The Iron Project (OSU): Large-Scale Computations of Atomic Data

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1 Introduction

The Iron Project (IP) [1] is devoted to the study of radiative and collisional atomic processes and the calculation of large-scale accurate atomic data, primarily for the iron-group elements for applications in astrophysical and laboratory plasmas. Among the processes of particular interest are: **electron impact excitation (EIE), photoionization, unified electron-ion recombination, and dipole allowed and forbidden transition probabilities**. Calculations are carried out in the close-coupling (CC) approximation using the R-matrix method. The computer codes developed under the Opacity Project (OP) [2] were extended to include relativistic effects in the Breit-Pauli (BP) approximation. The codes have been also adapted to massively parallel processors, the Cray T3E and the IBM SP2. We report some sample results for one single astrophysically important ion, Fe IV, calculated recently by the Ohio-State Atomic Astrophysics group.

2 Photoionization cross sections and oscillator strengths

Computations have been carried out for photoionization cross sections, σ_{PI}, and oscillator strengths (f-values) for dipole allowed transitions for Fe IV [3]. A 31-state eigenfunction expansion formed from the configurations $3d^4$, $3d^3 4s$, and $3d^3 4p$ of Fe V is used. The results include 746 LS bound states of sextet and quartet symmetries with $n \leq 10$, f-values for 34,635 LS transitions, and detailed σ_{PI} with extensive resonance structures for all bound states. The new σ_{PI} for the ground ^6S state of Fe IV exhibits a large resonance near the threshold (Fig. 1) not found in previous calculations for the OP and is likely to affect quantities such as the effective photoionization rate, the opacity, and the recombination rate significantly. The resonance has been identified as the $3s^2 3p^5 3d^6 (^6P^o)$ state [3].

3 Excitation collision strengths and rate coefficients

Excitation collision strengths, $\Omega(E)$, and maxwellian averaged rate coefficients, $\Upsilon(T)$, of Fe IV have been calculated for 8,771 non-vanishing transitions among 140 fine structure levels, dominated by the ground and excited configurations $3d^5$, $3d^4 4s$, and $3d^4 4p$ [4]. Calculations are carried out using a 49 term expansion in the CC approximation employing the R-matrx method. $\Omega(E)$ is obtained for electron energies up to 15 rydbergs, and $\Upsilon(T)$ is obtained at a wide range of temperatures. Fig. 2 presents $\Omega(E)$ for transitions between levels within the ground configuration $3d^5$.

4 Electron-ion recombination

Calculations of the total electron-ion recombination rate coefficient, $\alpha_R(T)$, of low charged iron ions, such as Fe I - V, are being carried out [5] through large-scale computations employing the unified treatment of Nahar and Pradhan [6]. The treatment subsumes the radiative recombination (RR) and dielectronic recombination (DR) in a unified, self-consistent manner. This work represents the first detailed study of electron-ion recombination for these iron ions. Previous results are from much simpler approximations, such as central-field and hydrogenic approximations for RR at lower temperatures and the Burgess general formula for DR at higher temperatures. Fig. 3(a) shows the general shape of $\alpha_R(T)$ for Fe IV in a wide temperature region. Starting with a high recombination rate, $\alpha_R(T)$ decreases to a minimum at $log_{10}(T) = 4.8$ K; above that the rate increases due to DR peaking at $log_{10}(T) = 5.3$ K, beyond which it falls monotonically. Fig. 3(b) presents a detailed comparison of our total rate (solid curve) with the currently used ones [9] for the temperature range of significant Fe IV abundance. The currently used rates are underestimated at lower T because autoionizing resonances are not included in the RR rates and are overestimated at higher T because interference effects with continuum and autoionization into lower states are not included in the Burgess formula for DR.

5 Resonance Averaged Photoionization Cross Sections for Astrophysical Modeling

Under the OP and the IP, accurate photoionization cross sections, σ_{PI}, have been calculated incorporating the complex autoionizing resonance structures. Owing to the complexity in the structures thousands of points are normally calculated to represent the detailed features for each bound state of the ion. While this is a great advance in terms of atomic physics and accuracy, the huge amount and the inherent details of the data do present a serious practical problem for numerical modeling. We present the resonance averaged σ_{PI} for the ground state of atoms and ions, available from the electronic OP database TOPbase [7] and the new data for the low ionization stages of iron Fe I - V. The average is obtained by convolving the detailed σ_{PI} with a Gaussian distribution over the autoionizing resonances. This preserves the overall resonant contribution to the cross sections in

the important near-threshold regions. The effective cross sections are then represented by a small number of points that can be readily interpolated linearly for practical applications. A Fortran subroutine and data will be available electronically. Sample averaged cross sections along with the detailed ones are presented in Fig. 4.

6 Conclusion

Large-scale *ab initio* calculations are carried out for atomic quantities of photoionization, oscillator strengths, excitation collision strengths and total electron-ion recombination rate coefficients. Resonance averaged photoionization cross sections are also presented for astrophysical models.

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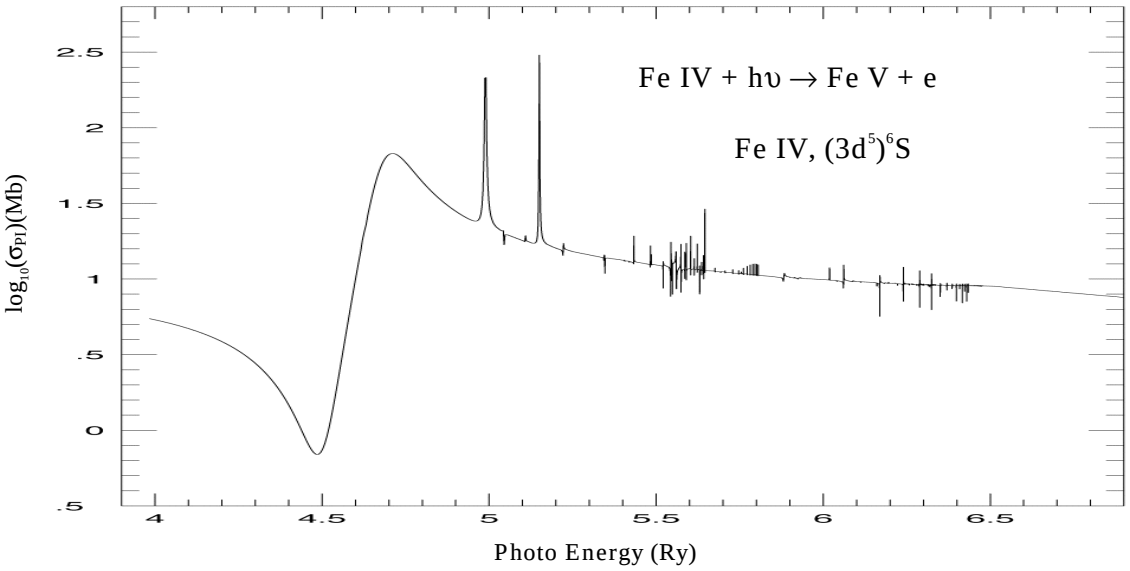
Fe IV + hυ → Fe V + e
Fe IV, (3d5)6S
log10(σPI)(Mb)
2.5
2
1.5
1
.5
0
.5
4
4.5
5
5.5
6
6.5
Photo Energy (Ry)

Figure 1

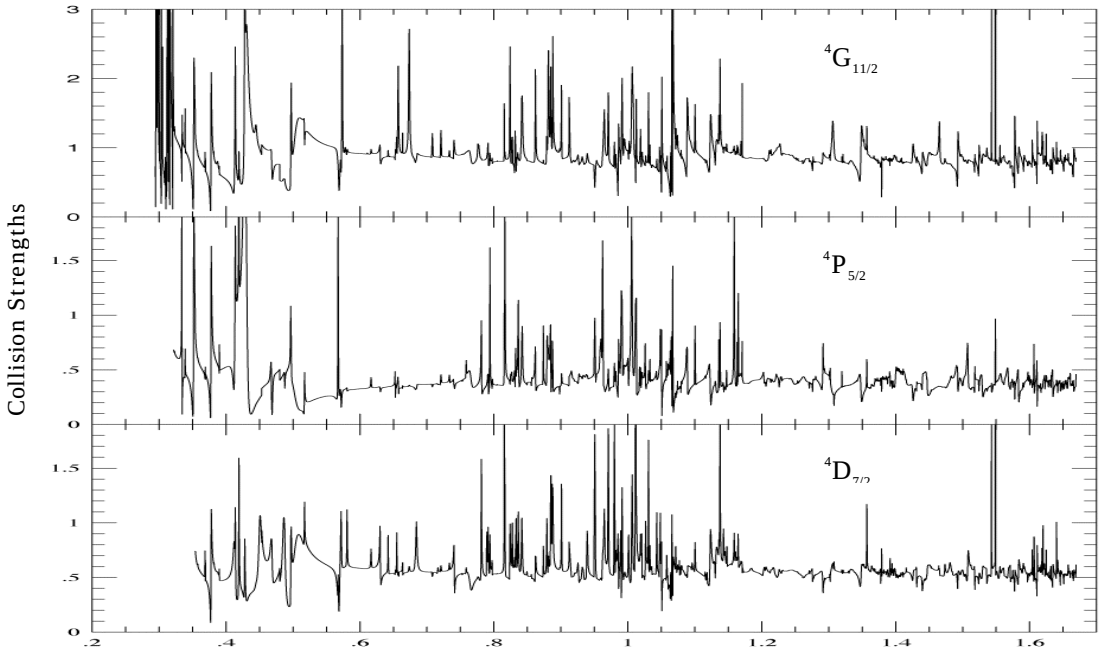

Figure 2

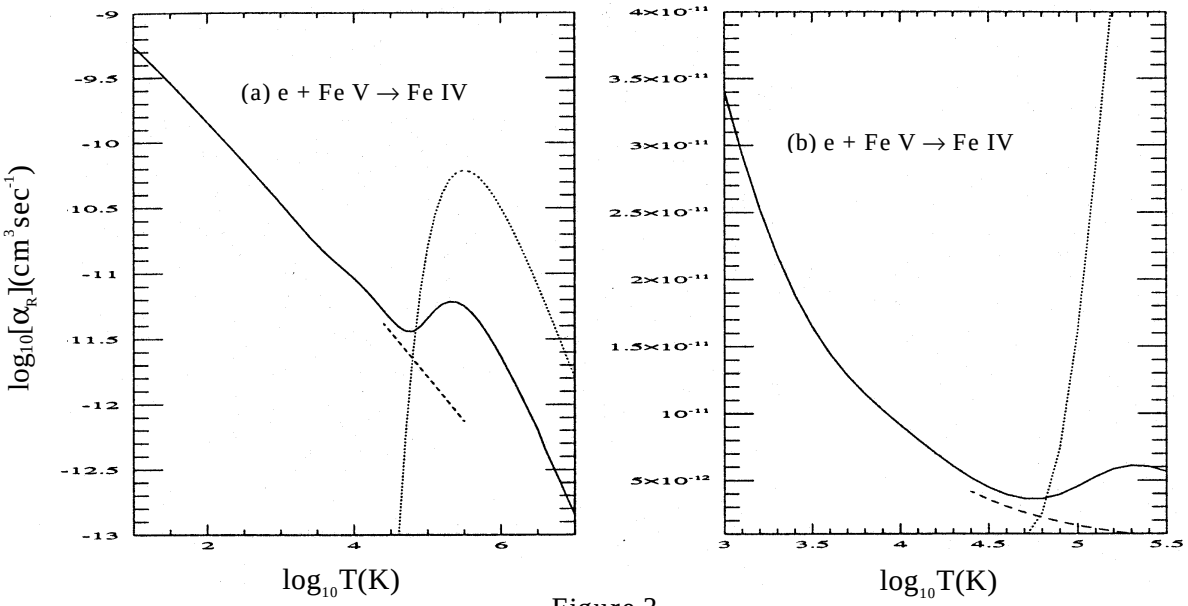

Figure 3

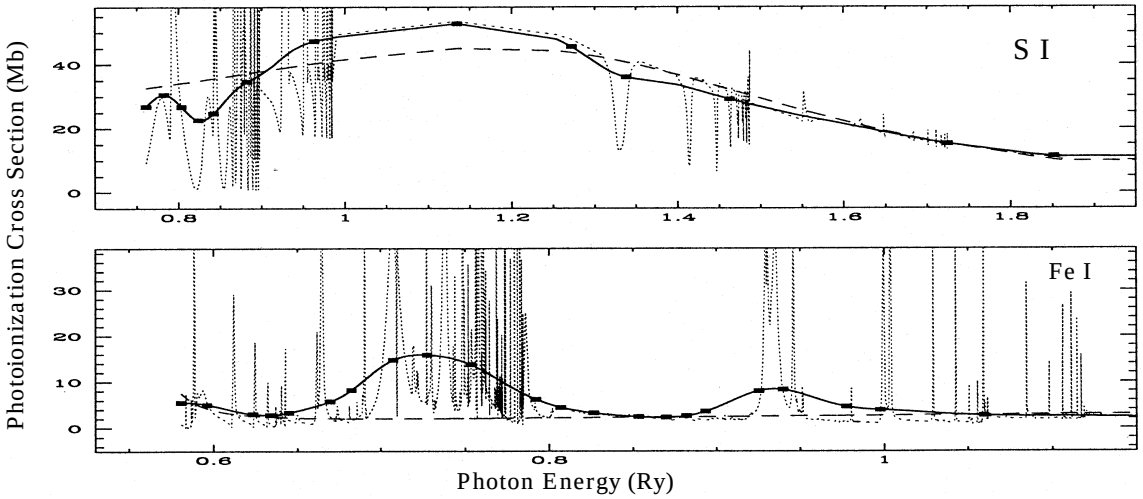

Figure 4