Photoionization cross sections for the Fe XVII ion

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1. Introduction

On the heavier side of the periodic table, iron is one of the most abundant element in the astronomical bodies. It is found in corona of the Sun in its higher degrees of ionized states. The radiative and non-radiative atomic data on the ions of iron, therefore, are very important for many applications in astrophysics - such as the analysis of the X-ray spectra of cataclysmic variables, X-ray binaries and AGNs, plasma modelling, fusion research and many other areas of study. The lack of good quality atomic data results in poor modelling of their environments.

In the present work, we attempt to calculate such data for Ne-like iron using sophisticated R-matrix method. The Photoionization cross sections for the Fe XVII ion from its ground and excited states in LS coupling are reported here extending our earlier work (Baliyan, 1993) Dr. Bhat. The calculation is also performed in the intermediate coupling for the ground level $2s^2 2p^6$ $^1S_0^e$ photoionization making use of the Breit-Pauli version of the RMATRX (Scott and Taylor 1982) package.

The main aspect of this calculation is that the photoionization cross sections below the highest N-electron excitation threshold are dominated by the Rydberg series of resonances. Most of the methods used earlier do not take account of their contribution to the total cross section.

2. Calculation

The configuration-interaction (CI) method of Hibbert 1975, Glass and Hibbert 1978 is used to construct the N-electron target state wavefunctions. In the intermediate (LSJ) coupling these CI wavefunctions take the form

$$\psi(J) = \sum_{i=1}^{M} a_i \Phi_i(\alpha_i LSJ).$$

The summation is over all the *m* configuration state functions with L and S values which couple to give a common J value. The coefficients $\{a_i\}$ are the eigen vectors of Hamiltonian matrix corresponding to specific eigenvalues. In the intermediate coupling calculation the relativistic

effects are included by adding spin dependent terms of Breit-Pauli operator in the non-relativistic Hamiltonian. The single-configuration functions $\{\Phi_i\}$ in quation (1) are constructed from one-electron orthogonal orbitals whose radial part is expressed as linear combination of the Slater-type functions. In this calculation we use 1s, 2s, 2p, 3s, 3p and 3d one electron orthogonal orbitals. The radial functions for 1s, 2s and 2p orbitals are taken from the tables of Clementi and Roetti (1974) and those of 3s, 3p and 3d are obtained by optimization using CIV3[3] program.

In the LS coupling case, we use lowest two target states, $2s^2 2p^5\ ^2P^0$ and $2sp^6\ ^2S^e$ in the wavefunction expansion. The $n = 3$ excited states lie considerably high in the $2s2p^6\ ^2S^e$ continuum and have not been included in the present calculation. The intermediate coupling calculation is carried out retaining lowest three levels, $2s^2 2p^5\ ^2P^0_{3/2}$, $^2P^0_{1/2}$ and $2s2p^6\ ^2S_{1/2}$ in the R-matrix basis function expansion. The initial bound and final continuum (N+1)-electron wavefunctions are expanded in terms of the R-matrix basis functions,

$$\Psi_k = A \sum_{ij} c_{ijk} \overline{\phi}_i(x_1, x_2, \ldots, x_N; \hat{r}_{N+1}, \sigma_{N+1})\, u_{ij}(r_{N+1}) \;\; + \sum_j d_{jk} \phi_j(x_1, \ldots, x_{N+1})$$

where A is the antisymmetrisation operator, $\overline{\phi}_i$ are channel functions formed by coupling the target states Φ_i to the l and s of the scattering channel, u_{ij} are the continuum basis orbitals and ϕ_j are the (N+1)-electron bound configurations which account for the short-range corelation effects.

The cross sections are obtained by matching the inner region solutions with the asymptotic region solutions at the R-matrix boundary. The R-matrix radius is chosen automatically and 15 continuum orbitals are introduced in each channel to obtain converged results in the required energy region. The observed energies of the target levels are used in the present calculation. The calculated value of the ionization potential of the ground level is 92.432Ryd which is in good agreement with the observed value.

3. Results

The photoionization cross sections in the dipole length approximation are obtained for the ground $2s^2 2p^6\ ^1S^e$ and excited $2s^2 2p^5\ ^{3,1}P^0$, $2s2p^6 3s\ ^3S^e$ states of Fe^{16+} ion. The partial cross sections for the photoionization of $^{3,1}P^0$ states are also calculated. $^{3,1}D^e$ partial cross sections, calculated in length and velocity forms, are in very good agreement. This indicates that the wavefunctions used here are of reasonably good quality. The $^{3,1}P^e$ final states do not couple to the $^2S^e$ excited state of the Fe^{17+} ion and therefore do not lead to any resonance structure. In the figure we plot the photoionization cross sections of the ground level $2s^2 2p^6\ ^1S^e_0$ in the Breit-Pauli approximation as a function of energy. Only the spin-orbit interaction is added to the non-

relativistic Hamiltonian. The figure compares the cross sections obtained in LS and relativistic calculations. The photoionization cross sections below the highest N-electron excitation threshold included in the calculation are dominated by the Rydberg series of resonances which converge onto the respective ionic threshold. A sufficiently fine energy mesh is used in order to resolve the resonance structure. The contribution from these resonance structures to the total cross sections is very important for the interpretation of astrophysical observations and should be taken into account while calculating the rates. The cross sections above the highest ionic threshold included in the calculation, vary smoothly with the photon energy.

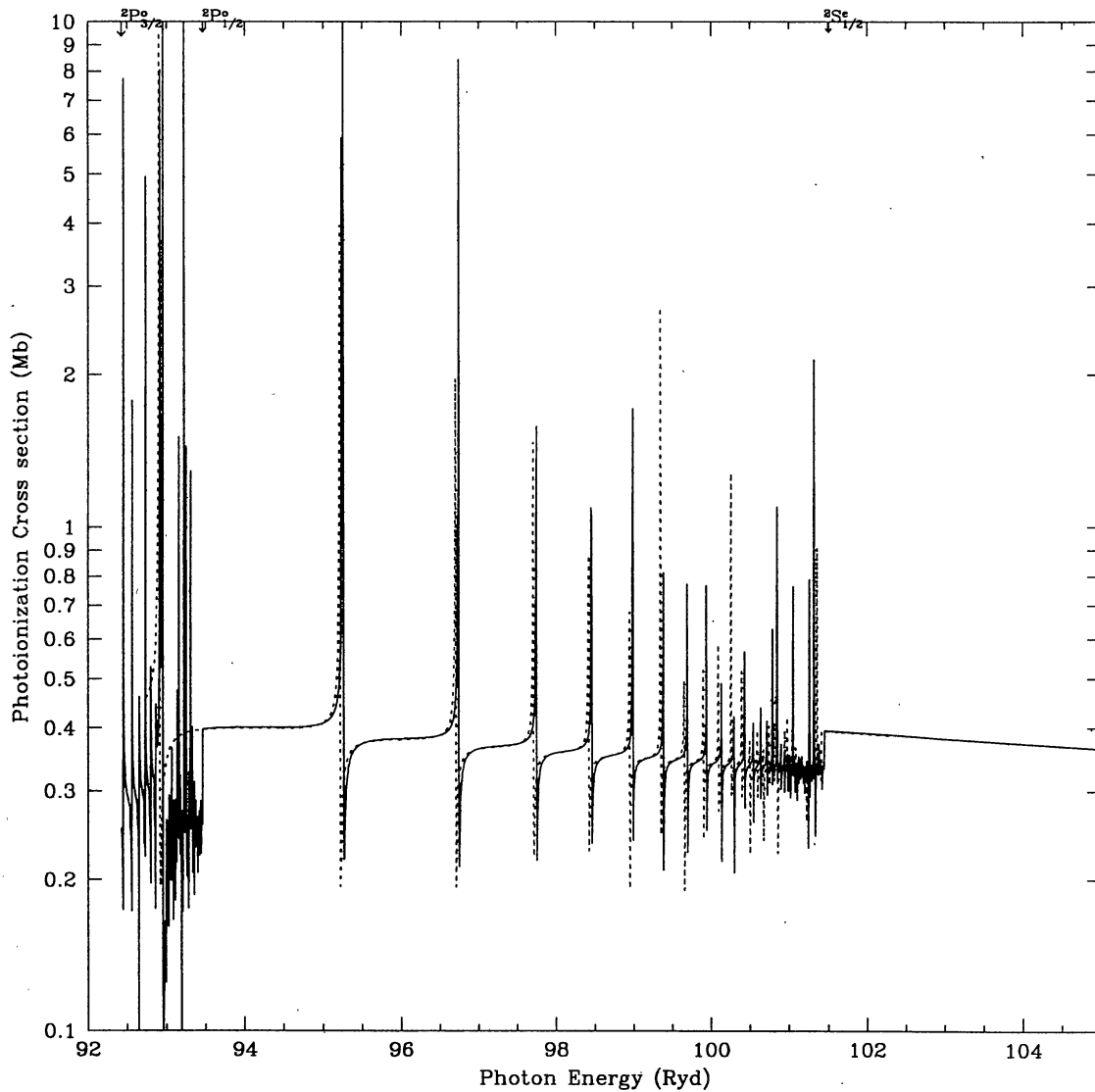This work is supported by the Department of Space, Government of India.

Figure 1. Photoionization of $Fe^{16+}(^1S_0^e)$ from ground state.

Table 1. The energies for the Fe^{17+} and Fe^{16+} states.

State	Energy (Ryd)
$E[2s2p^6\ ^2S - 2s^22p^5\ ^2P^0]$	8.6734
$E[2s^22p^5\ ^2P_{1/2} - 2s^22p^5\ ^2P^0_{3/2}]$	1.0267
$E[2s2p^6\ ^2S_{1/2} - 2s^22p^5\ ^2P^0_{3/2}]$	9.0162
$E[2s^22p5\ ^2P^0 - 2s^22p^6\ ^1S^e]$	92.7345
$E[2s^22p5\ ^2P^0 - 2s^22p^53s\ ^3P^0]$	39.1353
$E[2s^22p^5\ ^2P^0 - 2s^22p^53s\ ^1P^0]$	38.9049
$E[2s^22p^5\ ^2P^0 - 2s^22p^53p\ ^3S^e]$	37.2093
$E[2s^22p^5\ ^2P^0_{3/2} - 2s^22p^6\ ^1S^e_{1/2}]$	92.4322

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