

Photoionisation cross-sections for Fe XXIII and Fe XXIV

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Abstract. Photoionisation of Fe XXIII and Fe XXIV is investigated using the R-matrix method, with particular attention being given to photoejection of the $1s$ K-shell electron. In both cases, good agreement (to within 5%) is found with earlier calculations of the background cross-section. However, the present work is the first to determine resonance structure just below and above the $1s$ photoejection threshold energy.

Key words: atomic data – atomic processes

1. Introduction

The photoionisation cross-sections of highly ionised species of iron are important for modelling the emission-line spectra of cosmic X-ray sources (see, for example, Liedahl et al. 1992). However, for most ions, and in particular for photoionisation processes which remove the inner K-shell electron, the quality of current data is largely unassessed, and is generally obtained using approximate methods.

The photoionisation of Fe XXIII and Fe XXIV has been studied using various methods, but presently available theoretical results are not wholly consistent, while to the best of our knowledge no experimental data exist. For example, Verner et al. (1993, 1995) calculated the *partial* photoionisation cross-sections for all Fe XXIII and Fe XXIV subshells by employing the central field Hartree-Dirac-Slater method. This approach improved upon the earlier work of Clark et al. (1986), in which relativistic effects were ignored and the calculation was performed within the framework of the Hartree-Fock approximation. These investigations are the only studies which present, in their published data, the cross-sections for ejection of electrons from the individual sub-shells. The Hartree-Fock-Slater method was earlier used by Reilman & Manson (1979) and the *total* cross-section presented in their paper. The results of these different central field calculations are somewhat similar, but discrepancies do exist. Most importantly, the approximations used are not capable of taking resonance phenomena into consideration.

Only two other calculations exist, to the authors knowledge, for these two ions. Peach et al. (1988), as part of the International

Opacity Project, obtained cross-sections for several ions of the lithium isoelectronic sequence. The calculations were restricted to photoejection of the L-shell electron, and two independent approaches to the problem (a model potential method and a two-state R-matrix approximation) gave virtually the same result. These authors presented scaled cross-sections for the first six members of the sequence, together with the $Z=\infty$ cross-section, thus enabling interpolated data to be easily obtained. Again no resonance phenomena were taken into account.

For Fe XXIII, Tully et al. (1990), again as part of the International Opacity Project, used the R-matrix method to obtain the cross-section for L-shell photoejection. A five target-state calculation (i.e. $2s$, $2p$, $3s$, $3p$, $3d$ states of the Li-like target) was performed and so resonances converging on to the $2p$, $3s$, $3p$ and $3d$ states of the residual ion were found. This calculation is the most sophisticated carried out for either ion, but is severely restricted in that it takes no account of the K-shell photoionisation process.

There is clearly a need for a much more sophisticated calculation for the photoionisation processes associated with these ions. Configuration-interaction wavefunctions are required for the target states, a larger number of target states should be included in the calculation, resonance phenomena should be included and photoejection from the K-shell should be permitted. In this paper we present the results of such a sophisticated calculation for the photoionisation of Fe XXIII and FeXXIV from their respective ground states $1s^2 2s^2 \ ^2S$ and $1s^2 2s^2 \ ^1S$, i.e. the processes:

$$h\nu + Fe^{23+}(1s^2 2s^2 \ ^2S) \rightarrow e^- + Fe^{24+}(1s nl \ ^1,^3L) \quad (1)$$

$$h\nu + Fe^{22+}(1s^2 2s^2 \ ^1S) \rightarrow e^- + Fe^{23+}(1s nl n' l' \ ^2L) \quad (2)$$

where nl and $n'l'$ may be $1s$ or $2l$, $3l$.

2. Method

The present calculations employ the R-matrix method, using the computer codes as described by Berrington et al. (1987), with the associated theory being given by Seaton (1987). The calculations are performed in LS coupling, neglecting spin-orbit coupling and other relativistic effects. A recent relativistic study of electron-impact excitation of hydrogen-like ions (Kisielius et

al. 1995), coupled with a comparison of the existing relativistic and non-relativistic photoionisation cross-sections for the ions under consideration, indicate that neglect of relativistic effects is of minor importance in comparison with the sophistication of the LS coupling calculation. For each ion, the appropriate R-matrix wavefunction expansion is performed by including a certain number of target states. Each of these is represented by configuration-interaction wavefunctions determined from one-electron analytic functions of the form:

$$P_{nl}(r) = \sum_{j=1}^k c_{jnl} \frac{(2\zeta_{jnl})^{I_{jnl} + \frac{1}{2}}}{[(2I_{jnl})!]^{\frac{1}{2}}} r^{I_{jnl}} \exp(-\zeta_{jnl}r) \quad (3)$$

where the coefficients c_{jnl} and the exponents ζ_{jnl} are determined by a variational optimization on the energy of a particular target state, whilst the powers of r , I_{jnl} , remain fixed. The choice of parameters together with further details of the R-matrix calculation is given below for each ion.

2.1. Fe XXIV

The eleven lowest helium-like target states of Fe XXV were included in the R-matrix wavefunction expansion, namely, $1s^2 \ ^1S$; $1s2s \ ^{1,3}S$; $1s2p \ ^{1,3}P^o$; $1s3s \ ^{1,3}S$; $1s3p \ ^{1,3}P^o$ and $1s3d \ ^{1,3}D$. Seven one-electron functions, $P_{nl}(r)$, were included in the calculation: six real ($1s$, $2s$, $2p$, $3s$, $3p$, $3d$) and one pseudo-orbital, $\overline{4s}$. The parameters, as defined by Eq. (3) above, for these orbitals are given in Table 1 and were obtained as follows: the $1s$ orbital was taken as hydrogenic; those for the real nl orbitals were obtained by optimisation of the corresponding triplet state, $1snl \ ^3L$; the parameters for the $\overline{4s}$ pseudo-orbital were obtained by optimising the energy of the ground $1s^2 \ ^1S$ state using configurations arising from all two-electron combinations of the ns orbitals but with a common value for ζ_{jnl} . The pseudo-orbital was included in order to improve the ground state representation and to partially account for the difference between the $1s$ functions in the ground and excited states.

These one-electron functions were then employed in a configuration-interaction representation of the helium-like target states, by generating appropriate configurations through combining any pair of electrons from the set of functions described previously. The energies of the target states thus obtained, relative to the $1s^2 \ ^1S$ ground state, are compared in Table 2 with the critically reviewed data of Shirai et al. (1990). The agreement is highly satisfactory and it is noted that for all states the difference is fairly consistent at about 0.9%; this indicates that the excited states are well represented and that the main error of about 1% occurs in the ground state. We therefore feel confident that the target states are represented to a sufficiently high degree of accuracy.

The R-matrix program was then utilized, with 35 continuum orbitals included for each incident electron orbital angular momentum and the R-matrix boundary radius set at 1.8 au. The (N+1)-electron correlation terms were generated from all possible three electron combinations of the above orbital set; experience has shown that this is essential in order to achieve a

Table 1. Radial function parameters for helium-like Fe XXV orbitals

Function	c_{jnl}	I_{jnl}	ζ_{jnl}
$1s$	1.00000	1	26.00000
$2s$	0.69030	1	16.21412
	-1.38707	2	12.41452
$3s$	0.45896	1	14.16401
	-3.52474	2	7.22462
	3.90946	3	8.10903
$\overline{4s}$	3.64879	1	13.78670
	-11.63845	2	13.78670
	13.52881	3	13.78670
	-5.49668	4	13.78670
$2p$	1.00000	2	12.63522
$3p$	1.12965	2	9.73604
	-1.68978	3	8.21025
$3d$	1.00000	3	8.33762

Table 2. Comparison between *ab initio* energy levels (in Ryd) and assessed data (Shirai et al. 1990) relative to the ground state of Fe XXV

State	Present	Shirai et al.
$1s2s \ ^3S$	484.426	487.780
$1s2p \ ^3P^o$	486.346	490.642
$1s2s \ ^1S$	486.593	490.090
$1s2p \ ^1P^o$	487.981	492.471
$1s3s \ ^3S$	573.443	577.941
$1s3p \ ^3P^o$	573.975	578.570
$1s3s \ ^1S$	574.022	578.553
$1s3d \ ^3D$	574.285	—
$1s3d \ ^1D$	574.305	579.352
$1s3p \ ^1P^o$	574.424	579.254

correct balance in the various correlations. We obtained a value of 148.82 Ryd for the ionisation energy of the ground state of Fe XXIV, in excellent agreement with the result of 148.72 Ryd given by Shirai et al. (1990).

2.2. Fe XXIII

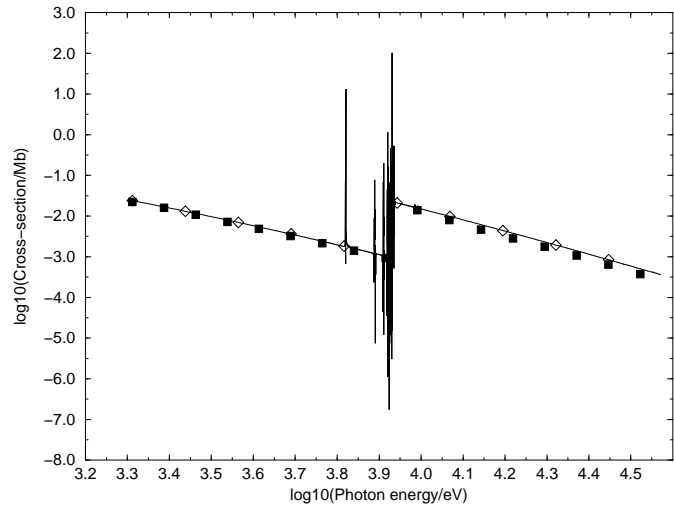
As specified in Eq. (2) above, we are interested in permitting $1s$ -electron removal, and so we included in the R-matrix wavefunction expansion target states which could be generated by keeping the $1s^2$ core fixed together with states generated by the addition of an electron (excluding $1s$) to $1s2s$ and $1s2p$ stems from the set of real orbitals: $1s$, $2s$, $2p$, $3s$, $3p$ and $3d$. The 31 states so generated are given in Table 4. In addition to these real orbitals a further four pseudo-orbitals ($\overline{4s}$, $\overline{4p}$, $\overline{4d}$, $\overline{4f}$) were included to allow for correlation in the target state representation. The parameters in the analytic function (3) were determined as follows: the $1s$ and $2s$ orbital parameters were taken to be the Hartree-Fock values derived by Clementi & Roetti (1974) for the ground state of Fe XXIII; the $2p$, $3s$, $3p$ and $3d$ orbital parameters were obtained by optimisation of the energy of the corresponding $1s^2nl \ ^2L$ state of Fe XXIV. Finally, the parame-

Table 3. Radial function parameters for Lithium-like Fe XXIV orbitals

Function	c_{jnl}	I_{jnl}	ζ_{jnl}
1s	0.98715	1	25.52450
	0.01133	1	45.77480
	-0.00008	2	11.73700
	0.00382	2	20.46870
2s	-0.33568	1	25.52450
	-0.00008	1	45.77480
	1.29072	2	11.73700
	-0.30212	2	20.46870
3s	0.39865	1	15.38554
	-3.53348	2	6.76540
	3.98649	3	7.73052
$\overline{4s}$	3.21113	1	9.20356
	-13.59461	2	9.22671
	22.16287	3	9.22593
	-12.13089	4	9.78159
2p	1.00000	2	12.17576
3p	1.07237	2	9.57623
	-1.62889	3	7.84995
$\overline{4p}$	1.14379	2	21.87541
	-2.91648	3	9.68465
	2.45324	4	9.64968
3d	1.00000	3	8.00504
$\overline{4d}$	3.73757	3	9.61722
	-3.64415	4	10.30303
$\overline{4f}$	1.00000	1	17.70126

ters for the four pseudo-orbitals $\overline{4s}$, $\overline{4p}$, $\overline{4d}$, $\overline{4f}$ were obtained as follows: the $\overline{4s}$ orbital parameters were obtained by optimisation on the $1s2s^2\ ^2S$ Fe XXIV excited state, to take into account the different 1s and 2s orbitals associated with this excited state; the $\overline{4p}$ orbital parameters were obtained by optimisation on the $1s2p^2\ ^2P$ Fe XXIV excited state, to account for the different 2p orbital associated with this state; the $\overline{4d}$ and $\overline{4f}$ orbital parameters were obtained by optimisation on the $1s2p^2\ ^2D$ Fe XXIV excited state, to include appropriate correlation effects. The parameters c , I , ζ for each of these functions are given in Table 3.

These one-electron functions were then employed in a configuration-interaction representation of the lithium-like target states, by generating appropriate configurations from the addition of any two orbitals from the above set to a 1s orbital. It is noted that the specific configurations arising from $1s^2\overline{4l}$ were excluded, since these give rise to target states which are embedded below the first ionisation threshold and which are not real spectroscopic terms. The energies of the 31 target states obtained, relative to the $1s^22s\ ^2S$ ground state, are given in Table 4. Also shown is a comparison with the critically reviewed data of Shirai et al. (1990). However we note that there is a lack of reliable results, and in addition a complete identification has not always been possible. Nevertheless, the agreement is highly satisfactory and it is noted that for all states, with the exception of the $1s^22p\ ^2P^o$ state, the difference is fairly consistent at about 1 – 2%. We are satisfied that, for this considerably more com-

**Fig. 1.** Total photoionisation cross-section of Fe XXIV. Solid line: present calculation; diamond: Verner et al. (1993, 1995); square: Clark et al. (1986)

plicated case, the target states are represented to a sufficiently high degree of accuracy.

The R-matrix program was then utilized with 37 continuum orbitals included for each incident electron orbital angular momentum. The R-matrix boundary radius was set at 1.8 au. The (N+1)-electron correlation terms were generated from all possible three electron combinations of the above orbital set added to a 1s orbital and, in order to achieve a correct balance in the various correlations, all configurations of type $1s^2\overline{4l}\overline{4l'}$ were excluded. We obtained a value of 142.04 Ryd for the ionisation energy of the ground state of Fe XXIII, in excellent agreement with the result of 143.34 Ryd given by Shirai et al. (1990).

3. Results and discussion

3.1. Photoionisation of Fe XXIV

We obtained 11 partial photoionisation cross-sections from the $1s^22s\ ^2S$ Fe XXIV ground state, corresponding to the final ion being left in one of the target states discussed in Sect. 2.1; from these the total photoionisation cross-section and the cross-section for 1s electron removal are readily derived.

The total photoionisation cross-section over the energy range considered is presented in Fig. 1. Only the data obtained in the length formulation will be considered, since the length and velocity formulation results are almost indistinguishable. In order to properly make comparison with previous calculations, we present in Fig. 2 the total photoionisation cross-section below the ionisation threshold corresponding to 1s electron photoejection. In both figures, we restrict comparison with the most recent work, namely that by Verner et al. (1993, 1995) and earlier data obtained using a similar approximation but neglecting relativistic effects (Clark et al. 1986). We note that the results of Reilman & Manson (1979) differ by $\lesssim 5\%$ from the present data whilst the values obtained by Peach et al. (1988) differ by

Table 4. Comparison between *ab initio* energy levels (in Ryd) and assessed data (Shirai et al. 1990) relative to the ground state of Fe XXIV

State	Present	Shirai et al.
$1s^2 2p^2 P^0$	3.437	4.353
$1s^2 3s^2 S$	83.453	84.476
$1s^2 3p^2 P^0$	84.409	85.675
$1s^2 3d^2 D$	84.789	86.247
$1s 2s^2 S$	481.761	485.000
$1s 2s(1S) 2p^2 P^0$	485.323	490.901
$1s 2s(3S) 2p^2 P^0$	486.406	489.416
$1s 2p^2 D$	487.774	492.908
$1s 2p^2 P$	488.408	493.680
$1s 2p^2 S$	490.187	495.472
$1s 2s(3S) 3s^2 S$	567.482	-
$1s 2s(3S) 3p^2 P^0$	567.887	-
$1s 2s(3S) 3d^2 D$	568.986	-
$1s 2s(1S) 3s^2 S$	569.090	-
$1s 2s(1S) 3p^2 P^0$	569.767	-
$1s 2p(3P^0) 3p^2 P$	569.878	-
$1s 2p(3P^0) 3s^2 P^0$	570.300	575.862 [†]
$1s 2p(3P^0) 3d^2 D^0$	570.511	-
$1s 2p(3P^0) 3p^2 D$	570.747	578.209 [†]
$1s 2s(1S) 3d^2 D$	570.848	-
$1s 2p(1P^0) 3s^2 P^0$	571.061	575.862 [†]
$1s 2p(3P^0) 3d^2 F^0$	571.153	579.589 [†]
$1s 2p(3P^0) 3p^2 S$	571.325	579.170 [†]
$1s 2p(3P^0) 3d^2 P^0$	571.640	-
$1s 2p(1P^0) 3p^2 D$	571.923	578.209 [†]
$1s 2p(1P^0) 3p^2 P$	571.925	-
$1s 2p(1P^0) 3d^2 D^0$	572.467	-
$1s 2p(1P^0) 3p^2 S$	572.510	579.170 [†]
$1s 2p(1P^0) 3d^2 F^0$	572.668	579.589 [†]
$1s 2p(1P^0) 3d^2 P^0$	573.036	-

[†] Coupling of electrons not identified by Shirai et al.

$\lesssim 3\%$. Fig. 2 shows that the present background cross-section agrees closely (within 1%) with that of Verner et al. In addition, the difference between the Verner et al. and Clark et al. calculations, previously attributed to relativistic effects, do not appear to be present.

The most significant feature of the present work in comparison with earlier studies is the resonances. Figs. 1 and 2 show these quite clearly; the two $1P^0$ lowest lying resonances together with the series of resonances converging on the $1s 2s^3 S$ threshold.

Fig. 3 presents the results for removal of the $1s$ electron, and again excellent agreement is found between the present data and those of Verner et al. (1993, 1995), the difference being within 2%. The results of Clark et al. (1986) are some 10-30 % lower than the present data.

3.2. Photoionisation of Fe XXIII

We obtained 31 partial photoionisation cross-sections from the $1s^2 2s^2 1S$ Fe XXIII ground state, corresponding to the final

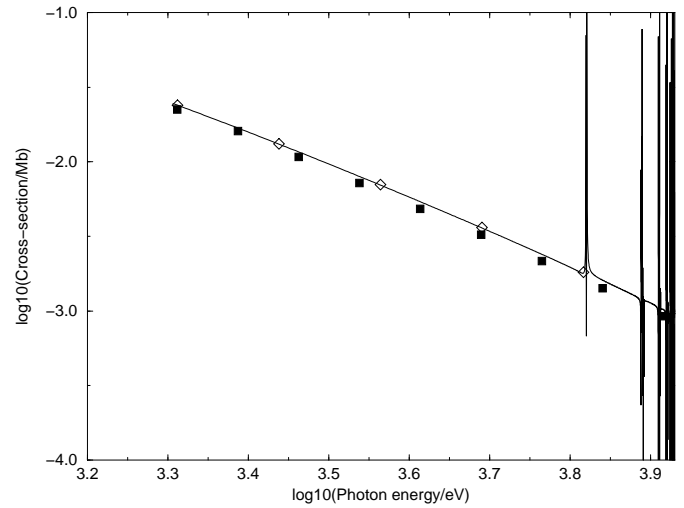


Fig. 2. Total photoionisation cross-section of Fe XXIV below the $1s$ photoejection threshold. Solid line: present calculation; diamond: Verner et al. (1993, 1995); square: Clark et al. (1986)

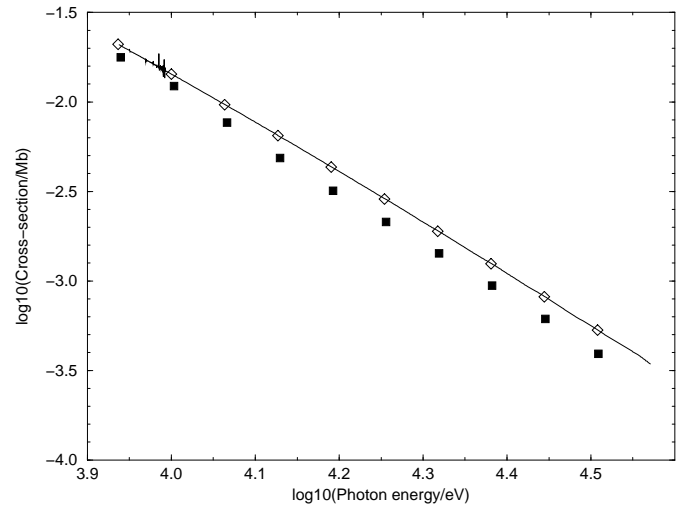


Fig. 3. Total $1s$ removal photoionisation cross-section of Fe XXIV. Solid line: present calculation; diamond: Verner et al. (1993, 1995); square: Clark et al. (1986)

ion being left in one of the target states discussed in Sect. 2.2, and from these both the total photoionisation cross-section and the cross-section for $1s$ electron removal are readily derived. We note that contributions to the $1s$ removal cross-section from final states other than $1s 2s^2$, $1s 2s 2p$ and $1s 2p^2$ are negligible.

The total photoionisation cross-section obtained in the length formulation over the energy range considered is presented in Fig. 4, whilst the $1s$ removal cross-section is shown in Fig. 5. The data obtained by Reilman & Manson (1979) are not shown, but differ by $\lesssim 5\%$ from the present results in the energy region below the $1s$ photoejection threshold. The five-state close-coupling values of Tully et al. (1990) only differ significantly as the $1s$ photoejection threshold is approached and,

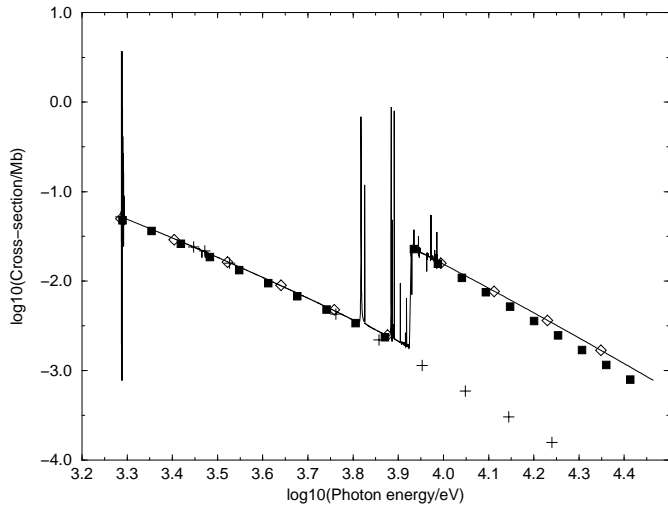


Fig. 4. Total photoionisation cross-section of Fe XXIII. Solid line: present calculation; diamond: Verner et al. (1993, 1995); square: Clark et al. (1986); cross: Tully et al. (1990)

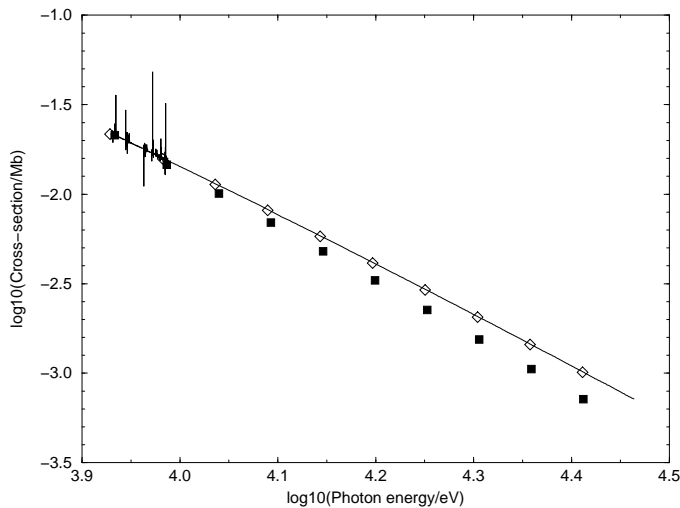


Fig. 5. Total $1s$ removal photoionisation cross-section of Fe XXIII. Solid line: present calculation; diamond: Verner et al. (1993, 1995); square: Clark et al. (1986)

although their data is plotted in Fig. 4, we recall that they did not include the possibility of $1s$ removal. An almost identical conclusion to that discussed above for Fe XXIV, applies also to Fe XXIII in comparing the present results, the data of Verner et al. (1993, 1995) and the values obtained by Clark et al. (1986). The present work and that of Verner et al. are in agreement to within 5% below the $1s$ removal threshold, and to within 1% above this threshold.

As in the case of Fe XXIV photoionisation, the total cross-section exhibits many large, well-defined resonances, several orders of magnitude greater than the background, before the onset of $1s$ photoejection. Soon after the $1s$ photoejection threshold,

some smaller resonances (about 20% greater than background) are observed in the cross-section.

4. Summary

In summary, the existing data for the total background cross-sections for the photoionisation of Fe XXIV and Fe XXIII have been validated by the present work, and it is probable that an accuracy of a few per cent can be assigned to the data. The inclusion of resonance phenomena in the present study should have significance in applications of the data.

Finally, we note that the individual partial cross-sections for the photoionisation processes may be obtained from the authors on request.

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