

Photoionisation cross sections for Fe XVII

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Abstract. This paper reports the first close-coupling photoionisation calculation of Fe XVII, and provides accurate total and partial cross sections for photon energies up to 450 Ryd. The total and first partial photoionisation cross sections, the latter obtained when the Fe XVIII ion is left in the $2s^2 2p^5 \ ^2P^o$ ground state, are dominated by resonance structure for photon energies in the range from threshold to excitation of the first excited state ($2s 2p^6 \ ^2S$) of Fe XVIII. This is the first time that such structure has been determined. The background cross section is found to be in good agreement (to within 10%) with the results of Verner and co-workers for the total cross section, and for the partial cross sections corresponding to $2p$ and $2s$ photoejection, respectively.

Key words: atomic data – atomic processes

1. Introduction

X-rays are widely detected from the low density, high temperature plasmas in the corona of the Sun and other stars (Doschek 1990; Haisch & Schmitt 1996), as well as from accretion-powered sources such as cataclysmic variables, X-ray binaries and active galactic nuclei (Mushotzky et al. 1993; Kahn & Liedahl 1995). The analysis of the X-ray spectra of such objects typically involves the inclusion of many atomic physics processes, and partially ionised ions of iron are often an important component in the modelling of the plasma emission (Liedahl et al. 1995; Netzer 1996). However the paucity of theoretical atomic data for these ions has hindered their quantitative analysis. The best existing theoretical data on the photoionisation spectrum of Fe XVII are those obtained by Verner et al. (1993) and Verner & Yakovlev (1995), who presented the results of an extensive calculation of photoionisation cross sections (including sub-shell partial cross sections) for ions with nuclear charge ranging from $Z = 2$ to 30. The method employed was a central field Hartree-Dirac-Slater approximation, which does not take into account resonance structure, and hence the accuracy of these data remains uncertain. Comparison with the calculations for Fe XXIII and Fe XXIV by Black et al. (1997)

Table 1. Radial function parameters for fluorine-like Fe XVIII orbitals

Function	c_{jnl}	I_{jnl}	ζ_{jnl}
1s	0.96227	1	25.93670
	0.01055	1	44.74550
	0.00048	2	10.58830
	0.03532	2	22.15850
2s	-0.30713	1	25.93670
	0.00009	1	44.74550
	1.16432	2	10.58830
	-0.18134	2	22.15850
3s	0.24213	1	19.05398
	-1.19322	2	8.30507
	1.64882	3	6.53483
	0.71092	2	10.56620
2p	0.13432	2	16.78830
	0.17053	2	9.65676
	0.00122	2	36.95710
	0.62697	2	10.60566
3p	-1.19016	3	6.02027
	0.99258	3	6.40818
	0.01003	3	11.60761
3d	1.33878	3	11.77954
	-0.98411	4	8.03752

reveals satisfactory accuracy for the background cross sections, but significant discrepancies with results based on a quantum close-coupled approach have been found near threshold for photoionisation of neutral iron (Bautista & Pradhan 1995).

The need for further investigation and for accurate data is clear, and in this paper we employ the R -matrix method to perform a sophisticated large scale calculation to obtain total and partial cross sections for photoionisation of Fe XVII. Our approach allows for resonance structure, and we believe that this is the first calculation to include such effects for Fe XVII.

2. Method

We present results for the photoionisation processes

$$h\nu + Fe^{16+}(1s^2 2s^2 2p^6 \ ^1S) \rightarrow e^- + Fe^{17+}(1s^2 m \ ^2L) \quad (1)$$

where m is given by $2s^2 2p^5$, $2s 2p^6$, $2s^2 2p^4 \ 3l$ or $2s 2p^5 \ 3l$ ($l=0,1,2$). The calculation was performed within the frame-

Table 2. Target state energies (in Ryd) relative to the ground state of Fe XVIII. Observed data are from Corliss & Sugar (1985) and Shirai et al. (1990)

State	Present	Observed	Cornille et al.
$2s^2 2p^5 \ ^2P^o$	0.0000	0.0000	0.0000
$2s 2p^6 \ ^2S$	8.579	9.391	9.538
$2s^2 2p^4 ({}^3P) 3s \ ^2P$	57.334	56.906	56.980
$2s^2 2p^4 ({}^1D) 3s \ ^2D$	58.019	58.023	58.097
$2s^2 2p^4 ({}^1S) 3s \ ^2S$	59.496	59.605	59.729
$2s^2 2p^4 ({}^3P) 3p \ ^2P^o$	59.509	–	59.596
$2s^2 2p^4 ({}^3P) 3p \ ^2D^o$	59.510	–	59.414
$2s^2 2p^4 ({}^3P) 3p \ ^2S^o$	59.653	–	59.969
$2s^2 2p^4 ({}^1D) 3p \ ^2F^o$	60.204	–	60.448
$2s^2 2p^4 ({}^1D) 3p \ ^2D^o$	60.495	–	60.735
$2s^2 2p^4 ({}^1D) 3p \ ^2P^o$	61.214	–	61.375
$2s^2 2p^4 ({}^1S) 3p \ ^2P^o$	61.890	–	62.328
$2s^2 2p^4 ({}^3P) 3d \ ^2F$	62.477	–	62.270
$2s^2 2p^4 ({}^3P) 3d \ ^2P$	62.558	62.997	62.931
$2s^2 2p^4 ({}^3P) 3d \ ^2D$	62.691	63.147	63.070
$2s^2 2p^4 ({}^1D) 3d \ ^2G$	63.086	–	63.472
$2s^2 2p^4 ({}^1D) 3d \ ^2S$	63.379	63.607	63.723
$2s^2 2p^4 ({}^1D) 3d \ ^2F$	63.441	–	63.772
$2s^2 2p^4 ({}^1D) 3d \ ^2D$	63.790	63.941	64.113
$2s^2 2p^4 ({}^1D) 3d \ ^2P$	63.821	63.936	63.979
$2s^2 2p^4 ({}^1S) 3d \ ^2D$	64.844	65.059	65.376
$2s 2p^5 ({}^3P^o) 3s \ ^2P^o$	65.255	–	66.066
$2s 2p^5 ({}^3P^o) 3p \ ^2D$	67.153	68.153	68.397
$2s 2p^5 ({}^3P^o) 3p \ ^2P$	67.235	67.984	68.106
$2s 2p^5 ({}^1P^o) 3s \ ^2P^o$	67.653	–	68.489
$2s 2p^5 ({}^3P^o) 3p \ ^2S$	67.959	68.939	69.009
$2s 2p^5 ({}^1P^o) 3p \ ^2D$	69.788	70.546	70.792
$2s 2p^5 ({}^1P^o) 3p \ ^2P$	69.948	70.691	70.981
$2s 2p^5 ({}^3P^o) 3d \ ^2F^o$	70.135	–	71.396
$2s 2p^5 ({}^3P^o) 3d \ ^2D^o$	70.283	–	71.240
$2s 2p^5 ({}^1P^o) 3p \ ^2S$	70.386	–	71.409
$2s 2p^5 ({}^3P^o) 3d \ ^2P^o$	70.822	–	71.930
$2s 2p^5 ({}^1P^o) 3d \ ^2F^o$	72.633	–	73.755
$2s 2p^5 ({}^1P^o) 3d \ ^2P^o$	72.885	–	73.999
$2s 2p^5 ({}^1P^o) 3d \ ^2D^o$	72.895	–	74.021

work of the R -matrix method, using the computer codes described by Berrington et al. (1987), with the associated theory being given by Seaton (1987). LS coupling was adopted, while spin-orbit coupling and other relativistic effects were neglected. The Fe^{16+} bound state and the 35 Fe^{17+} target states are described using sophisticated configuration-interaction wavefunctions constructed from one-electron orbitals.

The radial part of these one electron functions is given by a linear combination of Slater-type orbitals:

$$P_{nl} = \sum_{j=1}^k c_{jnl} \left[\frac{(2\zeta_{jnl})^{2I_{jnl}+1}}{(2I_{jnl})!} \right]^{1/2} r^{I_{jnl}} \exp(-\zeta_{jnl}r) \quad (2)$$

Details on the construction of the target wavefunctions and the photoionisation cross section calculation are given in Sects. 2.1 and 2.2, respectively.

Table 3. Oscillator strengths for dipole allowed transitions from the $2s^2 2p^5 \ ^2P^o$ ground state of Fe XVIII. BH and Cetal denote results from Blackford & Hibbert (1994) and Cornille et al. (1992), respectively, while f_L and f_V denote the length and velocity formulation values

Upper State	Present f_L	Present f_V	BH f_L	BH f_V	Cetal
$2s 2p^6 \ ^2S$	0.046	0.048	0.049	0.044	
$2s^2 2p^4 ({}^1S) 3s \ ^2S$	0.014	0.015	0.012	0.012	0.014
$2s^2 2p^4 ({}^1D) 3d \ ^2S$	0.197	0.200	0.167	0.172	0.179
$2s^2 2p^4 ({}^3P) 3s \ ^2P$	0.104	0.105	0.072	0.072	0.075
$2s^2 2p^4 ({}^3P) 3d \ ^2P$	0.022	0.023	0.029	0.029	0.030
$2s^2 2p^4 ({}^1D) 3d \ ^2P$	0.826	0.813	0.680	0.686	0.767
$2s^2 2p^4 ({}^1D) 3s \ ^2D$	0.063	0.065	0.064	0.063	0.067
$2s^2 2p^4 ({}^3P) 3d \ ^2D$	0.295	0.291	0.245	0.247	0.247
$2s^2 2p^4 ({}^1D) 3d \ ^2D$	1.195	1.188	0.870	0.878	1.054
$2s^2 2p^4 ({}^1S) 3d \ ^2D$	0.304	0.301	0.311	0.309	0.327

2.1. Target specifications

The configuration interaction wavefunctions for the Fe XVIII target states were constructed from 7 one-electron orbitals P_{nl} , corresponding to 6 spectroscopic orbitals ($1s$, $2s$, $2p$, $3s$, $3p$, $3d$) and one unphysical ($4d$) pseudo-orbital. For the orbitals $1s$, $2s$, and $2p$, the orbital function parameters c_{jnl} , ζ_{jnl} and I_{jnl} were taken to be the Hartree-Fock values obtained by Clementi & Roetti (1974) for the $1s^2 2s^2 2p^5 \ ^2P^o$ ground state of Fe XVIII. The remaining orbitals were generated using the general configuration-interaction code CIV3 (Hibbert 1975) as discussed below.

The $3s$ orbital was optimised on the energy of the $2s^2 2p^4 ({}^1D) 3s \ ^2D$ state using the single $2s^2 2p^4 3s$ configuration; the $3d$ orbital was then optimised on the energy of the $2s^2 2p^4 ({}^3P) 3d \ ^2P$ state using all configurations arising from $2s^2 2p^4 3d$ and $2s^2 2p^4 3s$; the $3p$ orbital was then optimised on the $2s 2p^5 ({}^1P^o) 3p \ ^2P$ state using configurations arising from $2s^2 2p^4 3s$, $2s^2 2p^4 3d$ and $2s 2p^5 3p$; finally, in order to take account of the important $2s \rightarrow nd$ correlation, a $4d$ pseudo-orbital was introduced by optimising on the energy of the $2s^2 2p^5 \ ^2P^o$ state with configurations arising from $2s^2 2p^5$, $2s 2p^5 3d$ and $2s 2p^5 4d$.

The values of the Slater function parameters obtained for these optimised orbitals are given in Table 1.

The configuration-interaction wavefunctions of the Fe XVIII target states were then constructed from these 7 one-electron orbitals using configurations obtained from two electron replacement in the basis $2s^2 2p^5$, with the restriction that only one $2s$ electron may be replaced. Resulting theoretical energies are presented in Table 2, where they are compared to the observed data (Corliss & Sugar 1985; Shirai et al. 1990). Also given in Table 2 are the multi-configurational relativistic theoretical estimates of Cornille et al. (1992), and we note that the values presented for both the observed and Cornille et al. data are weighted averages of the fine-structure results. In general the agreement is excellent, with differences no larger than 1.5% and often less than 1%, with the exception of the energy of the

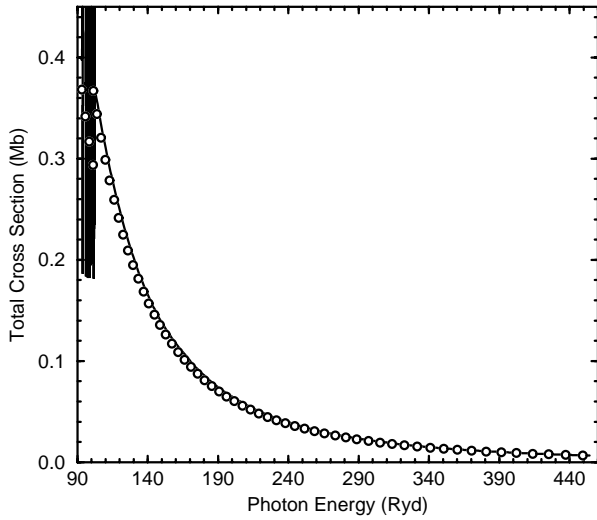


Fig. 1. Total photoionisation cross section for Fe XVII. Solid line: present calculation; circles: Verner et al. (1993) and Verner & Yakovlev (1995)

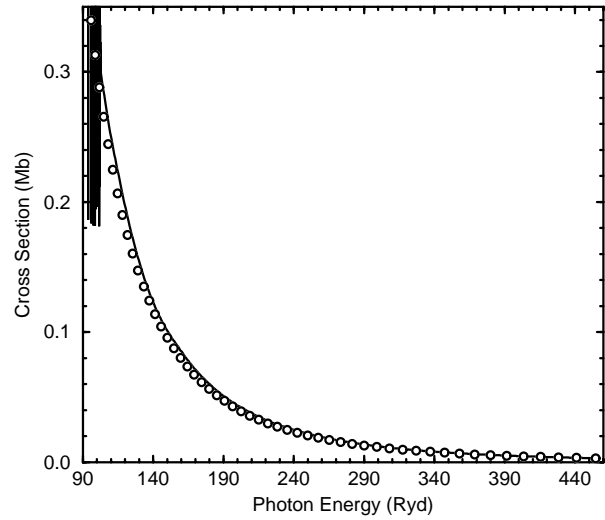


Fig. 3. Partial photoionisation cross section of Fe XVII, where the Fe XVIII ion is left in the $2s^2 2p^5 \ ^2P^o$ state. Solid line: present calculation; circles: Verner et al. (1993) and Verner & Yakovlev (1995)

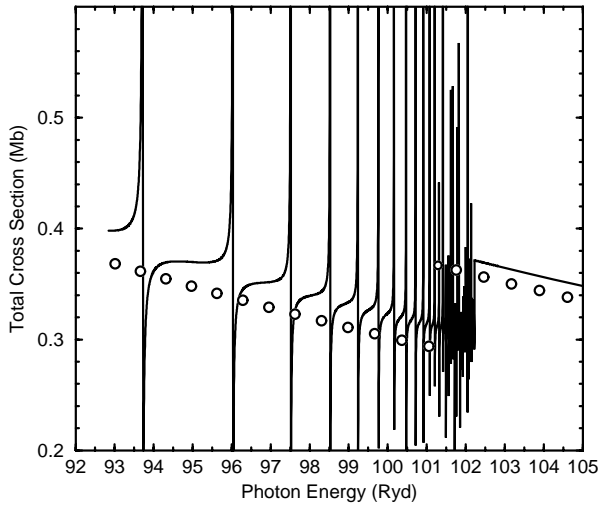


Fig. 2. Total photoionisation cross section for Fe XVII from threshold to the first excited state threshold. Solid line: present calculation; circles: Verner et al. (1993) and Verner & Yakovlev (1995)

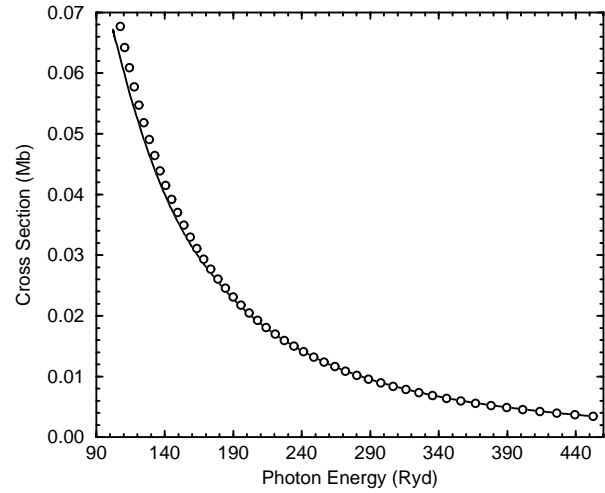


Fig. 4. Partial photoionisation cross section of Fe XVII, where the Fe XVIII ion is left in the $2s 2p^6 \ ^2S$ state. Solid line: present calculation; circles: Verner et al. (1993) and Verner & Yakovlev (1995)

first excited state $2s 2p^6 \ ^2S$, which was found to have an energy 8.6% lower than the observed value. This suggests that the target state wavefunctions are of high accuracy. A further test of their accuracy was performed by calculating the oscillator strengths for dipole allowed transitions between the states in Table 2. In Table 3 we present f-values for transitions from the ground state. Given that the present work is restricted to evaluation within LS coupling, satisfactory agreement is found with the results of Cornille et al. (1992) and Blackford & Hibbert (1994), both of the latter including relativistic effects. Similar accord is found for the other transitions not presented here. Although we are aware that the pair correlation energy for electrons in the $2s$ shell could be better described by the inclusion of further pseudo-orbitals, experience has demonstrated that the accuracy

of the wavefunctions (as assessed above) is sufficient to permit the calculation of reliable photoionisation cross sections.

2.2. Photoionisation cross section calculation

The calculation of the photoionisation cross section of Fe XVII was then performed using the R -matrix close coupling codes (Berrington et al. 1987). The $(N+1)$ -electron configurations were generated by allowing three electron replacement in the basis $2s^2 2p^5$, with the restriction that only one $2s$ electron may be replaced. Experience has shown that this is essential in order to achieve a correct balance in the various correlations. In constructing the total wavefunction in the R -matrix internal region, 25 continuum orbitals were used for each incident electron orbital angular momentum. Although it is customary to adjust

the target state bound state energies to their experimental values, in the present case we considered it unnecessary to perform such shifts, except for the first excited state $2s2p^6\ ^2S$. We noted above that this state had the largest error when compared with other data, and so it was shifted to the observed value relative to the Fe XVIII ground state. The R -matrix boundary was found to be 4.8 Ryd, and the ionisation energy of the ground state of Fe XVII was calculated to be 92.84 Ryd, in excellent agreement with the observed result of 93.08 Ryd (Corliss & Sugar 1985; Shirai et al. 1990).

3. Results and discussion

The total photoionisation cross section of Fe XVII along with the 35 individual partial cross sections, corresponding to the process which leaves the Fe XVIII ion in each of the spectroscopic states listed in Table 2, have been calculated. In Fig. 1 the total photoionisation cross section over the energy range considered is presented. Only the data obtained in the length formulation are considered, since these results are believed to be the most accurate, and in any event the differences between the length and velocity formulation values are insignificant. The most striking feature of the total cross section is the Rydberg resonance structure extending from threshold, and converging on the first excited state ($2s2p^6\ ^2S$) threshold. The importance of having this threshold in the correct place is clearly justified, since the resonances will also now be in their correct position. Fig. 2 illustrates this structure in more detail, and an energy mesh of 3×10^{-5} Ryd has been used in incrementing the photon energy, so that the resonances are well resolved. This structure will be of considerable significance in evaluating the radiative recombination rate inverse process.

In Figs. 1 and 2 we also display the central field calculation of Verner et al. (1993) and Verner & Yakovlev (1995), noting that they find the first excited state ($2s2p^6\ ^2S$) threshold at a photon energy of 101.2 Ryd, in comparison with the present value of 102.2 Ryd (the observed energy is 102.5 Ryd). We also note that, as expected, their results are devoid of structure. Nevertheless, their background cross section is in good agreement with the present work, and for energies above the $2s2p^6\ ^2S$ threshold the differences in the two sets of calculations are less than 5%.

Figs. 3 and 4 give the partial photoionisation cross sections for the cases where the Fe XVIII ion is left in the ground state $2s^22p^5\ ^2P^o$ or the first excited state $2s2p^6\ ^2S$, respectively. A comparison with the results of Verner et al. (1993) and Verner & Yakovlev (1995) reveals that, as the photon energy increases, their cross sections and the present data become almost indistinguishable. The remaining 33 partial cross sections, corresponding to the Fe XVIII ion being left in higher excited states, are all found to be at least 5 orders of magnitude smaller than the $2s2p^6\ ^2S$ data at all photon energies, and so make a negligible contribution to the total photoionisation cross section. All individual cross sections are available in tabular form from the authors (KLB and FPK).

4. Summary

In summary, existing data for the total background cross section for the photoionisation of Fe XVII has been demonstrated to be of high accuracy. However, the present work improves upon earlier calculations by performing a more sophisticated close-coupling treatment which, for the first time, has shown the resonance structure which dominates the cross section from threshold up to the first excited state threshold.

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