atomic data needed for these calculations have not been generated using modern theoretical methods and their reliability are often highly suspect. We have utilized state-of-the-art calculations of dielectronic recombination (DR) rate coefficients for the hydrogenic through Na-like ions of all elements from He to Zn. We have also utilized state-of-the-art radiative recombination (RR) rate coefficient calculations for the bare through Na-like ions of all elements from H to Zn. Using our data and the recommended electron impact ionization data of Mazzotta et al. (1998), we have calculated improved collisional ionization equilibrium calculations. We compare our calculated fractional ionic abundances using these data with those presented by Mazzotta et al. (1998) for all elements from H to Ni, and with the fractional abundances derived from the modern DR and RR calculations of Gu (2003a,b, 2004) for Mg, Si, S, Ar, Ca, Fe, and Ni.

1. Introduction

Electron-ionized plasmas (also called collisionally ionized plasmas) are formed in a diverse variety of objects in the universe. These range from stellar coronae and supernova remnants to the interstellar medium and gas in galaxies or in clusters of galaxies. The physical properties of these sources can be determined using spectral observations coupled with theoretical models. This allows one to infer electron and ion temperatures, densities, emission measure distributions, and ion and elemental abundances. Reliably determining these properties requires accurate fractional abundance calculations for the different ionization stages of the various elements in the plasma (i.e., the ionization balance of the gas).

Since many of the observed sources are not in local thermodynamic equilibrium, in order to determine the ionization balance of the plasma one needs to know the rate coefficients for all the relevant ionization and recombination processes. Often the observed systems are optically-thin, low-density, dust-free, and in steady-state or quasi-steady-state. Under these conditions the effects of any radiation field can be ignored, three-body collisions are unimportant, and the ionization balance of the gas is time-independent. This is commonly called collisional ionization equilibrium (CIE) or sometimes coronal equilibrium.

Our work has collected the most recent state-of-the-art theoretical DR and RR rate coefficients and, based on these data, calculated new CIE ionic fractional abundances of all elements from H to Zn.

2. Dielectronic Recombination

Badnell et al. (2003) have calculated the DR rate coefficients using the AUTOSTRUCTURE code for the H- through Na-like isoelectronic sequences of all elements from He through to Zn. We use the convention here of identifying the recombination process by the initial charge state of the ion. These new DR data have been collected together and are available online Badnell (2006a). In addition, some of the original data has been refitted so as to extend the validity of the fits to lower temperatures. Gu (2003a) has calculated DR rate coefficients using the FAC code for the H- through Ne-like isoelectronic sequences of Mg, Si, S, Ar, Ca, Fe and Ni and for the Na-like sequence for Mg through Zn (Gu 2004). For ionization stages not included in the calculations of Badnell (2006a) and Gu (2003a, 2004), we use the DR rate coefficients recommended by Mazzotta et al. (1998) for elements up to and including Ni and Mazzotta (private communication) for Cu and Zn.

3. Radiative Recombination

Gu (2003b) has calculated RR rate coefficients for ions of Mg, Si, S, Ar, Ca, Fe and Ni for bare through F-like ions using FAC. Badnell (2006c) has calculated RR rate coefficients for all elements from H through to Zn for the bare through Na-like isoelectronic sequences using AUTOSTRUCTURE. These are available online (Badnell 2006b). As for DR, we use the RR rate coefficients recommended by Mazzotta et al. (1998) and Mazzotta (private communication) for ions not calculated by Gu (2003b) or Badnell (2006b).

4. Results & Conclusions

The differences in our calculated CIE fractional abundances relative to those of Mazzotta et al. (1998) are, in general, much larger than the differences between our results and the results using the data of Gu (2003a,b, 2004). In the former case, peak abundance differences of nearly 60% are found and the differences can be larger than 1000% at fractional abundances down to 0.01. For the latter case, peak abundance differences are within 10% and differences for fractional abundances down to 0.01 are within 50%. This reflects the fact that the modern DR and RR data are in better agreement with one another than with the older data.

Full results can be found in Bryans et al. (2006) but, for illustrative purposes, we present here our calculated CIE fractional abundances for Fe. Fig. 1 shows how the AUTOSTRUCTUREbased results compare with those of Mazzotta et al. (1998), and Fig. 2 shows the comparison between the AUTOSTRUCTURE-based calculations and the FAC-based calculations.



Fig. 1.— Ionization fractional abundance versus electron temperature for Fe. The upper graph shows the AUTOSTRUCTURE-based results (*solid curves*, labeled 'AUTO') and the Mazzotta et al. (1998) results (*dashed curves*, labeled 'Mazz'). The lower graph shows the ratio of the calculated abundances.

Further progress in CIE calculations will require a concerted theoretical and experimental effort to generate the remaining needed atomic data. Modern DR and RR data are urgently needed for ions with 12 or more bound electrons. There is also a need for improved electron impact ionization (EII) and charge transfer (CT) data. There has been no significant revision or laboratory benchmarking of the recommended EII database since around 1990. Additionally, the latest compilation of recommended CT rate coefficients dates back to Kingdon & Ferland (1996). We propose that all future data for DR, RR, CT, and EII should be generated aiming for an accuracy that matches that of the modern electron-ion recombination measurements and calculations. Such an accurate and up-to-date database is crucial for being able to produce reliable CIE calculations for the astrophysics community.



Fig. 2.— Same as Fig. 1 but replacing the Mazzotta et al. (1998) results with the FAC-based results (*dashed curves*, labeled 'FAC').

This work was supported in part by the NASA APRA Program.

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