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

Calculation of Atomic Data for NASA Missions

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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 NASA-supported 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. Some additional details and examples of our recent findings are given below.

1. Dielectronic Recombination

We have completed the computation of DR rate coefficients, including fitting formula, for all H-like through Na-like ions up to nuclear charge $Z = 30$. For the Fe ions, we are able to benchmark R-matrix and AUTOSTRUCTURE results using storage ring experiments. These data are available electronically at `http://homepages.wmich.edu/~gorczyca/atomicdata` and `http://amdpp.phys.strath.ac.uk/tamoc/DATA/`. Our latest challenging work is for 3^{rd} and 4^{th} row elements where partially filled $n = 3$ and $n = 4$ shells lead to more complicated calculations (relaxation, larger configuration-interaction, etc.)

An example of our latest difficulties when addressing occupation of the $n = 3$ shell is DR of Ne-like Mg III. Figure 1 shows how the computed DR rate coefficients are extremely sensitive to the choice of atomic orbitals, and thus more sophisticated approaches for determining

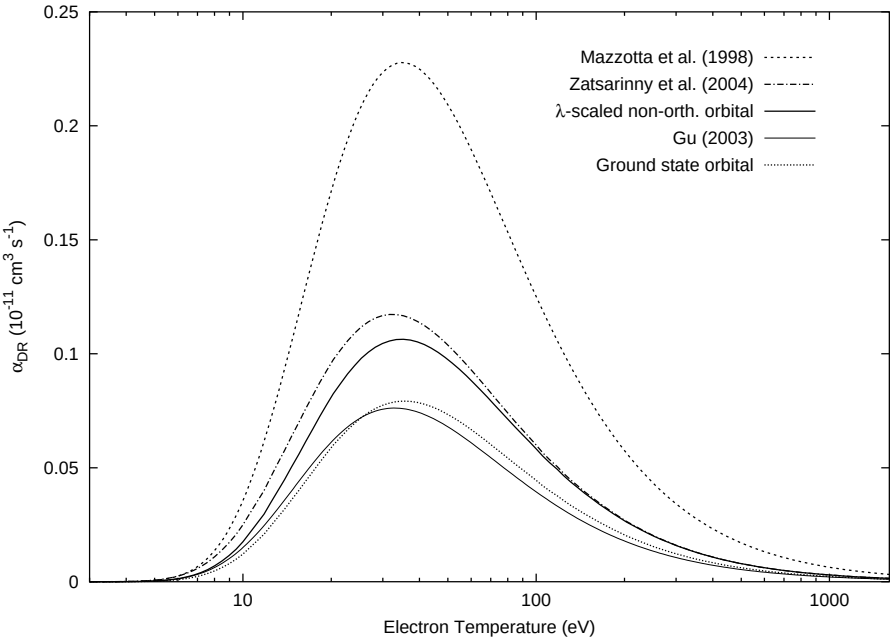

Fig. 1.— Sensitivity of Maxwellian DR rate coefficients to the choice of target orbitals used.

atomic structure is necessary. Our latest calculations utilizing λ-scaled non-orthogonal orbitals resolve a factor of ≈ 2 difference between our earlier results (Zatsarinny et al. 2004) and the results of Gu (2003), and are less than half the recommended data of Mazzotta et al. (1998).

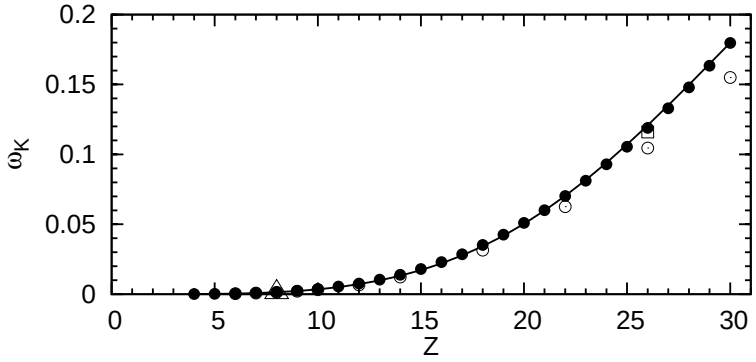

Fig. 2.— Calculated fluorescence yields ω_K^{CI} (solid circles) and fitted formula $\omega_K^{fit} = [1 + (aZ^4 - bZ^7)^{-1}]^{-1}$ (solid line) for K-shell vacancy Li-like $1s2s^2$ ions.

2. K-Shell Fluorescence Yields

We have also calculated new fluorescence yields for all second-row K-shell-vacancy isoelectronic sequences, where the inclusion of higher-order effects (fine structure, configuration interaction, term dependence, etc.) frequently give results (Gorczyca et al. 2003) that differ considerably from the currently recommended data of Kaastra & Mewe (1993). For instance, recent work on the Li-like sequence (Gorczyca et al. 2006) demonstrated the importance of $1s2s^2 + 1s2p^2$ CI: this state cannot radiate in a single-configuration model description. Further, we were able to develop a two-parameter fitting formula for all Z: $\omega_K^{fit} = [1 + (aZ^4 - bZ^7)^{-1}]^{-1}$. These results are shown in Figure 2.

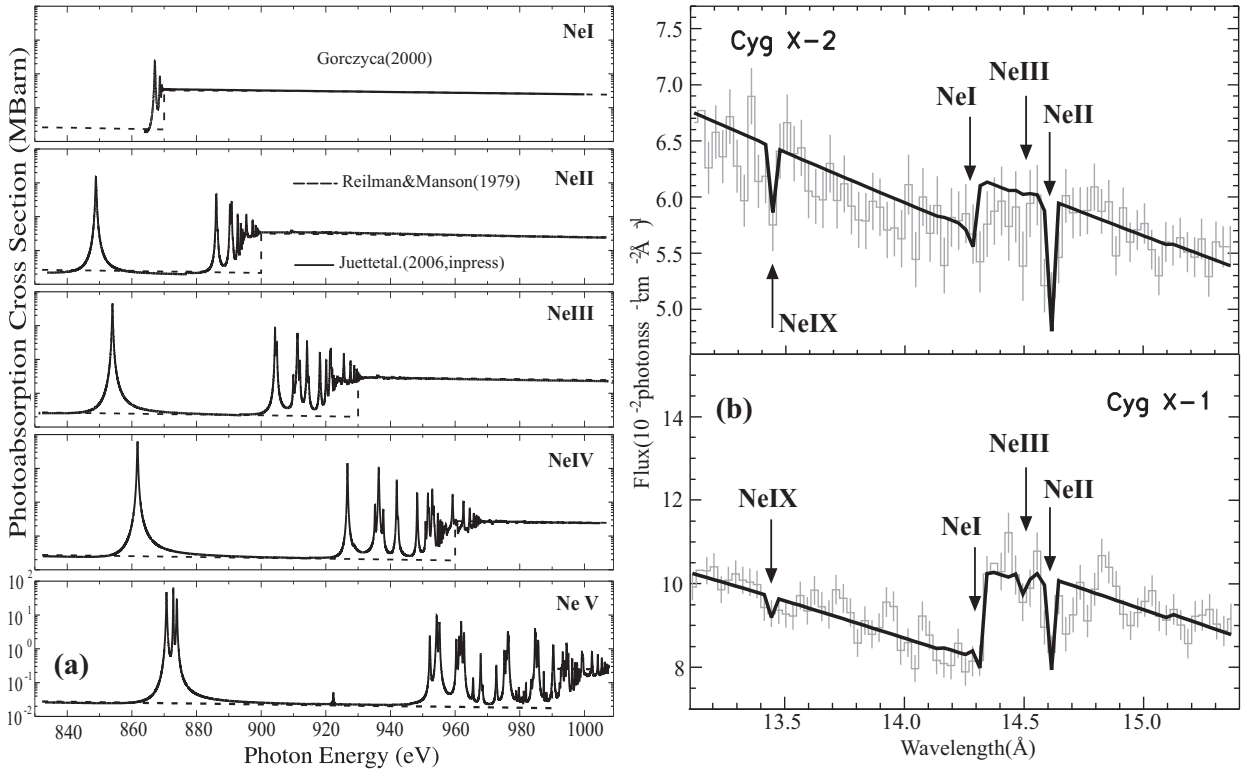

Fig. 3.— (a) Theoretical R-matrix photoabsorption cross sections for neutral neon (Gorczyca 2000) and ionized neon (Juett et al. 2006) compared to independent particle results (Reilman & Manson 1979) which do not include resonances. (b) Using our atomic cross sections $\sigma(\lambda)$, X-ray absorption spectra of the Cygnus black hole X-ray binary were fitted using intensities $I = I_0 e^{-\sigma(\lambda)N}$ to determine elemental abundances (column densities N) by Juett et al. (2006).

3. K-Shell Photoabsorption

We have recently calculated K-shell photoabsorption cross sections for all oxygen and neon ions (see Fig. 3a for neon ions). While results for the neutral O I and Ne I species compare favorably to experimental measurements (Gorczyca & McLaughlin 2000; Gorczyca 2000), our results for ionized oxygen (Garcia et al. 2005) and neon (Juett et al. 2006) are the only complete data available to our knowledge. These newly computed data have already been used to infer elemental abundances in the ISM by Juett et al. (2004, 2006) (see Fig. 3b for neon ion abundances).

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

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