Title: Calculations of Atomic Data for X-Ray Astrophysics

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Abstract: The interpretation of cosmic spectra relies on a vast sea of atomic data which are not readily obtainable from analytic expressions or simple calculations. Rather, their evaluation typically requires state-of-the-art atomic physics calculations, with the inclusion of weaker effects (spin-orbit and configuration interactions, relaxation, Auger broadening, etc.), to achieve the level of accuracy needed for use by astrophysicists. Our research program is focused on calculating data for three important atomic processes, 1) dielectronic recombination (DR), 2) inner-shell photoabsorption, and 3) fluorescence and Auger decay of inner-shell vacancy states. Our DR work has produced rate coefficients for all H-like through Na-like ions up to nuclear charge Z=30. Present work is focused on the more challenging third-row isoelectronic sequences, such as M-shell iron ions which are responsible for X-ray absorption in active galactic nuclei. K-shell photoabsorption cross sections for all oxygen and neon ions will also be presented and compared to existing experimental measurements. These newly computed data have already been used in conjunction with observed X-ray spectra to infer elemental abundances in the ISM. We also present new fluorescence yields for all second-row K-shell-vacancy isoelectronic sequences, where the inclusion of higher-order effects frequently give results that differ considerably from the currently recommended data, and where we show in particular the inadequacy of the commonly-used configuration-averaged approximation. This work is supported in part by the NASA APRA program.
Calculation of Atomic Data for X-Ray Astrophysics

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ABSTRACT

The interpretation of cosmic spectra relies on a vast sea of atomic data which are not readily obtainable from analytic expressions or simple calculations. Rather, their evaluation typically requires state-of-the-art atomic physics calculations, with the inclusion of weaker effects (spin-orbit and configuration interactions, relaxation, Auger broadening, etc.) to achieve the level of accuracy needed for use by astrophysicists. Our research program is focused on calculating data for important atomic processes: 1) dielectronic recombination (DR), 2) inner-shell photoabsorption, and 3) fluorescence and Auger decay of inner-shell vacancy states. Our DR work has produced rate coefficients for all Li-like through Na-like ions up to nuclear charge Z=30. Present work is focused on the more challenging third-row isoelectronic sequences, such as M-shell iron ions which are responsible for X-ray absorption in active galactic nuclei. K-shell photoabsorption cross sections for all oxygen and neon ions will also be presented and compared to existing experimental measurements. These newly computed data have already been used in conjunction with observed X-ray spectra to infer elemental abundances in the ISM. We also present new dielectronic yields for all second-row K-shell-isoelectronic sequences, where the inclusion of higher-order effects frequently give results that differ considerably from the currently recommended data, and where we show in particular the inadequacy of the commonly-used configuration-averaged approximation.

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1 Dielectronic Recombination

By performing state-of-the-art R-matrix calculations, including Auger broadening and relaxation effects, we have determined new photoabsorption data for all oxygen and neon ions. Previous calculations for ionized species had only considered non-resonant [15] or 1s→2p [16] contributions (see Figs. 3 and 4).

2 K-Shell Photoabsorption of O and Ne Ions

3 K-Shell Fluorescence and Auger Yields

Our investigations of K-shell fluorescence from second-row ions began with an assessment of the widely-used data base of [17], where we found several sources of inaccuracies [18]. More recently, we have assessed the importance of many-body interactions in the form of configuration interaction (CI) in the accurate calculation of a number of atomic properties relevant to astrophysics. The specific example of the K-shell fluorescence yields of core-excited Li-like ions was calculated, the inclusion of CI lead to significant values of the fluorescence yield as opposed to the single configuration result of zero [19]. For convenient astrophysical modeling, a two-parameter fit to the fluorescence yields is provided (see Fig. 5). It is expected that CI will be important in the accurate calculation of a variety of atomic processes occurring in astrophysical plasmas.

We have also shown that the fluorescence yields of the eight LSJ states arising from the five-electron K-shell-vacancy 1s212p2 configuration are strongly LSJ-dependent over the entire isoelectronic series [20]. This finding implicitly suggests that the individual transition rates, radiative and Auger, are also strongly LSJ-dependent (see Fig. 6). But there is nothing special about the five-electron K-shell-vacancy system; the same general phenomenology should be true for other isoelectronic sequences with fewer than ten electrons as well, i.e., the conclusions for the system considered should be quite general. For use in astrophysical modeling codes, then, fluorescence yields, and the radiative and Auger rates associated with them, need to be given for individual LSJ states; the oft-used [17] data compilation contains configuration-average fluorescence yields and these are quite inappropriate for most astrophysical situations. In other words, if configuration averages are sought, they cannot be general but must be tailored to the specific astrophysical situation being considered.

References


Figure 1 Total ground-level rate coefficient for FeII+. Blue solid curve, DRSCF; blue dashed curve, RR; all AuTOSTRUCTURE result from Badnell (2006) [1]. Red solid and dashed curves, recommended RR and RR data of Arnal and Raymon [2]. Shaded areas denote photoionization and electron-collisional plasma temperature ranges.

As an improvement to an earlier study [3], we have calculated dielectronic recombination rate coefficient spectra for ScII and TiII ions as a first step toward the assembly of a database I for the Arlike isoelectronic sequence required for modeling of dynamic finite-density plasmas [5]. Our theoretical spectra contain dominant ΔV=0 and ΔV=1 core excitations channels and exhibit nearly all features found in a recent storage ring experiments [6, 7]. In order to compare Maxwellian-averaged rate coefficients, which are of main interest to the astrophysics community, we have developed an iterative deconvolution procedure that enables us to extract the cross section from storage ring data.

Figure 2 Modeling of the resonant part of the experimental [7, 6] DR spectra in the vicinity of the 1S2 resonance. Solid (AS) red curve in both cases (a) for N<sub>c</sub> and (b) for T<sub>e</sub> is the relevant part of our computed spectra, and the solid blue curve is the best fit of the experiment (gray data points) to J-converted Fano profile. Each 1S2 Fano profile is illustrated as blue dotted curve. The fine structure splitting ∆E = E<sub>2S</sub> - E<sub>1S</sub> was fixed during the fit and fixed during the final stage of optimization. The shaded area below 4 meV is an unexplained enhancement that is present even in the spectra of base ions.

Figure 3 (left) While neutral iron cross sections had already been computed by Gorczyca et al. (2000) [9], we report for the first time the K-shell photoabsorption cross sections for all higher ionization stages of neon. Of particular importance, we find that Ne II and Ne III cross sections dominate over the neutral Ne I cross sections since the latter has a full 2p sub-shell and therefore cannot absorb any further 1s-2p photons. Therefore, even though the abundance of Ne II is typically reduced by a factor of 2-5 compared to the Ne I abundance, and Ne III is reduced even more, the observed X-ray spectra should show predominantly Ne II and Ne III absorption lines. These data are compared to the observed Ne X-ray emission data. (right) Jafft et al. (2006) [8] flux spectra of the neon K-shell absorption region for the Cygnus black hole X-ray binary. The dashed lines indicate the positions of the identified features.

Figure 4 (left) High-energy photoionization cross sections of Oxygen ions showing the structure of the K-edge: red solid curve, CREE-RB-R-matrix by Garcia et al. (2005) [14]. Yellow solid curve, CCC-BPR-matrix by Pradhan et al. (2003) [16]. Dashed curve, B** model by Reilman & Manson (1979) [17]. (right) Flux spectra and line identifications of the oxygen edge region for Cyg X-2 and Cyg X-1 ObsID 107 [18].

Figure 5 Calculated fluorescence yields of Li-like ions for K-shell vacancy 1s212p2 configuration is shown in the LSJ-states.