

# Atomic data from the Iron Project

## XXVI. Photoionization cross sections and oscillator strengths for Fe IV

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**Abstract.** Photoionization cross sections and dipole transition probabilities for the astrophysically important iron ion Fe IV are presented. The computations were carried out in the close coupling approximation using the R-matrix method including 31 LS terms with multiplicity  $(2S + 1) = 3$  and 5 of the target ion Fe V. All quartets and sextet bound states of Fe IV with  $n \leq 10$  and  $L \leq 8$  are considered. The results include 746 LS bound states, dipole oscillator strengths for 34 635 LS transitions, and, for all bound states, detailed photoionization cross sections with extensive resonance structures. These data differ significantly in many cases from the earlier data calculated under the Opacity Project and other theoretical calculations. In particular, the new cross section for the  $^6S$  ground state of Fe IV exhibits a large resonance near the threshold that is not present in previous calculations and is likely to affect the effective photoionization rate significantly. The autoionizing state that corresponds to that resonance as well as the Rydberg series to which it belongs are identified through supplementary close coupling calculations.

**Key words:** atomic data — plasmas — ultraviolet general

### 1. Introduction

Low ionization stages of iron, owing to their rich and complex structure and their relatively high abundance, dominate certain wavelength regions in the spectra of a variety of stellar and non-stellar objects, as well as the interstellar medium. Photoionization models of low excitation HII regions show Fe IV to be the dominant ionization state throughout most of the interior of the cloud, along with Fe I-III. Fe IV and Fe V have recently been identified in the EUV spectra of photospheres of hot, young white dwarfs, as recently observed by the *Extreme Ultraviolet*

*Explorer* (Pradhan 1995; Vennes 1995). In both cases accurate photoionization cross sections are needed to model these objects.

The interpretation and modeling of observations rely almost entirely on theoretical values of the atomic data, which until the recent advances made under the Opacity Project (OP, Seaton et al. 1994) and the Iron Project (IP, Hummer et al. 1993) could not be obtained with sufficient accuracy and on the large scale needed to fully determine the relevant astrophysical parameters. However, the OP calculations of radiative data and photoionization cross sections for the low ionization stages of Iron, i.e. Fe I-V, are not sufficiently accurate for modeling and lead to significant discrepancies with observations (e.g. Pradhan 1995). One of the goals of the IP is to carry out improved calculations for these ions (Bautista et al. 1996). This paper presents the results for Fe IV, which completes the set of improved radiative atomic data for the Fe I-V sequence. The calculations for the other ions were reported in Bautista & Pradhan (1995) and Bautista (1997) for Fe I, Nahar & Pradhan (1994) and Nahar (1995) for Fe II, Nahar (1996) for Fe III, and Bautista (1996) for Fe V.

A full list of papers from the IRON Project published to-date is given in the references. A complete list of papers including those in press can be found at <http://www.am.qub.uk/projects/iron/papers/>, where abstracts are also given for each paper. Information on other works by the present authors and their collaborators, including collisional excitation and recombination of ions of iron and other elements, can be found at <http://www-astronomy.mps.ohio-state.edu/~pradhan/>.

### 2. Target expansion

In the close coupling (CC) approximation the total wave function of the electron-ion system is represented as

$$\Psi(E; SL\pi) = A \sum_i \chi_i \theta_i + \sum_j c_j \Phi_j, \quad (1)$$

where  $\chi_i$  is the target ion wave function in a specific state  $S_i L_i$ ,  $\theta_i$  is the wave function for the free electron, and  $\Phi_j$  are short range correlation functions for the bound (e + ion) system. Accurate CC calculations of atomic processes require, first of all, a good representation of the target ion. For complex ions an accurate representation must include a large number of correlation configurations. However, in order for the computations to be computationally tractable, the configuration expansion must be carefully and economically chosen.

The CC expansion for this calculation includes 31 LS terms of the target ion Fe V. The atomic structure code SUPERSTRUCTURE (Eissner et al. 1974; Eissner 1991) was used to compute eigenfunctions for the 31 states of the Fe V target ion dominated by  $3d^4$ ,  $3d^3 4s$ , and  $3d^3 4p$ . Table 1 presents the complete list of configurations included in the target, as well as a comparison between the calculated target term energies and the observed energies, averaged over the fine structure, taken from Sugar & Corliss (1985). The agreement between the energies is very good; in all but six cases the agreement with the experimental values is within  $\sim 2\%$ . The overall agreement is better than 4%. Another indicator of the accuracy of the target representation is the good agreement between the length and the velocity oscillator strengths ( $f$ -values), which for the present case is typically about 10% (for a complicated atomic system such as Fe IV it is difficult to achieve higher accuracy for LS  $f$ -values).

### 3. Radiative calculations

The present calculations were carried out in LS coupling, since the relativistic effects in photoionizing the low ionization stages of iron should be small. Although they might be significant for some types of transitions in Fe IV, it would be impractical at this stage to carry through a large-scale relativistic calculation involving a number of channels several times larger than the already huge number in the LS coupling case. Also, the inclusion of fine structure has only a marginal effect on the calculation of the Rosseland or the Planck mean opacities (Seaton et al. 1994).

The second summation in the CC expansion (Eq. 1) represents short range correlation functions. These functions are very important in obtaining accurate (e + ion) wavefunctions, but may cause pseudo-resonances, particularly if the two summations in Eq. (1) are inconsistent (Berrington et al. 1987; also discussed later). Owing to the magnitude of the calculations, the set of  $\Phi_j$  functions for Fe IV was optimized to include only the minimum number of correlation functions having important effects on the bound states energies and bound-bound oscillator strengths. Nonetheless, this component of the close coupling expansion is large (Table 2).

The overall calculation was divided into two groups of total (e + ion) symmetries  $SL\pi$  according to their multi-

**Table 2.** Correlation functions for Fe IV included in the CC expansion

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$3p^6 3d^7, 3s3p^5 3d^7, 3p^5 d^7 4s, 3p^5 d^7 4p, 3p^5 d^7 4d, 3s^2 3p^4 3d^7,$ $3s3p^4 3d^7 4s, 3s3p^4 3d^7 4p, 3s3p^4 3d^7 4d, 3p^4 3d^7 4s^2, 3p^4 3d^7 4p^2,$ $3p^4 3d^6 4s4p^2, 3s^2 3p^6 3d^5, 3s^2 3p^6 3d^4 4s, 3s^2 3p^6 3d^4 4p,$ $3s^2 3p^5 3d^6, 3s^2 3p^5 3d^5 4s, 3s^2 3p^5 3d^5 4p, 3s^2 3p^5 3d^5 4d, 3p^6 3d^6 4s,$ $3p^6 3d^6 4p, 3p^6 3d^6 4d, 3p^6 3d^5 4s^2, 3p^6 3d^5 4p^2, 3p^6 3d^5 4s4p,$ $3p^6 3d^5 4s4d, 3s3p^6 3d^4 4s^2, 3s3p^6 3d^4 4p^2, 3s3p^6 3d^4 4s4d,$ $3s^2 3p^5 3d^4 4s4d, 3p^5 3d^6 4s4d, 3s3p^6 3d^6, 3p^6 3d^4 4s^2 4d,$ $3p^6 3d^4 4s4p^2, 3s^2 3p^4 3d^5 4p^2, 3s^2 3p^4 3d^5 4s^2, 3s3p^6 3d^5 4s,$ $3p^6 3d^7, 3s^2 3p^5 3d^4 4s^2, 3s^2 3p^5 3d^4 4p^2, 3s^2 3p^5 3d^4 4s4p,$ $3s^2 3p^5 3d^4 4p4d, 3s3p^6 3d^6, 3s3p^6 3d^4 4s^2, 3s3p^6 3d^4 4p^2,$ $3s3p^6 3d^4 4s4d, 3s3p^6 3d^4 4p4d, 3s^2 3p^4 3d^7, 3s^2 3p^4 3d^6 4s,$ $3s^2 3p^4 3d^5 4s^2, 3s^2 3p^4 3d^5 4p^2, 3s^2 3p^4 3d^5 4s4d, 3s^2 3p^4 3d^4 4s4p^2,$ $3s^2 3p^6 3d^4 4d, 3s3p^6 3d^4 4s4p, 3p^6 3d^4 4s^2 4p, 3s3p^6 3d^5 4d,$ $3s^2 3p^5 3d^4 4s4d, 3s3p^6 3d^4 4s4p, 3s^2 3p^4 3d^6 4d, 3s3p^4 3d^4 4s^2 4p^2$
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plicity, i.e.  $(2S + 1) = 4$ , and 6. For each multiplicity we consider total angular momenta  $L = 0 - 8$ , for both parities, and a total of 31  $SL\pi$ 's corresponding to the target terms in Table 1. Given the present large expansion, it was not possible to include the doublet symmetries, which are not connected to the ground state  ${}^6S$ , due to memory and disk space constraints (several tens of gigabytes). On the other hand, a calculation with a reduced number of terms would probably yield results similar to those of Sawey & Berrington (1992; SB) who included only the  $3d^4$  terms in their OP calculations.

### 4. Results

The results for the energy levels, oscillator strengths, and total and partial photoionization cross sections are described in the following sections.

#### 4.1. Energy levels of Fe IV

The calculations begin with the energies of 746 LS terms of Fe IV corresponding to all possible bound states with principal quantum number  $n \leq 10$ . In Table 3 we compare the computed energies for these terms with those calculated by SB, and experimental values from Sugar & Corliss (1985). The energies obtained in the present work, especially those for the low lying states, agree typically within 2% with the experimental values. This level of agreement, for most terms, is better than the results of SB.

#### 4.2. Oscillator strengths

Dipole oscillator strengths ( $f$ -values) for 34,635 transitions among the calculated states of Fe IV were obtained in LS coupling. This set includes transitions for which the lower state lies below the first ionization threshold and the

**Table 1.** Calculated and observed term energies (Rydbergs) for Fe V relative to the  $3d^4(^5D)$  ground state. The spectroscopic and correlation configurations for Fe V, and the values of the scaling parameters  $\lambda_{nl}$  for each orbital in the Thomas-Fermi-Dirac potential used in Superstructure, are also given

Level		$E_{obs}$	$E_{cal}$	Level		$E_{obs}$	$E_{cal}$		
1	$3d^4$	$^5D$	0.000000	0.000000	17	$3d^3(^2F)4s$	$^3F$	2.12336	2.161109
2	$3d^4$	$^3P$	0.227038	0.232252	18	$3d^3(^4F)4p$	$^5G^0$	2.33251	2.355847
3	$3d^4$	$^3H$	0.223059	0.259441	19	$3d^3(^4F)4p$	$^5D^0$	2.35148	2.386004
4	$3d^4$	$^3F$	0.237769	0.261593	20	$3d^3(^2D1)4s$	$^3D$	2.34905	2.419861
5	$3d^4$	$^3G$	0.267818	0.309157	21	$3d^3(^4F)4p$	$^5F^0$	2.36577	2.391652
6	$3d^4$	$^3D$	0.327553	0.379240	22	$3d^3(^4F)4p$	$^3D^0$	2.36838	2.397309
7	$3d^4$	$^3P$	0.561290	0.618696	23	$3d^3(^4F)4p$	$^3G^0$	2.40378	2.440669
8	$3d^4$	$^3F$	0.560546	0.618706	24	$3d^3(^4F)4p$	$^3F^0$	2.42943	2.469158
9	$3d^3(^4F)4s$	$^5F$	1.70206	1.695583	25	$3d^3(^4P)4p$	$^5P^0$	2.49342	2.534489
10	$3d^3(^4F)4s$	$^3F$	1.78024	1.782194	26	$3d^3(^4P)4p$	$^5D^0$	2.51746	2.556067
11	$3d^3(^4P)4s$	$^5P$	1.86264	1.874768	27	$3d^3(^4P)4p$	$^3P^0$	2.50752	2.551853
12	$3d^3(^2G)4s$	$^3G$	1.89927	1.910388	28	$3d^3(^2G)4p$	$^3H^0$	2.52243	2.558687
13	$3d^3(^4P)4s$	$^3P$	1.93610	1.963195	29	$3d^3(^2G)4p$	$^3G^0$	2.54016	2.585237
14	$3d^3(^2P)4s$	$^3P$	1.94802	1.975859	30	$3d^3(^2G)4p$	$^3F^0$	2.54951	2.597140
15	$3d^3(^2D)4s$	$^3D$	1.96486	1.984966	31	$3d^3(^2P)4p$	$^3P^0$	2.60523	2.623293
16	$3d^3(^2H)4s$	$^3H$	1.96974	1.985141					

Fe V configurations.

Spectroscopic:  $3s^2 3p^6 3d^4$ ,  $3s^2 3p^6 3d^3 4s^1$ ,  $3s^2 3p^6 3d^3 4p^1$ .

Correlation:  $3s^2 3p^5 3d^5$ ,  $3s^2 3p^4 3d^6$ ,  $3s^2 3p^6 3d^2 4p^2$ ,  $3s^1 3p^6 3d^4 4s^1$ ,  $3s^1 3p^6 3d^4 4p^1$ ,  $3p^6 3d^6$ ,  $3p^6 3d^5 4s^1$ ,  $3p^6 3d^4 4s^2$ ,  $3s^2 3p^6 3d^2 4s^1 4p^1$ ,  $3s^2 3p^6 3d^2 4s^1 4d^1$ .

$\lambda_{nl}$ : 0.92092(1s), 1.12967(2s), 1.30081(2p), 1.30177(3s), 1.10895(3p), 1.08238(3d), 1.08360(4s), 1.08238(4p), 1.19316(4d).

upper state lies above. These transitions can be important in opacity calculations because they contribute to the total photo-absorption, but do not appear as resonances in the photoionization cross sections (strictly speaking, the upper bound state does autoionize if departure from LS coupling is considered and fine structure continua are explicitly allowed).

In the absence of experimental  $f$ -values it is difficult to ascertain the overall accuracy of the data. However, a comparison of length and velocity oscillator strengths provides a systematic consistency check on the accuracy of the wavefunctions and, therefore, on the reliability of the  $f$ -values. In Fig. 1 we plot  $\log gf_V$  vs.  $\log gf_L$ . We have included all the symmetries since each exhibits roughly the same dispersion. The dispersion between length and velocity values with  $gf$ 's greater than unity  $< 13\%$  for the quartets, and  $< 22\%$  for the sextets. This, added to the good agreement between the calculated energies and those observed experimentally, suggests that the overall uncertainty for such transitions should be 20% or less. However, weaker transitions are likely to have greater uncertainties.

Table 4 presents a comparison of the present  $gf$ -values with those of SB and Fawcett (1989) for a small sample of transitions. Fawcett's work is based on a semi-empirical adjustment of Slater parameters in the relativistic Hartree-Fock code by Cowan (1981) to minimize the differences between calculated and observed wavelengths. Very good agreement between the present results and Fawcett's values is observed for most transitions.

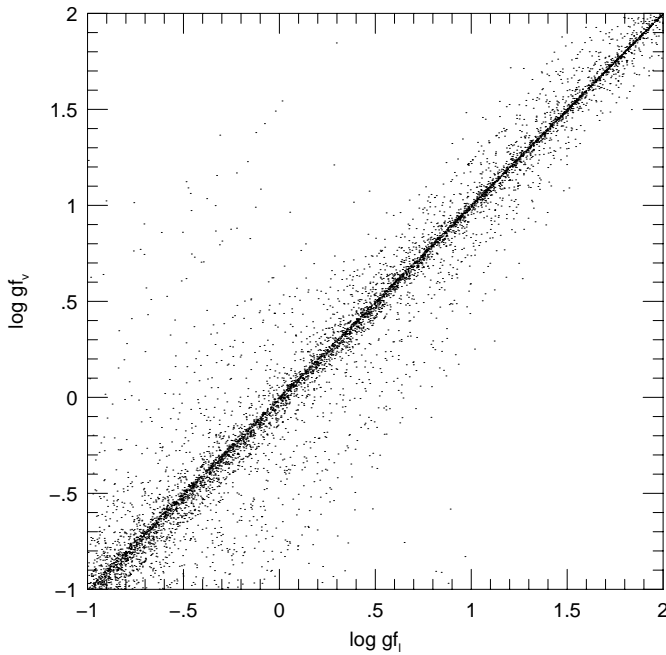
#### 4.3. Photoionization cross sections

Photoionization cross sections were calculated for all 746 bound states of Fe IV considered here. These cross sections include detailed autoionization resonances resulting from the coupling to states dominated by  $3d^4$ ,  $3d^3 4s$ , and  $3d^2 4p$  configurations in the core ion. Figure 2a shows the photoionization cross section of the  $3d^5(^6S)$  ground state of Fe IV. In the same figure we have plotted the results of Reilman & Manson (1979) and those of SB. One interesting feature in the present cross section is the huge resonance, more than 1 Ry wide and two orders of magnitude higher than the background, just above the ionization threshold. Such a feature should have a large effect on the ionization rate and the opacity of Fe IV; thus a careful and detailed study of this resonance is worthwhile.

The first thing to investigate is what electron configuration of the Fe IV system is responsible for the resonance, and whether this is possibly a pseudo-resonance that sometimes arise in close coupling calculations owing to inconsistencies between the two summations in Eq. (1). Pseudo-resonances can arise if the first summation involving all channels coupled to the target terms does *not* explicitly include the parent configurations of some  $(N+1)$ -electron correlation configurations included in the second summation. Such configurations then do not have corresponding thresholds for the Rydberg series of resonances in the target expansion (first summation in Eq. (1)). These manifest themselves as large pseudo-resonances, which in

**Table 3.** Comparison of the calculated energies for Fe IV,  $E_{\text{cal}}$ , with the previous OP results,  $E_{\text{TOP}}$ , by Sawey & Berrington (1992), and observed energies,  $E_{\text{obs}}$ , from Sugar & Corliss (1985)

Conf.	Term	$E_{\text{cal}}$	$E_{\text{OP}}$	$E_{\text{obs}}$	Conf.	Term	$E_{\text{cal}}$	$E_{\text{OP}}$	$E_{\text{obs}}$
$3d^5$	$^6S$	-3.984	-3.961	-4.028	$3d^4(5D)4p$	$^6D^\circ$	-2.229	-2.214	-2.266
$3d^5$	$^4G$	-3.665	-3.640	-3.734	$3d^4(5D)4p$	$^4F^\circ$	-2.184	-2.189	-2.237
$3d^5$	$^4P$	-3.660	-3.585	-3.706	$3d^4(5D)4p$	$^4D^\circ$	-2.115	-2.135	-2.184
$3d^5$	$^4D$	-3.613	-3.563	-3.674	$3d^4(3H)4p$	$^4H^\circ$	-2.005	-2.035	-2.090
$3d^5$	$^4F$	-3.485	-3.426	-3.548	$3d^4(3P2)4p$	$^4D^\circ$	-1.971	-2.024	-2.075
$3d^4(5D)4s$	$^6D$	-2.941	-2.774	-2.857	$3d^4(3F2)4p$	$^4G^\circ$	-1.967	-2.035	-2.065
$3d^4(5D)4s$	$^4D$	-2.795	-2.685	-2.767	$3d^4(3H)4p$	$^4I^\circ$	-1.972	-2.006	-2.058
$3d^4(3P2)4s$	$^4P$	-2.648	-2.531	-2.616	$3d^4(3P2)4p$	$^4P^\circ$	-1.936	-1.997	-2.048
$3d^4(3H)4s$	$^4H$	-2.618	-2.531	-2.620	$3d^4(3F2)4p$	$^4F^\circ$	-1.932	-1.987	-2.038
$3d^4(3F2)4s$	$^4F$	-2.613	-2.516	-2.605	$3d^4(3H)4p$	$^4G^\circ$	-1.949	-1.988	-2.040
$3d^4(3G)4s$	$^4G$	-2.580	-2.488	-2.578	$3d^4(3F2)4p$	$^4D^\circ$	-1.910	-1.970	-2.026
$3d^4(3D)4s$	$^4D$	-2.523	-2.427	-2.519	$3d^4(3G)4p$	$^4H^\circ$	-1.906	-1.956	-2.010
$3d^4(5D)4p$	$^6F^\circ$	-2.275	-2.256	-2.303	$3d^4(3G)4p$	$^4F^\circ$	-1.902	-1.959	-2.012
$3d^4(5D)4p$	$^6P^\circ$	-2.267	-2.250	-2.296	$3d^4(3G)4p$	$^4G^\circ$	-1.877	-1.929	-1.982
$3d^4(3P1)4s$	$^4P$	-2.280	-2.194	-2.292	$3d^4(3D)4p$	$^4D^\circ$	-1.819	-1.900	-1.959
$3d^4(3F1)4s$	$^4F$	-2.270	-2.198	-2.293	$3d^4(3D)4p$	$^4P^\circ$	-1.816	-1.895	-1.947
$3d^4(5D)4p$	$^4P^\circ$	-2.226	-2.224	-2.274	$3d^4(3D)4p$	$^4F^\circ$	-1.806	-1.882	-1.939

**Fig. 1.**  $\log gf_V$  plotted against  $\log gf_L$  for transitions between calculated LS terms

a sense represent the entirety of resonance series belonging to the missing thresholds. In order to rule out this possibility, the ground state cross section was calculated several times with different subsets of the  $(N+1)$ -electron correlation configurations list given in Table 2.

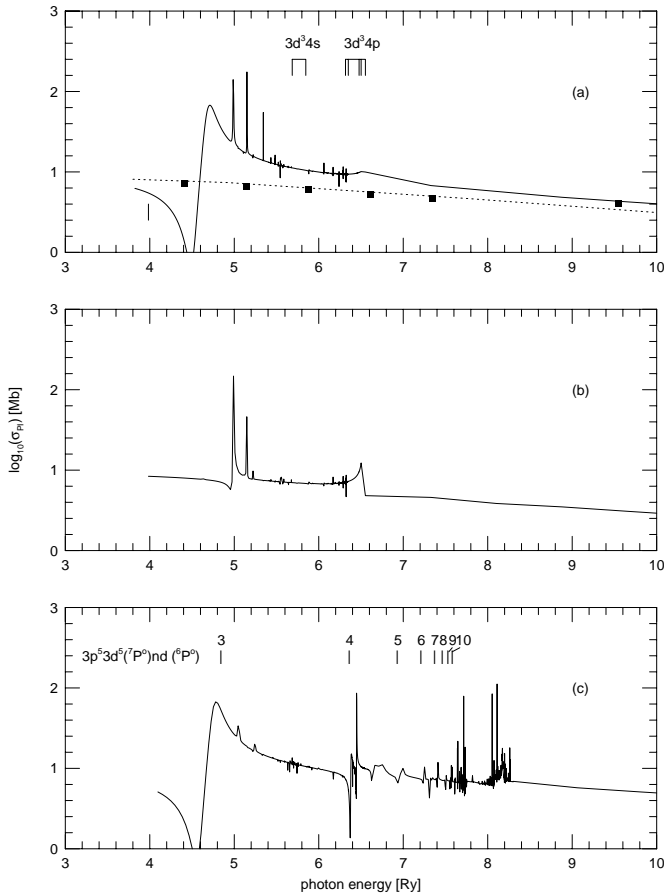
It appears that the configuration  $3s^23p^53d^6$  gives rise to the particular resonance. Figure 2b shows the cross section obtained when this configuration is

excluded. The  $3s^23p^53d^6$  configuration of Fe IV corresponds directly to the  $3s^23p^53d^5$  correlation configuration in the expansion for the Fe V core ion. Thus, this resonance appear to be real. In addition, the term energies for Fe IV calculated with an accurate CI expansion that includes the  $3s^23p^53d^6$  configuration, using the code SUPERSTRUCTURE (Eissner 1991), indicates that an autoionizing  $3s^23p^53d^6(^6P^\circ)$  state is indeed expected at about 4.58 Ry above the ground state. That the energy of this state agrees well with the position of the resonance adds weight to our identification.

**Table 4.** Comparison of calculated  $gf$  values in LS coupling for Fe IV with the OP calculations by Sawey & Berrington (1992), and the semi-empirical results by Fawcett (1989) using Cowan's code

Configuration	Transition	Present	SB	Fawcett
$3d^4(5D)4s - 3d^4(5D)4p$	$^6D - ^6P^\circ$	6.11	5.92	6.11
	$^6D - ^6D^\circ$	10.2	9.83	8.49
	$^6D - ^6F^\circ$	13.8	13.3	13.9
	$^4D - ^4P^\circ$	3.77	3.64	2.20
	$^4D - ^4D^\circ$	7.02	6.67	6.57
	$^4D - ^4F^\circ$	9.17	8.79	8.75
$3d^4(3H)4s - 3d^4(3H)4p$	$^4H - ^4H^\circ$	12.7	11.5	12.0
	$^4H - ^4I^\circ$	17.5	16.6	16.9
$3d^4(3F)4s - 3d^4(5D)4p$	$^4F - ^4F^\circ$	0.11	0.08	0.10
$3d^4(3G)4s - 3d^4(5D)4p$	$^4G - ^4F^\circ$	0.11	0.08	0.10
$3d^4(3G)4s - 3d^4(3H)4p$	$^4G - ^4H^\circ$	1.90	2.24	1.94

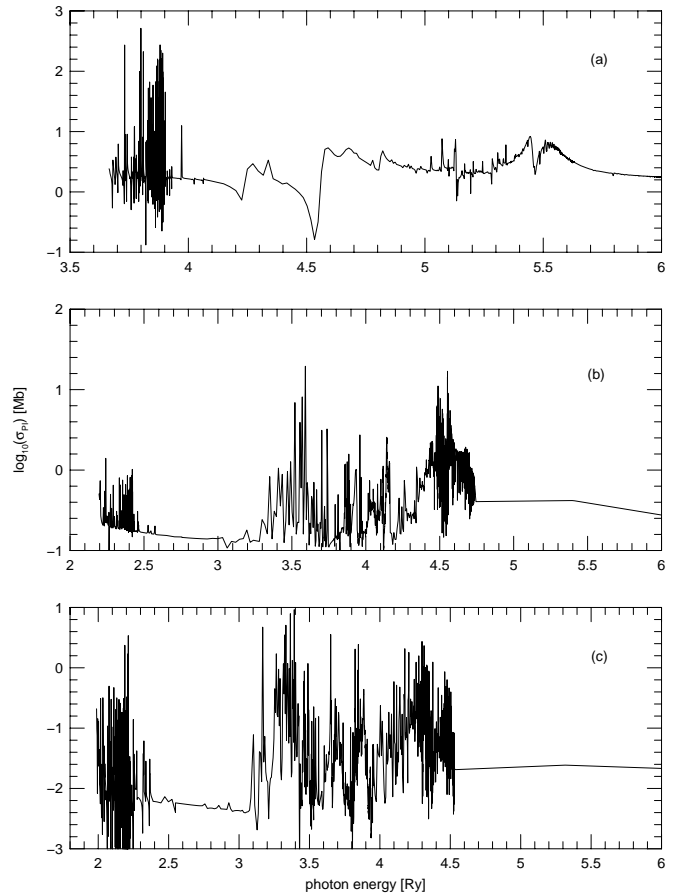
As this resonance arises from the  $3s^23p^53d^6$  configuration in Fe IV, one might expect that explicit



**Fig. 2.** Photoionization cross section ( $\sigma$  (Mb)) of the ground state  $3d^5(^6S)$  of Fe IV as a function of photon energy (Rydbergs). **a)** the cross section obtained with the present 31CC expansion (solid curve); **b)** the cross section excluding the  $3s^2 3p^5 3d^6$  configuration; **c)** the cross section with the  $3s^2 3p^5 3d^5$  target terms of Fe V included explicitly (the Rydberg series  $3s^2 3p^5 3d^5(^7P^o)nd(^6P^o)$  for  $n = 3$  to 10 is marked). The dashed curve shows the results of Sawey & Berrington (1992) and the filled dots, those of Reilman & Manson (1979)

inclusion in the calculation of the thresholds due to the  $3s^2 3p^5 3d^5$  parent configuration in the Fe V target would change the shape of the resonance and even break it into a series of narrow Rydberg resonances. The list of term energies for Fe V in the present target expansion reveals that above these 31 terms the next higher terms coupled to the ground  $^6S$  state of Fe IV are  $3s^2 3p^5 3d^5(^7P^o)$ ,  $(^5P^o)$ ,  $(^5F^o)$ ,  $(^5H^o)$ . Therefore, the ground state cross section was re-calculated including these states; the result is shown in Fig. 2c. A number of narrow resonances converging on to the new thresholds are present; however, the large resonance under investigation remains unchanged.

The more extended calculation also allows for a better identification of the origin of the resonance, which seems to belong to the  $3s^2 3p^5 3d^5(^7P^o)nd(^6P^o)$  Rydberg series,

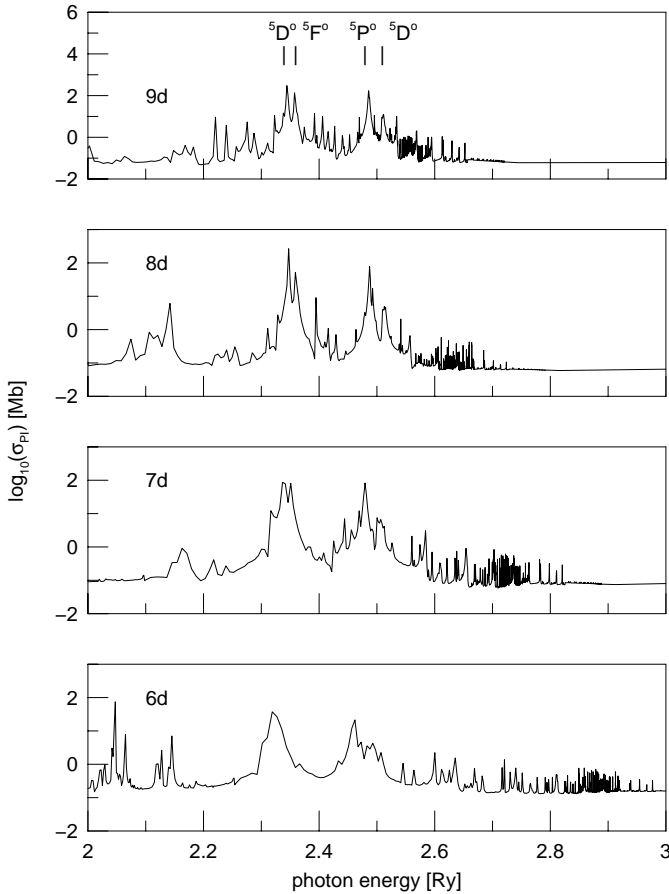


**Fig. 3.** Partial photoionization cross sections of some excited states ( $3d^5\ ^4G$ , panel **a**); ( $3d^4(^5D)4p\ ^4F^o$ , panel **b**); ( $3d^4(^3F2)4p\ ^4G^o$ , panel **c**) of Fe IV into the ground state of Fe V

as indicated in Fig. 2c, for  $n = 3$  to 10. An alternative series could be the  $3s^2 3p^5 3d^5(^5P^o)nd(^6P^o)$ ; however, the percentage channel contribution with the  $^5P^o$  parent is smaller.

Thus the nature of the large resonance in the ground state cross section seems to be understood, and its identification as the autoionizing equivalent electron state  $3s^2 3p^5 3d^6(^6P^o)$  explains in large part the broadness of the feature. Nevertheless, one should be aware that the position of the resonance may be uncertain in the absence of experimental data for the  $3s^2 3p^5 3d^5$  thresholds in Fe V. Also, the position of the resonance in the present calculation relies entirely on the accuracy of the  $3s^2 3p^5 3d^5$  wavefunctions, which is rather difficult to assess.

The failure of other authors to obtain resonance structures in the cross sections is due to the absence of the relevant electron correlations in those calculations. This is always the case for the central field approximation used by Reilman & Manson (1979). The close-coupling calculation by SB included only the 16 states of the target ion dominated by the  $3d^4$  configuration. This means that



**Fig. 4.** Photoionization of bound states in the  $3d^4(^5D)nd(^4G)$  Rydberg series showing PEC resonances

only contributions from the  $3d^4(^5D)$  ground state of the Fe V core ion were included in the photoionization cross sections of states with multiplicity  $(2S+1) = 6$ . Therefore, all coupling effects for the cross sections of these states and, in particular, of the the ground state of Fe IV, were also missing.

#### 4.3.1. Partial photoionization cross sections

In constructing non-LTE spectral models of astrophysical objects it may be important to determine accurately the populations of *excited* levels of the residual ion following photoionization. This requires not only total photoionization cross section but also *partial* cross sections into the excited states of product ion. Therefore, we have obtained the partial cross sections for photoionization of the states of Fe IV into at least the lowest few (particularly the metastable) terms of Fe V. These partial photoionization cross sections are also necessary in the calculation of unified electron-ion recombination rate coefficients (Nahar & Pradhan 1995). Fig. 3 presents these partial cross sections for photoionization of some excited states of Fe IV into the ground state of Fe V.

#### 4.3.2. Photoexcitation-of-core resonances

One interesting feature observed in certain photoionization cross sections is the so-called photoexcitation-of-core (PEC) resonances that result from strong dipole transitions between the ground state and opposite parity states within the target ion (Yu & Seaton 1987; see also Bautista & Pradhan 1995, for Fe I). The PEC features are prominent in the photoionization of excited bound states along a Rydberg series, as the outer electron is weakly bound and photo-excitation takes place within the ion core – the PEC process is thus the inverse of the di-electronic recombination process with the outer electron as a “spectator” (Nahar & Pradhan 1995). Such PEC resonances are seen in Fig. 4 which displays the photoionization cross sections of Fe IV bound states in the Rydberg series  $3d^3(^4F)nd(^5D)$  with  $n = 5 - 9$ . At the Fe V target thresholds  $3d^34p(^4F^o, ^4D^o, ^4S^o)$ , the incident photon energies equal those of the strong dipole transitions from the ground state  $3d^3(^4F)$  and large PEC autoionizing resonances are formed, enhancing the effective cross section up to several orders of magnitude above the background. The prominent peaks shown in Fig. 4 correspond to these dipole transition energies  $a^4F \rightarrow z^4F^o, z^4D^o$ .

## 5. Conclusion

Extensive radiative calculations for Fe IV are presented which are expected to be applicable to a variety of astrophysical problems such as the calculation of improved Iron opacities, non-LTE models, and spectroscopic interpretation of Fe IV spectra. The present calculations include a number of target terms of both parities and therefore exhibit resonance structures absent from previous calculations, especially the near-threshold resonance structure in the ground state photoionization cross section. Oscillator strengths for 34 635 dipole allowed transitions among the quartet and the sextet terms in Fe IV were calculated. This data set expands the data set of transitions currently in the Opacity Project database TOPbase (Cunto & Mendoza 1993) and should be more accurate than that of SB.

All radiative data reported here will be included in TOPbase at CDS (Cunto et al. 1993). These data can also be accessed electronically via Internet by request to the authors.

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**References**

- Bautista M.A., 1997, A&A Suppl. (in press) (Paper XXI)  
Bautista M.A., 1996, A&AS 119, 105 (Paper XVI)  
Bautista M.A., Nahar S.N., Peng J.F., Pradhan A.K., Zhang H.L., 1995, in *Astrophysics in the Extreme Ultraviolet*, Bowyer S. (Ed.), IAU Symposium No. 152  
Bautista M.A., Pradhan A.K., 1996, A&AS 115, 551 (Paper XIII)  
Bautista M.A., Pradhan A.K., 1995b, J. Phys. B: At. Mol. Phys. 28, L173  
Berrington K.A., 1995, A&AS 109, 193 (Paper VIII)  
Berrington K.A., Burke P.G., Butler K., et al., 1987, J. Phys. B: At. Mol. Phys. 20, 6379  
Butler K., Zeippen C.J., 1994, A&AS 108, 1 (Paper V)  
Cowan R.D., 1981, *The theory of Atomic Structure and Spectra*. University of California Press, Berkeley, California  
Cunto W., Mendoza C., Ochsenbein F., Zeippen C.J., 1993, A&A 275, L5-L8  
Eissner W., Jones M., Nussbaumer H., 1974, *Comput. Phys. Commun.* 8, 270  
Eissner W., 1991, J. Phys. IV (Paris) C1, 3  
Hummer D.G., Berrington K.A., Eissner W., et al., 1993, A&A 279, 298 (Paper I)  
Kisielius R., Berrington K.A., Norrington P.H., 1996, A&AS 118, 157 (Paper XV)  
Lennon D.J., Burke V.M., 1994, A&AS 103, 273 (Paper II)  
Nahar S.N., 1995, A&AS 293, 967 (Paper VII)  
Nahar S.N., 1996, Phys. Rev. A 53, 1545  
Nahar S.N., Pradhan A.K., 1996, A&AS 119, 509 (Paper XVII)  
Nahar S.N., Pradhan A.K., 1994, J. Phys. B: At. Mol. Phys. 27, 429  
Nahar S.N., Pradhan A.K., 1995, ApJ 447, 966  
Pelan J., Berrington K.A., 1995, A&AS 110, 209 (Paper IX)  
Pradhan A.K., 1995, in *Astrophysics in the Extrema Ultraviolet*, Bowyer S. (ed.), IAU Symposium No. 152  
Reilman R.F., Manson S.T., 1979, ApJS 40, 815  
Saraph H.E., Storey P.J., 1996, A&AS 115, 151 (Paper XI)  
Saraph H.E., Tully J.A., 1994, A&AS 107, 29 (Paper IV)  
Seaton M.J., Yu Yan, Mihalas D., Pradhan A.K., 1994, MNRAS 266, 805  
Storey P.J., Mason H.E., Saraph H.E., 1996, A&A 309, 677 (Paper XIV)  
Sugar J., Corliss C., 1985, J. Phys. Chem. Ref. Data 14 Suppl. No. 2  
Vennes S., 1995, in *Astrophysics in the Extrema Ultraviolet*, Bowyer S. (ed.), IAU Symposium No. 152  
Yu Yan, Seaton M.J., 1987, J. Phys. B: At. Mol. Phys. 20, 6409  
Zhang H.L., Graziani M., Pradhan A.K., 1994, A&A 283, 319 (Paper III)  
Zhang H.L. Pradhan A.K., 1995b, A&A 293, 953 (Paper VI)  
Zhang H.L. 1996, A&AS 119, 523 (Paper XVIII)