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Final Progress Report for NAG5-9581

Dear Dr. Crane,

This letter is the final progress report for the SARA grant **NAG5-9581** entitled **"Improved Simulations of Astrophysical Plasmas: Computation of New Atomic Data"** which began on 1 March 2001 and ended on 28 February 2004.

1 Introduction

Our research program is designed to carry out state-of-the-art atomic physics calculations crucial to advancing our understanding of fundamental astrophysical problems. We redress the present inadequacies in the atomic data base along two important areas: dielectronic recombination and inner-shell photoionization and multiple electron ejection/Auger fluorescence therefrom. All of these data are disseminated to the astrophysical community in the proper format for implementation in spectral simulation codes.

2 Review of Progress

2.1 Brief Summary

The following is an initial, brief summary of the atomic physics research we have performed over the grant period, which was funded by NASA Space Astrophysics Research and Analysis Program grant NAG5-10448:

- Benchmarking of our MCBP and R-matrix DR calculations with experimental measurements performed at the Test Storage Ring (5 iron ions, 4 papers);

- Systematic calculations and fitting formulas for DR of C-like, O-like, F-like, and Ne-like isoelectronic sequences (95 ions, 3 published papers and one more in preparation, tables of fitting coefficients on our web page);
- Assesment of the exisiting fluorescence/Auger database (1 paper);
- Peripheral collisional (5 papers), photoionization (2 papers), photodetachment (3 papers), and DR perturbative vs. R-matrix comparison (1 paper) studies.

A more detailed description of each of these accomplishments is given below.

2.2 General Considerations

Our research program is designed to carry out state-of-the-art atomic physics calculations crucial to advancing our understanding of fundamental astrophysical problems. We have redressed the present inadequacies in the atomic data base along two important areas: dielectronic recombination and multiple fluorescence/Auger decay of inner-shell vacancy states. All of these data have been disseminated to the astrophysical community in the proper format for implementation in spectral simulation codes.

With the available funding, we were able to support a postdoctoral fellow for only two of the three years of the grant period. On November 1^{st}, 2001, we hired Dr. Oleg Zatsarinny, an expert in atomic collision calculations, and the former director of theoretical physics at Uzhgorod University, Ukraine.

Dr. Zatsarinny thus worked at WMU for two years. During that time, he diligently performed DR calculations for *95 different ionic systems*, as is detailed below.

Besides this large comprehensive effort of computing along isoelectronic sequences, our other two main areas of research have been 1) the benchmarking of theoretical and experimental DR rate coefficients for several iron ions, and 2) the assessment of the fluorescence/Auger data base in current use. Further work in collisional excitation, photoionization, and photodetachment made up smaller peripheral projects.

2.3 DR of O-like Fe XIX: Laboratory Measurements and Theoretical Calculations

In Savin et al. (2002) we presented our results for DR measurements and calculations of oxygen-like Fe XIX forming Fe XVIII. Measurements were carried out using the heavy ion Test Storage Ring (TSR) at the Max Planck Institute for Nuclear Physics in Heidelberg, Germany. We also calculated the relevant DR resonance strengths and energies using our state-of-the-art AUTOSTRUCTURE code which uses a perturbative MCBP method (Badnell 1986). Overall reasonable agreement is found between experiment and our theoretical calculations.

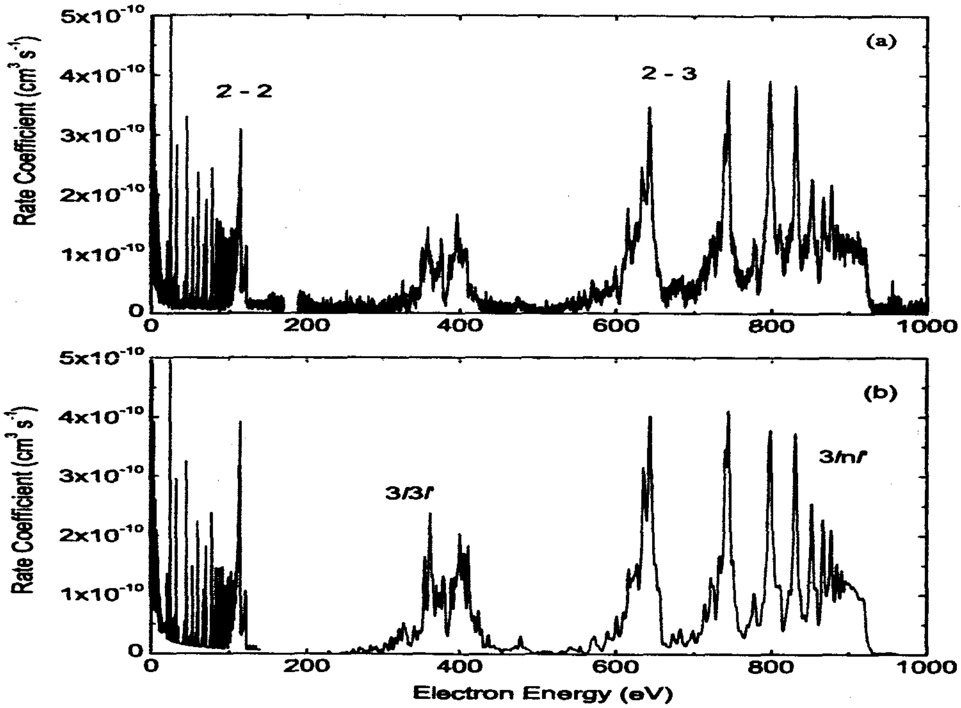


Figure 1: Fe XIX DR laboratory rate coefficients due to $2 \to 2$ ($e^- + 2s^2 2p^4 \to 2\ell^6 nl'$) and $2 \to 3$ ($e^- + 2s^2 2p^4 \to 2\ell^6 3lnl'$) core excitation; the latter are clearly seen in the collisionally ionized zone ($kT \approx 300 - 1000$ eV, Mazzotta et al. 1998) as the $3l3l'$ ($kT \approx 400$ eV), $3l4l'$ ($kT \approx 600$ eV), $3l5l'$ ($kT \approx 750$ eV), etc., manifolds: (a) the TSR experiment (Savin et al. 1999, 2002), and (b) the present MCBP calculations.

We have used our measurements to produce a Maxwellian-averaged rate coefficients for DR of Fe XIX. Our experimentally-derived rate coefficient is estimated to be good to better than 20%. Our AUTOSTRUCTURE results are in excellent agreement with our experimental rate coefficient, as seen in Fig. 1. However, these investigations turn up inaccuracies in the earlier recommended data by Mazzotta et al. (1998), Roszman (1987), and Jacobs et al. (1977), as seen in Fig. 2, indicating the utility of the newly computed data.

2.4 Calculations of Fluoresence and Auger Yields

In Gorczyca et al. (2003), we have investigated the accuracy of the fluoresence and Auger yields due to innershell ionization of boron-like ions and neon-like ions producing a $1s$ hole, thereby creating, respectively, beryllium-like and fluorine-like ions which can then either radiatively stabilize or autoionize. We have carried out calculations up to and including zinc. The currently used $1s$ fluoresence data base currently being used is based on 30 year old atomic calculations and simplistic isoelectronic extrapolations. Our results provide reliable new atomic data for two important isoelectronic sequences and cast doubt on the reliability

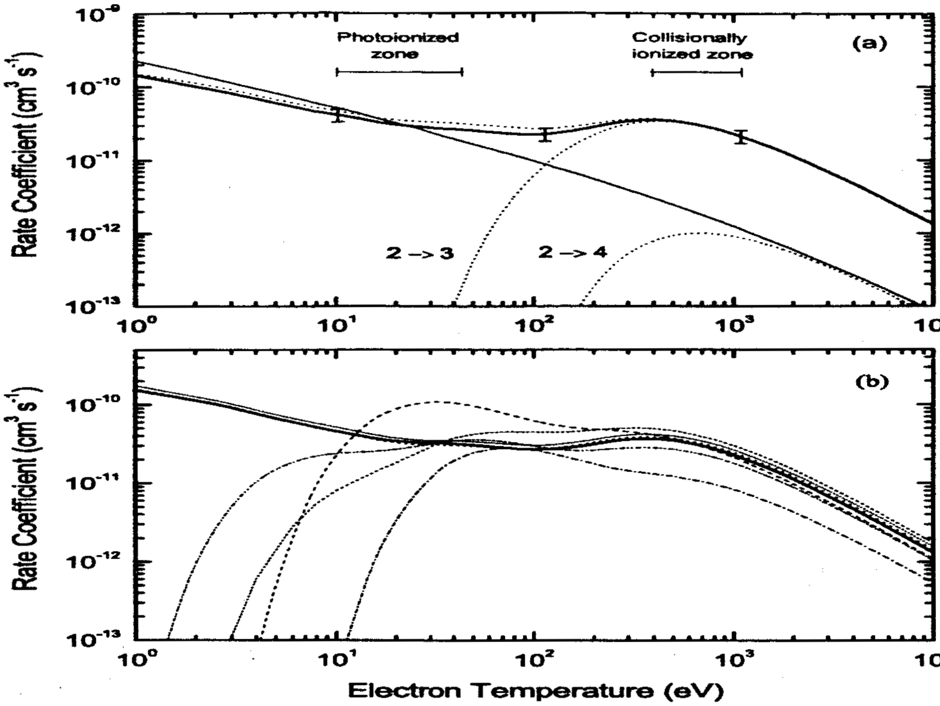


Figure 2: Fe XIX DR Maxwellian rate coefficients: (a) Thick solid curve – experimental data, dotted curve – MCBP calculations, thin solid curve – RR rate coefficient. (b) solid curve – present results, dot-dashed curve – Jacobs et al. (1977), dot-dot-dashed curve – Roszman (1987), dashed curve – recommended data of Mazzotta et al.(1998), dotted curve – MCDF (Savin et al. 2002).

of the $1s$ fluoresence database currently being used for the isoelectronic sequences of other second row elements.

2.5 Calculated DR data for dynamic finite-density plasmas

In Badnell et al. (2003) we outlined a program for the assembly of a comprehensive dielectronic recombination database within a generalized collisional-radiative (GCR) framework. It is valid for modeling ions of elements in dynamic finite-density plasmas. The resolution and precision of the data are tuned to spectral analysis and so are sufficient for prediction of the dielectronic recombination contributions to individual spectral line emissivities. The fundamental data are structured according to the format prescriptions of the Atomic Data and Analysis Structure (ADAS) and the production of relevant GCR derived data for application is described and implemented following ADAS. The requirements on the dielectronic recombination database are reviewed and the new data are placed in context and evaluated with respect to older and more approximate treatments. We have benchmarked our results using laboratory measurements where available and found good agreement. All data produced are

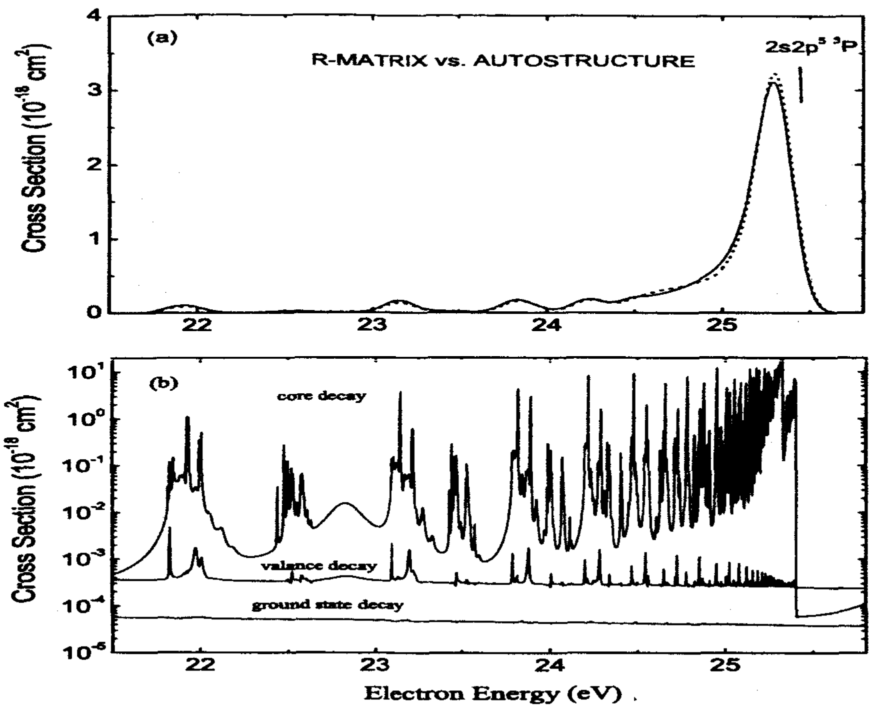


Figure 3: DR cross sections for Ne^{2+} for 2s $\rightarrow$ 2p core excitation. (a) Comparison of cross sections obtained with R-matrix (*solid curve*) and AUTOSTRUCTURE (*dotted curve*) codes. The cross sections were convoluted with a Gaussian electron distribution of 0.1 eV FWFM. (b) Contribution of different decay modes to the total DR cross section. The region below 21 eV is devoid of resonances formed due to a 2s $\rightarrow$ 2p core excitation.

publicly available via the website `http://homepages.wmich.edu/~gorczyca/drdata`.

2.6 Calculations of DR and RR Data for the Oxygen Isoelectronic Sequence

In Zatsarinny et al. (2003), we have calculated DR and RR data for oxygen-like ions forming fluorine-like ions as part of the assembly of a level-resolved DR and RR database necessary for modeling of dynamic finite-density plasmas (see above). In this paper we presented total DR and RR rate coefficients for F^+ to Zn^{22+} and discussed the results. By comparison between perturbative and R-matrix results, we find that RR/DR interference effects are negligible even for the lowest-charged (where interference is most likely) F^+ member (see Fig. 3). These RR and DR data are suitable for modeling of plasmas under conditions of collisional ionization equilibrium and non-equilibrium ionization.

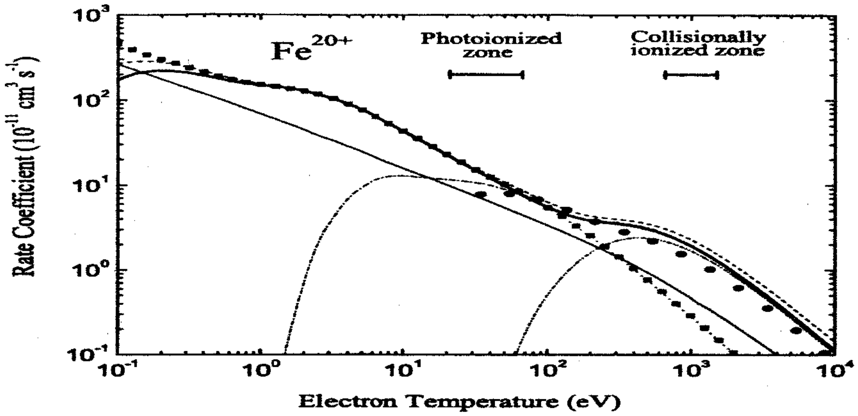
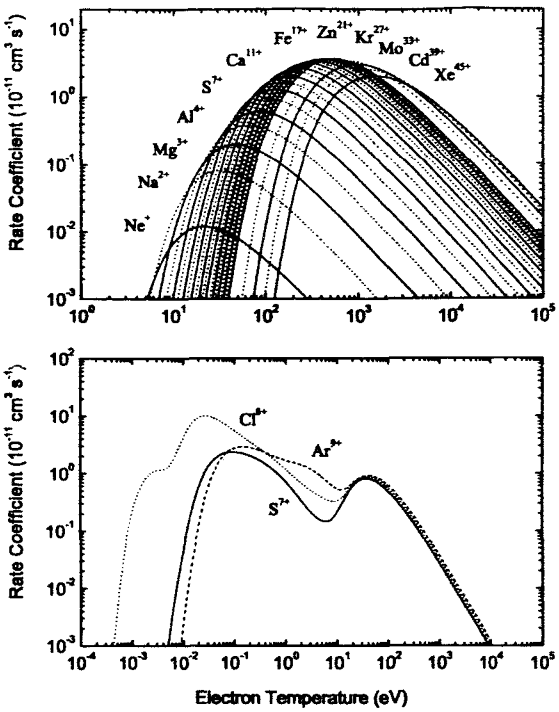


Figure 4: Maxwellian-average DR rate coefficients for Fe^{20+} as a function of electron temperature (in eV). The *thick solid curve* represents our MCBP calculations, the *solid squares* represent the experimentally derived rate coefficients for just the $2 \rightarrow 2$ core excitations (Savin et al 2003). Also shown are our contributions due to just the $2 \rightarrow 2$ core excitations (*dotted line*), the $2 \rightarrow 3$ core excitations (*dash-dot-dotted line*), and RR (*thin solid curve*). Comparison is given with the LS-coupling calculations of Jacobs et al. (1977, *solid circles*), the unpublished LS-calculations of Rozmann as given by Arnaud & Raymond (1992, *dot-dashed curve*), and the recent calculations of Gu (2003a, *short-dashed curve*). For reference we have plotted up the temperature ranges where Fe^{20+} is predicted to form in photoionization equilibrium (Kallman & Bautista 2001) and collisional ionization equilibrium (Gu 2003b).

2.7 Calculations of DR and RR Data for the Carbon Isoelectronic Sequence

In Zatsarinny et al. (2004a), we have calculated DR and RR data for carbon-like ions forming nitrogen-like ions as part of the assembly of a level-resolved DR and RR database necessary for modeling of dynamic finite-density plasmas (see above). In this paper we presented total DR and RR rate coefficients for N^{+} to Zn^{24+} and discussed the results – see fig. 4 for a comparison between our theoretical results, the experimental ones of our collaborator Dr. Daniel Wolf Savin, and earlier theoretical results the accuracy of which were compromised by the computational limitations at that time and the resulting theoretical approximations required to make the calculations tractable. These RR and DR data are suitable for modeling of plasmas under conditions of collisional ionization equilibrium and non-equilibrium ionization.



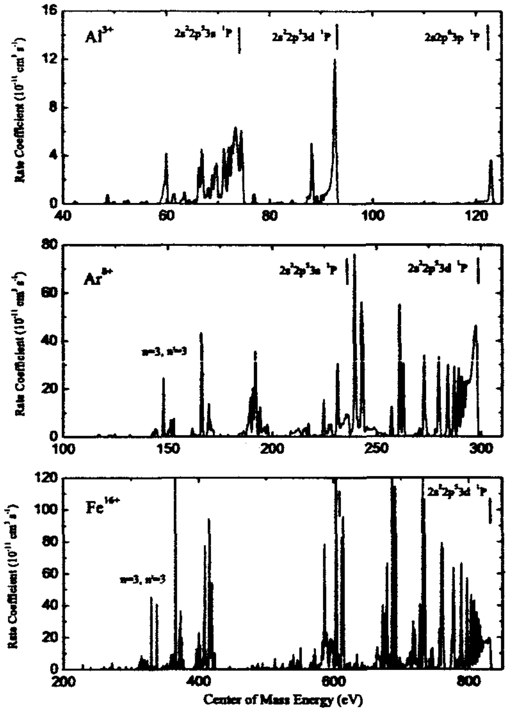


Figure 5: Behavior of Maxwellian averaged DR rate coefficients for the fluorine-like sequence as a function of atomic number. Whereas the rate coefficients for $2 \rightarrow 3$ DR scale smoothly with Z (a), the rate coefficients for $2 \rightarrow 2$ DR show irregular dependence on Z (b).

Figure 6: Computed DR resonance structure for neon-like ions Al^{3+}, Ar^{8+}, and Fe^{16+}. These data are subsequently convoluted analytically to yield Maxwellian-averaged DR rate coefficients, which are then condensed further into simple formulas using fitting coefficients.

2.8 Calculations of DR and RR Data for the Fluorine and Neon Isoelectronic Sequences

We also completed studies for the fluorine-like and neon-like sequences. These data have been made available on our web page (`http://homepages.wmich.edu/~gorczyca/drdata`). In Fig. 5, we show our computed results for the entire sequence (Zatsarinny et al., in preparation). For Ne-like ions, where no experimental data exists, typical detailed resonance structure for selected ions is shown in Fig. 6 (Zatsarinny et al., 2004b).

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IV. The Neon Isoelectronic Sequence].

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1. **O. Zatsarinny, T. W. Gorczyca, K. T. Korista, N. R. Badnell**, and **D. W. Savin**, *Dielectronic Recombination Data for Dynamic Finite-Density Plasmas. VII. The Fluorine Isoelectronic Sequence*, Astronomy and Astrophysics, in preparation.

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Thank you for your continued support.

Sincerely,

Thomas W. Gorczyca and Kirk T. Korista