ASTRONOMY & ASTROPHYSICS
SUPPLEMENT SERIES

Astron. Astrophys. Suppl. Ser. **135**, 347–357 (1999)

Atomic data from the Iron Project

XXXV. Relativistic fine structure oscillator strengths for Fe XXIV and Fe XXV

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Received August 27; accepted October 21, 1998

Abstract. The first large-scale calculations of relativistic radiative transition probabilities from the Iron Project is reported for dipole allowed and intercombination (E1) transitions in Li-like Fe XXIV and He-like Fe XXV. The ab intio calculations are carried out in the close coupling approximation using the Breit-Pauli R-matrix method in intermediate coupling characterized by SLJ, with total $(2S+1) = 2,4$, $L = 7$, $J = 1/2 - 11/2$ even and odd parity, for Fe XXIV, and with total $(2S+1) = 1,3$, $L = 9$, and $J = 0 - 4$ for Fe XXV. The eigenfunction expansions for the target ions include 13 levels up to the $n = 3$ for Fe XXV, and 16 levels up to the $n = 4$ for Fe XXVI, respectively. The calculated number of bound levels, 83 for Fe XXIV and 138 for Fe XXV, is much larger than experimentally observed. The level energies are in good agreement for the common levels. All dipole and intercombination fine structure transitions involving the calculated bound levels up to $n = 10$ and $\ell = 5$ or 6 are considered. Oscillator strengths, line strengths, and Einstein A-coefficients are tabulated for 802 transitions in Fe XXIV and 2579 transitions in Fe XXV. The results compare well with limited subsets of transitions considered in previous works including fully relativistic and QED corrections. Additional comparisons between the length and the velocity formulations indicate an overall accuracy between $1 - 10\%$. The range of uncertainty is indicative of the relatively small influence of atomic effects, such as the two-body Breit interaction terms and finite nuclear mass term, that are not included in the Breit-Pauli approximation employed in the present calculations. The extensive set of data is expected to be useful in the analysis of X-ray and XUV spectra from astrophysical sources[1].

Key words: atomic data — X-ray: galaxies

1. Introduction

Extensive and accurate datasets for radiative transitions in atomic species are required for studies of many astrophysical and laboratory plasma sources. These range from diagnostics of specific spectral features to the calculation of mean opacities of stellar and non-stellar astronomical objects. Previous calculations of large radiative datasets were carried out under the Opacity Project (hereafter OP; 1995, 1996), and have been archived in the electronically accessible database TOPbase by C. Mendoza and collaborators (Cunto et al. 1993). However, the non-relativistic OP calculations were in LS coupling and for dipole allowed transitions; fine structure transitions within the LS multiplets, and intercombination type transitions, were not considered. The OP datasets, primarily intended for the calculation of mean stellar opacities, are therefore of limited value for diagnostic purposes involving the analysis of observed transitions between fine structure levels. For light elements, and for low ionization stages, the OP datasets for a number of ions have been reprocessed to obtain fine structure oscillator strengths through purely algebraic transformation of line strengths (often utilising observed energies for improved accuracy). Among such works is the recent compilation of transition probabilities at the U.S. National Institute for Standards and Technology (NIST) for C, N, O ions (Wiese et al. 1996). Similarly, fine structure oscillator strengths have been obtained (using experimental level energies where available) for Fe II (IP.VII, Nahar 1995), Fe III (IP.XVII, Nahar and Pradhan 1996; this work also includes forbidden transitions), Si II (Nahar 1998), S II (Nahar 1997), and Si-ions Si I, S III, Ar V and Ca VII (Nahar 1993).

In addition to the non-relativistic fine structure oscillator strengths derived from the OP data in LS coupling, several relativistic calculations for forbidden (E2,

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[1] The complete table of transition probabilities is available in electronic form at the CDS via anonymous ftp to cdsarc.u-strasbg.fr (130.79.128.5) or via http://cdsweb.u-strasbg.fr/Abstract.html

M1) and intercombination transitions have been reported by members of the Iron Project (IP.I, Hummer et al. 1993) using the Breit-Pauli mode of the atomic structure code SUPERSTRUCTURE (Eissner et al. 1974; Eissner 1991, 1998). The latter works include: transition probabilities for forbidden lines in Fe II (IP.XIX, Quinet et al. 1996), radiative rates for forbidden transitions within the ground state configurations of ions in the carbon and oxygen isoelectronic sequences (IP.XXII, Galavis et al. 1997), transitions within the $n = 2$ complex in ions of the boron isoelectronic sequence (IP.XXIX, Galavis et al. 1998), and intercombination transitions in the carbon isoelectronic sequence (IP.XXXIII, Mendoza et al. 1998). A complete list and abstracts of IP papers can be found at http://www.am.qub.uk/projects/iron/papers/. Information on other radiative calculations by the authors and collaborators, including photoionization and recombination of ions of iron and other elements, can be found at http://www-astronomy.ohio-state.edu/∼pradhan/.

The Iron Project work has so far concentrated primarily on collisional excitation of atomic ions including relativistic effects using the Breit-Pauli R-matrix (BPRM) method. However, analogous to the earlier LS coupling OP codes (Berrington et al. 1987), the BPRM atomic collision codes extended and developed for the IP, (Scott & Taylor 1982; Hummer et al. 1993; Berrington et al. 1995) can also be employed for radiative work. The present work represents the first such IP effort for systematic and large-scale calculation of transition probabilities, akin to the earlier OP work (Seaton et al. 1994). We describe the calculations, together with the nomenclature and formats used to identify the transitions and tabulate the data. The accuracy is ascertained from the overall level of agreement between the length and the velocity forms of the oscillator strengths, as well as by comparisons with previous calculations for more limited but accurate data.

2. Theory

As described in IP.I (Hummer et al. 1993), the basic methods are derived from atomic collision theory and the coupled channel approximation or the close coupling (CC) method. The computational method is based on the powerful R-matrix formalism that enables efficient, accurate, and large-scale calculations of compound (bound and continuum), state wavefunctions of the (e + ion) system at all positive or negative energies (in accordance with the terminology of collision theory the "ion" core is often referred to as the "target ion"). At positive energies the "channels", characterized by the spin and angular quantum numbers of the (e + ion) system, describe the scattering process with the free electron interacting with the target ion. However, at *negative* total energies of the (e + ion) system, the solutions of the close coupling equations occur at discrete eigenvalues of the (e + ion) Hamiltonian that correspond to pure bound states (all scattering channels are then "closed"). The positive and negative energy solutions yield many atomic parameters of practical interest: electron impact excitation cross sections, photoionization and recombination cross sections, and radiative transition probabilities.

Table 1. Energy Levels of Fe XXV and Fe XXVI in the eigenfunction expansion of Fe XXIV and Fe XXV respectively

Level		E(Ry)	Level		E(Ry)
Fe XXV: 13CC			Fe XXVI: 16CC		
$1s^2$	$^1S_0$	0.	1s	$^2S_{1/2}$	0.
1s2s	$^3S_1$	487.774760	2p	$^2P^o_{1/2}$	511.2020874
1s2p	$^3P^o_0$	489.899743	2s	$^2S_{1/2}$	511.2250584
1s2p	$^3P^o_1$	490.071608	2p	$^2P^o_{3/2}$	512.7378860
1s2s	$^1S_0$	490.091292	3p	$^2P^o_{1/2}$	606.3387185
1s2p	$^3P^o_2$	491.132414	3s	$^2S_{1/2}$	606.3463027
1s2p	$^1P^o_1$	492.448740	3p	$^2P^o_{3/2}$	606.7831354
1s3s	$^3S_1$	579.251214	3d	$^2D_{5/2}$	606.9330548
1s3p	$^3P^o_0$	579.251214	3d	$^2D_{3/2}$	606.7822943
1s3s	$^1S_0$	579.251214	4p	$^2P^o_{1/2}$	639.5703607
1s3p	$^3P^o_1$	579.251214	4s	$^2S_{1/2}$	639.5735718
1s3p	$^3P^o_2$	579.251214	4d	$^2D_{3/2}$	639.7513049
1s3p	$^1P^o_1$	579.251214	4p	$^2P^o_{3/2}$	639.7517913
			4f	$^2F^o_{5/2}$	639.8139450
			4d	$^2D_{5/2}$	639.8141276
			4f	$^2F^o_{7/2}$	639.8456304

The non-relativistic $(N + 1)$-electron Hamiltonian for the N-electron target ion and a free electron is

$$H_{N+1} = \sum_{i=1}^{N+1} \left\{ -\nabla_i^2 - \frac{2Z}{r_i} + \sum_{j>i}^{N+1} \frac{2}{r_{ij}} \right\}. \quad (1)$$

Relativistic effects are incorporated into the R-matrix formalism in the Breit-Pauli approximation with the Hamiltonian

$$H^{\rm BP}_{N+1} = H_{N+1} + H^{\rm mass}_{N+1} + H^{\rm Dar}_{N+1} + H^{\rm so}_{N+1}, \quad (2)$$

where H_{N+1} is the non-relativistic Hamiltonian defined by Eq. (1), together with the one-body mass correction term, the Darwin term and the spin-orbit term resulting from the reduction of the Dirac equation to Pauli form. The mass-correction and Darwin terms do not break the LS symmetry, and they can therefore be retained with significant effect in the computationally less intensive LS calculations. Spin-orbit interaction does, however, split the LS terms into fine-structure levels labeled by $J\pi$, where J is the total angular momentum.

In the coupled channel or close coupling (CC) approximation the wavefunction expansion, $\Psi(E)$, for a total spin and angular symmetry $SL\pi$ or $J\pi$, of the $(N+1)$ electron system is represented in terms of the target ion states as:

$$\Psi(E) = A \sum_i \chi_i \theta_i + \sum_j c_j \Phi_j, \quad (3)$$

Table 2. Comparison of Fe XXIV and Fe XXV level energies in Breit-Pauli approximation, E_c, with the observed ones, E_o (Sugar & Corliss 1985)

Level		E_c(Ry)	E_o(Ry)	Level		E_c(Ry)	E_o(Ry)
Fe XXIV							
$1s^2 2s$	$^2S_{1/2}$	150.77	150.36	$1s^2 4d$	$^2D_{3/2}$	36.080	36.077
$1s^2 2p$	$^2P^o_{3/2}$	145.93	145.61	$1s^2 5p$	$^2P^o_{3/2}$	23.169	23.246
$1s^2 2p$	$^2P^o_{1/2}$	147.25	146.79	$1s^2 5p$	$^2P^o_{1/2}$	23.253	23.246
$1s^2 3s$	$^2S_{1/2}$	66.241	65.863	$1s^2 5d$	$^2D_{5/2}$	23.063	23.101
$1s^2 3p$	$^2P^o_{3/2}$	64.874	64.545	$1s^2 5d$	$^2D_{3/2}$	23.089	23.137
$1s^2 3p$	$^2P^o_{1/2}$	65.265	64.900	$1s^2 6p$	$^2P^o_{3/2}$	16.080	16.093
$1s^2 3d$	$^2D_{5/2}$	64.070	64.044	$1s^2 6p$	$^2P^o_{1/2}$	16.129	16.093
$1s^2 3d$	$^2D_{3/2}$	64.190	64.162	$1s^2 6d$	$^2D_{5/2}$	16.020	16.047
$1s^2 4s$	$^2S_{1/2}$	36.806	36.779	$1s^2 6d$	$^2D_{3/2}$	16.034	16.084
$1s^2 4p$	$^2P^o_{3/2}$	36.236	36.205	$1s^2 7d$	$^2D_{5/2}$	11.768	11.764
$1s^2 4p$	$^2P^o_{1/2}$	36.401	36.350	$1s^2 7d$	$^2D_{3/2}$	11.778	11.764
$1s^2 4d$	$^2D_{5/2}$	36.029	36.032				
Fe XXV							
$1s^2$	$^1S_0$	649.57	648.85	1s4s	$^3S_1$	39.738	39.695
1s2s	$^3S_1$	161.16	161.07	1s4p	$^3P^o_2$	39.335	39.298
1s2p	$^3P^o_2$	157.75	157.72	1s4p	$^3P^o_1$	39.509	39.433
1s2p	$^3P^o_1$	158.94	158.78	1s4p	$^3P^o_0$	39.516	39.449
1s2p	$^3P_0$	159.21	158.95	1s4s	$^1S_0$	39.499	39.448
1s2s	$^1S_0$	158.96	158.76	1s4p	$^1P^o_1$	39.158	39.150
1s2p	$^1P^o_1$	156.38	156.40	1s5s	$^3S_1$	25.325	25.327
1s3s	$^3S_1$	70.967	70.909	1s5s	$^1S_0$	25.206	25.204
1s3p	$^3P^o_2$	69.999	69.961	1s5p	$^3P^o_2$	25.119	25.126
1s3p	$^3P^o_1$	70.367	70.280	1s5p	$^3P^o_1$	25.194	25.195
1s3p	$^3P^o_0$	70.430	70.320	1s5p	$^3P^o_0$	25.212	25.203
1s3s	$^1S_0$	70.392	70.301	1s5p	$^1P^o_1$	25.044	25.051
1s3p	$^1P^o_1$	69.614	69.598				

where χ_i is the target ion wave function in a specific state $S_iL_i\pi_i$ or level $J_i\pi_i$, and θ_i is the wave function for the $(N+1)$th electron in a channel labeled as $S_iL_i(J_i)\pi_i\ k_i^2\ell_i(SL\pi\ or\ \ J\pi)$; k_i^2 is the incident kinetic energy. In the second sum the Φ_j's are correlation wavefunctions of the $(N+1)$ electron system that (a) compensate for the orthogonality conditions between the continuum and the bound orbitals, and (b) represent additional short-range correlation that is often of crucial importance in scattering and radiative CC calculations for each $SL\pi$. In the relativistic BPRM calculations the set of $SL\pi$ are recoupled to obtain (e + ion) states with total $J\pi$, followed by diagonalisation of the $(N+1)$-electron Hamiltonian, i.e.

$$H^{\rm BP}_{N+1}\Psi = E\Psi. \tag{4}$$

The oscillator strength (or photoionization cross section) is proportional to the generalised line strength (Seaton 1987) defined, in either length form or velocity form, by the equations

$$S_{\rm L} = \left| \left\langle \Psi_{\rm f} | \sum_{j=1}^{N+1} r_j | \Psi_i \right\rangle \right|^2 \tag{5}$$

and

$$S_{\rm V} = \omega^{-2} \left| \left\langle \Psi_{\rm f} | \sum_{j=1}^{N+1} \frac{\partial}{\partial r_j} | \Psi_i \right\rangle \right|^2 . \tag{6}$$

In these equations ω is the incident photon energy in Rydberg units, and $\Psi_{\rm i}$ and $\Psi_{\rm f}$ are the wave functions representing the initial and final states respectively. The boundary conditions satisfied by a bound state with negative energy correspond to exponentially decaying partial waves in all "closed" channels, whilst those satisfied by a free or continuum state correspond to a plane wave in the direction of the ejected electron momentum $\hat{\underline{k}}$ and ingoing waves in all open channels.

Using the energy difference, E_{ji}, between the initial and final states, the oscillator strength, f_{ij}, for the transition can be obtained from S as

$$f_{ij} = \frac{E_{ji}}{3g_i} S, \tag{7}$$

and the Einstein's A-coefficient, A_{ji}, as

$$A_{ji}({\rm a.u.}) = \frac{1}{2}\alpha^3 \frac{g_i}{g_j} E_{ji}^2 f_{ij}, \tag{8}$$

Table 3. Energy levels of Fe XXIV in Breit-Pauli approximation. N_b is the total number of bound levels of the ion and TL is total number of bound levels of quantum number $J\pi$

l_v	Level		E(Ry)
	Fe XXIV: $N_b = 83$		
	$(J = 0.5)^e$ $TL = 9$		
1	$1s^2 2s$	$^2S^e_{0.5}$	−150.7655
2	$1s^2 3s$	$^2S^e_{0.5}$	−66.2407
3	$1s^2 4s$	$^2S^e_{0.5}$	−36.8057
4	$1s^2 5s$	$^2S^e_{0.5}$	−23.4580
5	$1s^2 6s$	$^2S^e_{0.5}$	−16.2461
6	$1s^2 7s$	$^2S^e_{0.5}$	−11.9109
7	$1s^2 8s$	$^2S^e_{0.5}$	−9.1046
8	$1s^2 9s$	$^2S^e_{0.5}$	−7.1846
9	$1s^2 10s$	$^2S^e_{0.5}$	−5.8136
	$(J = 0.5)^o$ $TL = 9$		
1	$1s^2 2p$	$^2P^o_{0.5}$	−147.2479
2	$1s^2 3p$	$^2P^o_{0.5}$	−65.2645
3	$1s^2 4p$	$^2P^o_{0.5}$	−36.4007
4	$1s^2 5p$	$^2P^o_{0.5}$	−23.2528
5	$1s^2 6p$	$^2P^o_{0.5}$	−16.1286
6	$1s^2 7p$	$^2P^o_{0.5}$	−11.8371
7	$1s^2 8p$	$^2P^o_{0.5}$	−9.0552
8	$1s^2 9p$	$^2P^o_{0.5}$	−7.1500
9	$1s^2 10p$	$^2P^o_{0.5}$	−5.7884
	$(J = 1.5)^e$ $TL = 8$		
1	$1s^2 3d$	$^2D^e_{1.5}$	−64.1901
2	$1s^2 4d$	$^2D^e_{1.5}$	−36.0796
3	$1s^2 5d$	$^2D^e_{1.5}$	−23.0892
4	$1s^2 6d$	$^2D^e_{1.5}$	−16.0344
5	$1s^2 7d$	$^2D^e_{1.5}$	−11.7776
6	$1s^2 8d$	$^2D^e_{1.5}$	−9.0154
7	$1s^2 9d$	$^2D^e_{1.5}$	−7.1220
8	$1s^2 10d$	$^2D^e_{1.5}$	−5.7681
	$(J = 1.5)^o$ $TL = 9$		
1	$1s^2 2p$	$^2P^o_{1.5}$	−145.9275
2	$1s^2 3p$	$^2P^o_{1.5}$	−64.8742
3	$1s^2 4p$	$^2P^o_{1.5}$	−36.2359
4	$1s^2 5p$	$^2P^o_{1.5}$	−23.1688
5	$1s^2 6p$	$^2P^o_{1.5}$	−16.0803
6	$1s^2 7p$	$^2P^o_{1.5}$	−11.8067
7	$1s^2 8p$	$^2P^o_{1.5}$	−9.0348
8	$1s^2 9p$	$^2P^o_{1.5}$	−7.1356
9	$1s^2 10p$	$^2P^o_{1.5}$	−5.7779
	$(J = 2.5)^e$ $TL = 8$		
1	$1s^2 3d$	$^2D^e_{2.5}$	−64.0700
2	$1s^2 4d$	$^2D^e_{2.5}$	−36.0288
3	$1s^2 5d$	$^2D^e_{2.5}$	−23.0633
4	$1s^2 6d$	$^2D^e_{2.5}$	−16.0196
5	$1s^2 7d$	$^2D^e_{2.5}$	−11.7682
6	$1s^2 8d$	$^2D^e_{2.5}$	−9.0090
7	$1s^2 9d$	$^2D^e_{2.5}$	−7.1176
8	$1s^2 10d$	$^2D^e_{2.5}$	−5.7648
	$(J = 2.5)^o$ $TL = 7$		
1	$1s^2 4f$	$^2F^o_{2.5}$	−36.0225
2	$1s^2 5f$	$^2F^o_{2.5}$	−23.0591
3	$1s^2 6f$	$^2F^o_{2.5}$	−16.0166
4	$1s^2 7f$	$^2F^o_{2.5}$	−11.7661
5	$1s^2 8f$	$^2F^o_{2.5}$	−9.0078
6	$1s^2 9f$	$^2F^o_{2.5}$	−7.1168
7	$1s^2 10f$	$^2F^o_{2.5}$	−5.7643
	$(J = 3.5)^e$ $TL = 6$		
1	$1s^2 5g$	$^2G^e_{3.5}$	−23.0466
2	$1s^2 6g$	$^2G^e_{3.5}$	−16.0085
3	$1s^2 7g$	$^2G^e_{3.5}$	−11.7612
4	$1s^2 8g$	$^2G^e_{3.5}$	−9.0047
5	$1s^2 9g$	$^2G^e_{3.5}$	−7.1147
6	$1s^2 10g$	$^2G^e_{3.5}$	−5.7628
	$(J = 3.5)^o$ $TL = 7$		
1	$1s^2 4f$	$^2F^o_{3.5}$	−35.9975
2	$1s^2 5f$	$^2F^o_{3.5}$	−23.0463
3	$1s^2 6f$	$^2F^o_{3.5}$	−16.0095
4	$1s^2 7f$	$^2F^o_{3.5}$	−11.7616
5	$1s^2 8f$	$^2F^o_{3.5}$	−9.0047
6	$1s^2 9f$	$^2F^o_{3.5}$	−7.1147
7	$1s^2 10f$	$^2F^o_{3.5}$	−5.7627
	$(J = 4.5)^e$ $TL = 6$		
1	$1s^2 5g$	$^2G^e_{4.5}$	−23.0390
2	$1s^2 6g$	$^2G^e_{4.5}$	−16.0044
3	$1s^2 7g$	$^2G^e_{4.5}$	−11.7586
4	$1s^2 8g$	$^2G^e_{4.5}$	−9.0029
5	$1s^2 9g$	$^2G^e_{4.5}$	−7.1135
6	$1s^2 10g$	$^2G^e_{4.5}$	−5.7619
	$(J = 4.5)^o$ $TL = 5$		
1	$1s^2 6h$	$^2H^o_{4.5}$	−16.0029
2	$1s^2 7h$	$^2H^o_{4.5}$	−11.7592
3	$1s^2 8h$	$^2H^o_{4.5}$	−9.0033
4	$1s^2 9h$	$^2H^o_{4.5}$	−7.1136
5	$1s^2 10h$	$^2H^o_{4.5}$	−5.7618
	$(J = 5.5)^e$ $TL = 4$		
1	$1s^2 7i$	$^2I^e_{5.5}$	−11.7567
2	$1s^2 8i$	$^2I^e_{5.5}$	−9.0015
3	$1s^2 9i$	$^2I^e_{5.5}$	−7.1124
4	$1s^2 10i$	$^2I^e_{5.5}$	−5.7611
	$(J = 5.5)^o$ $TL = 5$		
1	$1s^2 6h$	$^2H^o_{5.5}$	−16.0001
2	$1s^2 7h$	$^2H^o_{5.5}$	−11.7577
3	$1s^2 8h$	$^2H^o_{5.5}$	−9.0023
4	$1s^2 9h$	$^2H^o_{5.5}$	−7.1128
5	$1s^2 10h$	$^2H^o_{5.5}$	−5.7613

where α is the fine structure constant, and g_i, g_j are the statistical weight factors of the initial and final states, respectively. In terms of c.g.s. unit of time,

$$A_{ji}(\mathrm{s}^{-1}) = \frac{A_{ji}(\mathrm{a.u.})}{\tau_0}, \tag{9}$$

where $\tau_0 = 2.4191\ 10^{-17}$ s is the atomic unit of time.

The BP Hamiltonian in the present work (Eq. 2) does not include the full Breit-interaction in that the two-body spin-spin and spin-other-orbit terms are not included. A discussion of these terms is given by Mendoza et al. in a recent IP paper (IP.XXXIII, 1998). Their study on the

Table 4. Energy levels of Fe XXV in Breit-Pauli approximation. N_b is the total number of bound levels of the ion and TL is total number of bound levels of quantum number $J\pi$

l_v	Level		E(Ry)
	Fe XXIV: $N_b = 138$		
	$(J=0)^e$ $TL=10$		
1	$1s^2$	$^1S^e_0$	−649.5738
2	1s2s	$^1S^e_0$	−158.9648
3	1s3s	$^1S^e_0$	−70.3923
4	1s4s	$^1S^e_0$	−39.4994
5	1s5s	$^1S^e_0$	−25.2065
6	1s6s	$^1S^e_0$	−17.4844
7	1s7s	$^1S^e_0$	−12.8364
8	1s8s	$^1S^e_0$	−9.8203
9	1s9s	$^1S^e_0$	−7.7545
10	1s10s	$^1S^e_0$	−6.2781
	$(J=0)^o$ $TL=9$		
1	1s2p	$^3P^o_0$	−159.2099
2	1s3p	$^3P^o_0$	−70.4299
3	1s4p	$^3P^o_0$	−39.5165
4	1s5p	$^3P^o_0$	−25.2117
5	1s6p	$^3P^o_0$	−17.4867
6	1s7p	$^3P^o_0$	−12.8375
7	1s8p	$^3P^o_0$	−9.8212
8	1s9p	$^3P^o_0$	−7.7553
9	1s10p	$^3P^o_0$	−6.2788
	$(J=1)^e$ $TL=17$		
1	1s2s	$^3S^e_1$	−161.1560
2	1s3s	$^3S^e_1$	−70.9669
3	1s3d	$^3D^e_1$	−69.6921
4	1s4s	$^3S^e_1$	−39.7376
5	1s4d	$^3D^e_1$	−39.2092
6	1s5s	$^3S^e_1$	−25.3249
7	1s5d	$^3D^e_1$	−25.0550
8	1s6s	$^3S^e_1$	−17.5517
9	1s6d	$^3D^e_1$	−17.3966
10	1s7s	$^3S^e_1$	−12.8782
11	1s7d	$^3D^e_1$	−12.7809
12	1s8s	$^3S^e_1$	−9.8485
13	1s8d	$^3D^e_1$	−9.7830
14	1s9s	$^3S^e_1$	−7.7745
15	1s9d	$^3D^e_1$	−7.7284
16	1s10s	$^3S^e_1$	−6.2927
17	1s10d	$^3D^e_1$	−6.2592
	$(J=1)^o$ $TL=18$		
1	1s2p	$^3P^o_1$	−158.9379
2	1s2p	$^1P^o_1$	−156.3811
3	1s3p	$^3P^o_1$	−70.3675
4	1s3p	$^1P^o_1$	−69.6136
5	1s4p	$^3P^o_1$	−39.5087
6	1s4p	$^1P^o_1$	−39.1576
7	1s5p	$^3P^o_1$	−25.1939
8	1s5p	$^1P^o_1$	−25.0444
9	1s6p	$^3P^o_1$	−17.4768
10	1s6p	$^1P^o_1$	−17.3906
11	1s7p	$^3P^o_1$	−12.8313
12	1s7p	$^1P^o_1$	−12.7776
13	1s8p	$^3P^o_1$	−9.8170
14	1s8p	$^1P^o_1$	−9.7805

Table 4. continued

l_v	Level		E(Ry)
	$(J=1)^o$ $TL=18$		
15	1s9p	$^3P^o_1$	−7.7523
16	1s9p	$^1P^o_1$	−7.7264
17	1s10p	$^3P^o_1$	−6.2766
18	1s10p	$^1P^o_1$	−6.2576
	$(J=2)^e$ $TL=16$		
1	1s3d	$^3D^e_2$	−69.6910
2	1s3d	$^1D^e_2$	−69.5368
3	1s4d	$^3D^e_2$	−39.2166
4	1s4d	$^1D^e_2$	−39.1329
5	1s5d	$^3D^e_2$	−25.0524
6	1s5d	$^1D^e_2$	−25.0218
7	1s6d	$^3D^e_2$	−17.3952
8	1s6d	$^1D^e_2$	−17.3773
9	1s7d	$^3D^e_2$	−12.7800
10	1s7d	$^1D^e_2$	−12.7687
11	1s8d	$^3D^e_2$	−9.7824
12	1s8d	$^1D^e_2$	−9.7747
13	1s9d	$^3D^e_2$	−7.7280
14	1s9d	$^1D^e_2$	−7.7225
15	1s10d	$^3D^e_2$	−6.2589
16	1s10d	$^1D^e_2$	−6.2549
	$(J=2)^o$ $TL=16$		
1	1s2p	$^3P^o_2$	−157.7502
2	1s3p	$^3P^o_2$	−69.9986
3	1s4p	$^3P^o_2$	−39.3348
4	1s4f	$^3F^o_2$	−39.1456
5	1s5p	$^3P^o_2$	−25.1189
6	1s5f	$^3F^o_2$	−25.0220
7	1s6p	$^3P^o_2$	−17.4335
8	1s6f	$^3F^o_2$	−17.3772
9	1s7p	$^3P^o_2$	−12.8043
10	1s7f	$^3F^o_2$	−12.7682
11	1s8p	$^3P^o_2$	−9.7986
12	1s8f	$^3F^o_2$	−9.7747
13	1s9p	$^3P^o_2$	−7.7392
14	1s9f	$^3F^o_2$	−7.7228
15	1s10p	$^3P^o_2$	−6.2670
16	1s10f	$^3F^o_2$	−6.2551
	$(J=3)^e$ $TL=14$		
1	1s3d	$^3D^e_3$	−69.5560
2	1s4d	$^3D^e_3$	−39.1514
3	1s5d	$^3D^e_3$	−25.0078
4	1s5g	$^3G^e_3$	−25.0078
5	1s6d	$^3D^e_3$	−17.3688
6	1s6g	$^3G^e_3$	−17.3688
7	1s7d	$^3D^e_3$	−12.7702
8	1s7g	$^3G^e_3$	−12.7625
9	1s8d	$^3D^e_3$	−9.7758
10	1s8g	$^3G^e_3$	−9.7712
11	1s9d	$^3D^e_3$	−7.7233
12	1s9g	$^3G^e_3$	−7.7204
13	1s10d	$^3D^e_3$	−6.2554
14	1s10g	$^3G^e_3$	−6.2534
	$(J=3)^o$ $TL=14$		
1	1s4f	$^3F^o_3$	−39.1487
2	1s4f	$^1F^o_3$	−39.1140
3	1s5f	$^3F^o_3$	−25.0219

Table 4. continued

l_v	Level		E(Ry)
	$(J=3)^o$ $TL=14$		
4	1s5f	$^1F^o_3$	−25.0075
5	1s6f	$^3F^o_3$	−17.3772
6	1s6f	$^1F^o_3$	−17.3688
7	1s7f	$^3F^o_3$	−12.7682
8	1s7f	$^1F^o_3$	−12.7631
9	1s8f	$^3F^o_3$	−9.7747
10	1s8f	$^1F^o_3$	−9.7711
11	1s9f	$^3F^o_3$	−7.7228
12	1s9f	$^1F^o_3$	−7.7203
13	1s10f	$^3F^o_3$	−6.2550
14	1s10f	$^1F^o_3$	−6.2533
	$(J=4)^e$ $TL=12$		
1	1s5g	$^3G^e_4$	−25.0078
2	1s5g	$^1G^e_4$	−24.9991
3	1s6g	$^3G^e_4$	−17.3688
4	1s6g	$^1G^e_4$	−17.3638
5	1s7g	$^3G^e_4$	−12.7625
6	1s7g	$^1G^e_4$	−12.7625
7	1s8g	$^3G^e_4$	−9.7712
8	1s8g	$^1G^e_4$	−9.7691
9	1s9g	$^3G^e_4$	−7.7204
10	1s9g	$^1G^e_4$	−7.7190
11	1s10g	$^3G^e_4$	−6.2534
12	1s10g	$^1G^e_4$	−6.2524
	$(J=4)^o$ $TL=12$		
1	1s4f	$^3F^o_4$	−39.1173
2	1s5f	$^3F^o_4$	−25.0075
3	1s6f	$^3F^o_4$	−17.3639
4	1s6h	$^3H^o_4$	−17.3639
5	1s7f	$^3F^o_4$	−12.7588
6	1s7h	$^3H^o_4$	−12.7588
7	1s8f	$^3F^o_4$	−9.7712
8	1s8h	$^3H^o_4$	−9.7712
9	1s9f	$^3F^o_4$	−7.7191
10	1s9h	$^3H^o_4$	−7.7191
11	1s10f	$^3F^o_4$	−6.2524
12	1s10h	$^3H^o_4$	−6.2524

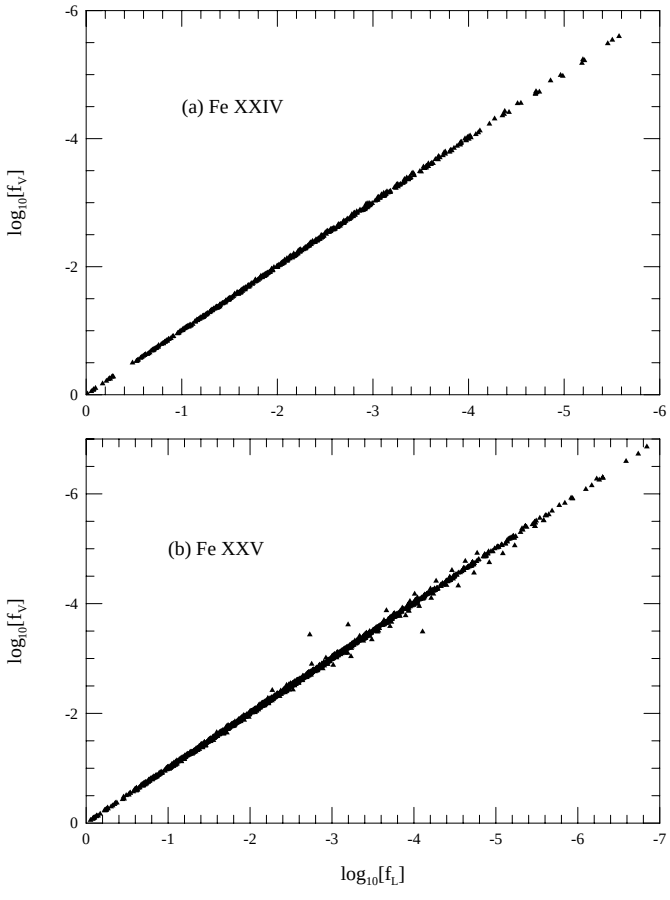

Fig. 1. Comparison between the length and the velocity forms of f-values for **a)** Fe XXIV and **b)** Fe XXV

intercombination transitions in C-like ions shows that the effect of the two-body Breit terms, relative to the one-body operators, decreases with Z such that for $Z = 26$ the computed A-values with and without the two-body Breit terms differ by less than 0.5%. However, the differences towards the neutral end of the C-sequence is up to about 20%.

For the few-electron systems it is possible to calculate transition energies and probabilities including electron-correlation, relativistic, and QED effects. Several investigators have done very elaborate ab intio calculations. Highly accurate calculations for transition probabilities have been carried out by Drake (1979, 1988), Lin et al. (1977a,b) for helium-like ions and Yan et al. (1998), and Johnson et al. (1996) for lithium-like ions. In addition to these latest works, relativistic calculations have been done using perturbation theory and the $1/Z$ expansion method by Vainshtein & Safronova (1985) for He-like and Li-like ions. The calculations by Drake (1988) on the He-sequence include quantum electrodynamic (QED) corrections (screened nuclear charge for the Bethe logarithm) in a more accurate manner than the earlier works. In an elaborate relativistic calculation, using many-body perturbation theory up to third order, Johnson et al. (1996) obtain transition probabilties for a few transitions in Fe XXIV. In the work on Li-like ions, Yan et al. (1998) employ a fully correlated Hylleraas-type variational method and relativistic corrections derived from the relativistic many-body perturbation theory by Johnson et al. (1996). Yan et al. (1998) investigate both the relativistic and the finite nuclear mass corrections and show those to be important for high accuracy. The slight differences between the calculations by Yan et al. (1998) and earlier work by Johnson et al. (1996) are attributable essentially to the nuclear term not included in the latter calculations. In addition, multi-configuration Dirac-Fock (MCDF) calculations, that include the relativistic one-body operators exactly but not the Breit terms, have been carried

Table 5. Comparison of Fe XXIV f- and A-values in Breit-Pauli R-matrix (BPRM) approximation with other works

Transition	Multiplet	g_i	g_f	f_{ij}			$A_{ji}(s^{-1})$	
				f_L	f_V	Others	BPRM	Others
2s − 2p	^{2}S −^{2} P^o	2	2	0.0173		0.0176[a],0.0177[b],0.0177[f]	1.722[9]	1.804[9][c],1.83[9][d]
		2	4	0.0484		0.0475[a],0.0478[b],0.0479[f]	4.554[9]	4.299[9][c],4.32[9][d]
2s − 3p	^{2}S −^{2} P^o	2	2	0.129		0.128[e],0.129[f]	7.561[12]	7.51[12][g],7.69[12][d]
		2	4	0.246		0.246[e],0.247[f]	7.285[12]	7.28[12][g],7.78[12][d]
2s − 4p	^{2}S −^{2} P^o	2	2	0.0317	0.0323	0.033[h],0.0319[f]	3.33[12]	3.19[12][d]
		2	4	0.0617	0.0628	0.0655[h],0.0623[f]	3.25[12]	3.20[12][d]
2p − 3s	^{2}P^o −^{2} S	2	2	0.0171	0.0166	0.015[i],0.0167[f]	8.998[11]	8.981[11][c],8.47[11][d]
		4	2	0.0188	0.0182	0.0176[i],0.0182[f]	1.914[12]	1.905[12][c],1.62[12][d]
2p − 3d	^{2}P^o −^{2} D	2	4	0.674	0.671	0.670[e],0.660[f]	1.87[13]	1.88[13][d]
		4	4	0.0684	0.0684	0.068[e],0.0669[f]	3.67[12]	3.60[12][d]
		4	6	0.614	0.611	0.611[e]	2.20[13]	2.17[13][d]
2p − 4s	^{2}P^o −^{2} S	2	2	0.0037	0.0036	0.0037[h],0.0036[f]	3.61[11]	3.53[11][d]
		4	2	0.0040	0.0039	0.0036[h],0.0039[f]	7.64[11]	6.84[11][d]
2p − 4d	^{2}P^o −^{2} D	2	4	0.122	0.122	0.124[h],0.122[f]	6.06[12]	5.87[12][d]
		4	4	0.0122	0.0122	0.0122[h],0.0124[f]	1.17[12]	1.14[12][d]
		4	6	0.110	0.110	0.110[h]	7.10[12]	6.83[12][d]
3s − 4p	^{2}S −^{2} P^o	2	2	0.14		0.15[j]	1.02[12]	1.16[12][d]
		2	4	0.27	0.27	0.30[j]	9.77[11]	1.17[12][d]
3p − 4d	^{2}P^o −^{2} D	2	4	0.584	0.576	0.63[j]	2.0[12]	2.1[12][d]
		4	4	0.060	0.058	0.06[j]	4.02[11]	4.05[11][d]
		4	6	0.538	0.530	0.55[j]	2.40[12]	2.44[12][d]
4p − 7d	^{2}P^o −^{2} D	2	4	0.0607	0.0614	0.0620[j]		
		4	4	0.0062	0.0062	0.0062[j]		
		4	6	0.0552	0.0558	0.0554[j]		

a) Yan et al. (1998), b) Cheng et al. (1979), c) Johnson et al. (1996), d) Vainshtein & Safronova (1985), e) Armstrong et al. (1977), f) Zhang et al. (1990), g) Burkhalter et al. (1978), h) Doschek et al. (1972), i) Hayes (1979), j) Fuhr et al. (1988).

out by Cheng et al. (1979). Other previous works are also discussed later.

We compare with available data from previous calculations. The agreement between the present values and these previous calculations shows that the relativistic and QED terms omitted from the BP Hamiltonian (Eq. 2) do not affect the transition probabilities of the highly charged ions considered herein by more than a few percent – the accuracy sought in the present large-scale calculations intended for applications in laboratory and astrophysical plasmas.

3. Atomic calculations

The Breit-Pauli R-matrix calculations are carried out using an eigenfunction expansion for Fe XXIV↔ (e + Fe XXV) containing 13 fine structure levels from configurations, $1s^2$, 1s2s, 1s2p, 1s3s and 1s3p of the core ion Fe XXV (Table 1). For Fe XXV↔ (e + Fe XXVI) the expansion contains 16 levels corresponding to the hydrogenic orbitals 1s, 2s, 2p, 3s, 3p, 3d, 4s, 4p, 4d, and 4f of Fe XXVI (Table 1). The orbital wavefunctions of the target are obtained using the atomic structure code SUPERSTRUCTURE (Eissner et al. 1974) which are input for the BPRM codes (Hummer et al. 1993). Table 1 lists the target level energies which are obtained from stage RECUPD which reconstructs the target states developed from SUPERSTRUCTURE.

The BPRM codes (also called the RMATRX1 codes; Berrington et al. 1995) from the IP, consisting of several stages similar to those in the OP codes (Berrington et al. 1987), are used for computations of the oscillator strengths for bound-bound levels. For each $J\pi$ of Fe XXIV, all possible combinations of doublets and quartets of Fe XXIV with $L \leq 7$ and $l \leq 9$ are included, and to those of Fe XXV, singlets and triplets of Fe XXV with $L \leq 5$ and $l \leq 9$ are included. The level energies of Fe XXIV and Fe XXV are obtained from the code STGB of the BPRM suite of codes. As the bound levels are scanned out by the effective quantum numbers ν through the poles in the (e + ion) Hamiltonian, the mesh for ν should be fine enough to avoid any missing levels and to obtain accurate energies

Table 6. Comparison of Fe XXV f-values in Breit-Pauli R-matrix (BPRM) approximation with other works

Transition	Multiplet	$g_{\rm i}$	$g_{\rm f}$	f_{ij}		
				$f_{\rm L}$	$f_{\rm V}$	Others
			Fe XXV			
$1s^2 - 1s2p$	^{1}S $-^3$ P$^{\rm o}$	1	3	0.0652	0.0672	0.0687[a],0.0667[b], 0.06876[f]
	^{1}S $-^1$ P$^{\rm o}$	1	3	0.7115	0.735	0.703[a],0.731[b]
$1s^2 - 1s3p$	^{1}S $-^3$ P$^{\rm o}$	1	3	0.0154	0.0161	0.017[e],0.0145[b]
	^{1}S $-^1$ P$^{\rm o}$	1	3	0.138	0.143	0.138[c],0.142[b]
$1s^2 - 1s4p$	^{1}S $-^3$ P$^{\rm o}$	1	3	0.0076	0.0079	0.0060[e]
	^{1}S $-^1$ P$^{\rm o}$	1	3	0.0493	0.0514	0.0507[c]
$1s^2 - 1s5p$	^{1}S $-^3$ P$^{\rm o}$	1	3	0.0024	0.0025	0.0030[e]
	^{1}S $-^1$ P$^{\rm o}$	1	3	0.0251	0.0261	0.0244[c]
1s2s − 1s2p	^{3}S $-^3$ P$^{\rm o}$	3	1	0.00297		0.00347[d]
		3	3	0.00934		0.0103[d]
		3	5	0.0264		0.0273[d]
	^{3}S $-^1$ P$^{\rm o}$	3	3	0.00187		0.00197[d]
	^{1}S $-^1$ P$^{\rm o}$	1	3	0.0336		0.0329[d]
1s2s − 1s3p	^{3}S $-^3$ P$^{\rm o}$	3	5	0.217		0.231[b]
	^{3}S $-^3$ P$^{\rm o}$	3	3	0.120	0.122	0.122[c],0.125[b]
	^{1}S $-^1$ P$^{\rm o}$	1	3	0.359	0.369	0.364[c],0.384[b]
	^{3}S $-^1$ P$^{\rm o}$	3	3	0.0140		0.0129[b]
1s2s − 1s4p	^{3}S $-^3$ P$^{\rm o}$	3	3	0.0273	0.0278	0.030[c]
	^{1}S $-^1$ P$^{\rm o}$	1	3	0.084	0.087	0.088[c]
1s2s − 1s5p	^{3}S $-^3$ P$^{\rm o}$	3	3	0.012	0.013	0.012[c]
	^{1}S $-^1$ P$^{\rm o}$	1	3	0.037	0.038	0.036[c]
1s2p − 1s3d	^{3}P$^{\rm o}$ $-^3$ D	3	3	0.155	0.156	0.159[b]
	^{3}P$^{\rm o}$ $-^3$ D	3	5	0.476	0.481	0.495[b]
	^{3}P$^{\rm o}$ $-^3$ D	5	3	0.00685	0.00694	0.00683[b]
	^{3}P$^{\rm o}$ $-^1$ D	3	5	0.0438	0.0438	0.0422[b]
	^{1}P$^{\rm o}$ $-^3$ D	3	3	0.0147	0.0147	0.0142[b]

a) Drake (1979), b) Vainshtein & Safronova (1985), c) Lin et al. (1977a), d) Lin et al. (1977b), e) Fuhr et al. (1988), f) Johnson et al. (1995).

for the higher levels. For example, for Fe XXV, $\Delta\nu = 0.01$ is adequately fine for the lower levels, but it is necessary to refine it to 0.001 in order to obtain a number of the higher energy levels for $J \geq 2$.

The large number of bound levels yield very large sets of fine structure transitions for both Fe XXIV and Fe XXV. The code STGBB of the BPRM codes computes the gf-values for the bound-bound transitions. The transitions are identified by the "good" quantum numbers $J\pi$ only. The datasets are processed, following the NIST format, for oscillator strengths (f-values), line strengths ($\mathcal{S}$-values) and transition probabilites (A-values) using a code BPRAD (Nahar, unpublished). The format is similar to that used for the OP data (OP 1995) in that the energies and transitions are labeled by level indices.

Identification of the calculated energy levels is a major task for BPRM calculations since a large number of energy levels are generated (and indeed exist). The BP Hamiltonian matrix yields energies corresponding to the different J-values. While STGB of the R-matrix codes from the Opacity Project is capable of sorting out the possible configurations contributing to a given LS term, the BP version of the code does not link the J-values with the corresponding LS terms and configurations, making the task of level identification difficult. The problem is particularly acute in the BPRM calculations since many levels may be very closely spaced within a small range of effective quantum number but corresponding to different *interacting* Rydberg series. This problem is not too severe for the highly charged ions under consideration in this work, since the Rydberg series can be relatively easily identified. For example, the total $J = 2^{\rm o}$ (odd parity) levels in Fe XXV correspond to the two Rydberg series $1snp$ and $1snf$. For each ν there are two bound states; for example, for $\nu \approx 4.0$ there are the 1s4p $^3P^{\rm o}$ ($J = 2$) and 1s4f $^3F^{\rm o}$ ($J = 2$) levels. For more complicated atomic systems however, such as the ongoing BPRM intermediate coupling calculations for Fe V (e + Fe VI), the interacting Rydberg series problem is far more complex, and level identifications are much more difficult, since many levels corresponding approximately to the same ν lie close together (Nahar & Pradhan, in preparation).

Table 7a. Sample of the complete table for A_{ik}, f_{ik} and S values for fine structure transitions in Fe XXIV. $N_{\rm f}$ is the total number of bound-bound transitions for the ion and $T_{\rm f}$ is the number of transitions for a pair of JJ'

i	k	g_i	g_k	A_{ki} $\rm s^{-1}$	f_{ik}	S (a.u.)
Fe XXIV, $N_{\rm f}$ = 802						
$(J=0.5)^{\rm e}-(J=0.5)^{\rm o}$ $T_{\rm f}=81$						
1	1	2	2	1.721E+09	−1.731E-02	2.953E-02
1	2	2	2	7.561E+12	−1.288E-01	9.035E-03
1	3	2	2	3.331E+12	−3.171E-02	1.663E-03
1	4	2	2	1.716E+12	−1.314E-02	6.183E-04
1	5	2	2	9.923E+11	−6.815E-03	3.037E-04
1	6	2	2	6.231E+11	−4.019E-03	1.736E-04
1	7	2	2	4.166E+11	−2.583E-03	1.093E-04
1	8	2	2	2.922E+11	−1.764E-03	7.368E-05
1	9	2	2	2.128E+11	−1.260E-03	5.217E-05
2	1	2	2	8.998E+11	1.707E-02	1.264E-03

Table 7b. Sample of the complete table for A_{ik}, f_{ik} and S values for fine structure transitions in Fe XXV. $N_{\rm f}$ is the total number of bound-bound transitions for the ion and $T_{\rm f}$ is the number of transitions for a pair of JJ'

i	k	g_i	g_k	A_{ki} $\rm s^{-1}$	f_{ik}	S (a.u.)
Fe XXIV, $N_{\rm f}$ = 2579						
$(J=0.0)^{\rm e}-(J=1.0)^{\rm o}$ $T_{\rm f}=180$						
1	1	1	3	4.205E+13	−6.524E-02	3.989E-04
1	2	1	3	4.655E+14	−7.148E-01	4.348E-03
1	3	1	3	1.383E+13	−1.540E-02	7.976E-05
1	4	1	3	1.245E+14	−1.382E-01	7.149E-04
1	5	1	3	7.527E+12	−7.553E-03	3.714E-05
1	6	1	3	4.921E+13	−4.932E-02	2.424E-04
1	7	1	3	2.464E+12	−2.360E-03	1.134E-05
1	8	1	3	2.618E+13	−2.507E-02	1.204E-04
1	9	1	3	1.446E+12	−1.352E-03	6.417E-06
1	10	1	3	1.495E+13	−1.397E-02	6.629E-05
1	11	1	3	9.092E+11	−8.375E-04	3.946E-06
1	12	1	3	9.327E+12	−8.590E-03	4.047E-05
1	13	1	3	6.263E+11	−5.715E-04	2.680E-06
1	14	1	3	6.267E+12	−5.718E-03	2.681E-05
1	15	1	3	4.351E+11	−3.945E-04	1.844E-06

The energy levels of ions in the present work have been identified by matching the J-values with the possible combination of total spin multiplicity and total orbital angular momentum of the ion whose LS term is derived, in turn, from combinations of the target term S_iL_i and angular momentun of the outer electron ℓ_i. The target S_iL_i is determined from the spectroscopic configurations included in the eigenfunction expansion, and the n and l quantum numbers of the outer electron are determined from its effective quantum number. Hund's rule is followed to identify the positions of levels, e.g. the triplets lie below the singlets of same L, π and configuration of He-like ions. The code BPRAD is written to process these data for complete identification of energy levels and corresponding transitions.

4. Results and discussions

The BPRM intermediate coupling calculations in principle, and the present work in particular, should yield all possible atomic energy levels. We have obtained 83 bound fine structure levels of Fe XXIV in the range of SLJ with total spin multiplicity $(2S+1)$ = 2,4, total orbital angular momentum, $L \leq 7$, with total angular momentum, $J = 1/2 - 11/2$, even and odd parities, and 138 of Fe XXV in the range of SLJ with total $(2S+1)$ = 1,3, $L = 9$, and $J = 0-4$, even and odd parities. These numbers far exceed the observed or previously calculated ones. Accuracy of the energies is checked against the observed values from NIST (Sugar & Corliss 1985). All 23 observed bound levels of Fe XXIV and 25 of Fe XXV have been identified in the calculated dataset and are compared in Table 2. The calculated energies of both Fe XXIV and Fe XXV agree very well with the observed ones, differing by less than 1% for all levels (the accuracy may not be quite so good for more complicated atomic systems). These are the most detailed close coupling calculations for the two ions. The complete energy levels of Fe XXIV and Fe XXV are presented in Tables 3 and 4 respectively where they are listed in terms of $J\pi$ quantum numbers.

We obtain the transition probabilities for 802 transitions in Fe XXIV and for 2579 transitions in Fe XXV. These correspond to both dipole allowed and intercombination transitions in intermediate coupling. The two forms of oscillator strengths, length ($f_{\rm L}$) and velocity ($f_{\rm V}$), show less than 10% difference for almost all transitions. Figures 1a,b display $f_{\rm L}$ versus $f_{\rm V}$ for Fe XXIV and Fe XXV respectively to show the close correlation between the two sets going down to $f \sim 10^{-7}$. For some transitions the velocity form were not obtained and are not included in the figures. One tolerence criterion for the R-matrix codes is that $f_{\rm V}$ is not calculated for transitions for which the transition energy is extremely small. There is almost no dispersion of $f_{\rm L}$ and $f_{\rm V}$ for Fe XXIV even for the very weak transitions of the order of 10^{-6}. Although there are some transitions in Fe XXV where the $f_{\rm L}$ and $f_{\rm V}$ differ by about 10% or higher, most are in closer agreement with each other.

Present f- and A-values for Fe XXIV and Fe XXV are compared with the best previous calculations and experiments in Tables 5 and 6 repectively. Most of the previous values have been compiled by the NIST (Fuhr et al. 1988; Shirai et al. 1990). In Table 5 most of the BPRM f-values for Fe XXIV agree quite well with those in the NIST compilation (Fuhr et al. 1988), obtained by several investigators, such as by Cheng et al. (1979), Armstrong et al. (1976), Doschek et al. (1972). Although the NIST rating for the accuracy of these transitions varies from B+

to D ($< 10\% - 30\%$), nearly all of the available f-values agree to better than 10% with the present ones. As mentioned earlier, Yan et al. (1998) have calculated the level energies and oscillator strengths for lithium like ions up to $Z = 20$ using Hylleras type variational method including finite nuclear mass effects. They extend the results to higher Z ions including relativistic corrections. Present f-values for Fe XXIV compare very well with their values obtained for the transitons, $2s(^2S_{1/2}) - 2p(^2P^o_{1/2,3/2})$. Present A-values agree with those by Johnson et al. (1996) obtained from relativistic third-order many-body perturbation theory to about 5% for the two transitions $2s(^2S_{1/2}) - 2p(^2P^o_{1/2,3/2})$, and by less than 1% for the two transitions, $2s(^2S_{1/2}) - 3p(^2P^o_{1/2,3/2})$. We also find very good agreement with most of the transition probabilities, A-values, by Vainshtein & Safronova (1985) obtained using the Z^{-1}-expansion method, which yields more accurate A-values with increasing Z. Present f-values for the transitions $2s(^2S_{1/2}) - 2p(^2P^o_{1/2,3/2})$ agree within error bars with the measured values of Buchet et al. (1984).

The BPRM f-values for Fe XXV are compared with the previous calculations in Table 6. Present f-values agree within 5% with detailed calculations by Drake (1979) and Johnson et al. (1995) for the dipole allowed and within 1% with Drake (1979) for the intercombination transitions, $1s^2(^1S_0) - 1s2p(^{1,3}P^o_1)$. We agree very well with Vainshtein & Safronova (1985) for the dipole allowed transition who employed the Z^{-1}-expansion method. Very good agreement is obtained of the present f-values with those by Lin et al. (1977a) for all the transitions compared in Table 6. Of the transitions, $1s^2(^1S_0) - 1s(3,4,5)p(^{1,3}P^o_1)$, the dipole allowed ones were calculated by Lin et al. (1977a), and agree quite well with the present values. However, f-values for the intercombination transitions were obtained by Fuhr et al. (NIST 1988) through extrapolation of the data by Johnson & Lin (1976). The present values differ by more than 10% with the extrapolated NIST values. Since our results are in better than 10% agreement with the actual calculated results from other investigators, it appears that the NIST data for these intercombination transitions might not be accurate. The agreement between the present results and those by Lin et al. (1977b) is better than 10% for all transitions except the two transitions $1s2s(^3S_1) - 1s2p(^3P^o_{0,1})$ whose f-values are of the order of 10^{-3}. However, for the stronger intercombination transition $1s2s(^3S_1) - 1s2p(^3P^o_2)$ the agreement with Lin et al. is about 3%, and also in good agreement with the measured value of Buchet et al. (1984). Present f-values agree to a similar degree with those by Vainshtein & Safronova (1985) for the dipole allowed as well as the intercombination transitions.

Owing to the large volume of the present data and the number of transitions computed, the complete set of data will be made available electronically. The tables include: transition probabilities A, oscillator strengths f, and line strengths S for all the fine structure transitions. These electronic files will include the calculated level energies also for level identifications. Samples of these data are presented in Tables 7a,b for Fe XXIV and Fe XXV, respectively. Indices "i" and "k" correspond to the two levels with the even/odd parity total $J\pi$ symmetries specified in the column headings. Transition probabilities can also be identified from the energy Tables 3 and 4. Negative values of f_{ik} imply $E_i > E_k$ (emission), and positive values imply $E_i < E_k$. The format of the tables follow closely that of the OP (1995), with the main exception that the present results are in intermediate coupling with $J\pi$ as the defining quantum numbers instead of $SL\pi$.

5. Conclusion

Accurate and large-scale datasets of level energies and fine structure transition probabilities for Fe XXIV and Fe XXV are reported under the Iron Project. The transitions include both the dipole allowed and intercombination obtained in intermediate coupling including relativistic effects through the Breit Pauli R-matrix method (BPRM) in the close coupling approximation. Both the energies and the transition probabilities agree generally to within $1-10\%$ with nearly all of the most accurate calculated and measured values available. It might be concluded that for highly charged ions the relativistic and QED effects omitted from consideration in the BPRM calculations should lead to an error not exceeding the estimated uncertainty. However, much more work needs to be done to investigate the precise magnitude of the various effects on increasingly complex atomic systems. Calculations are presently under way for Fe V and Fe XVI. We should expect the present data to be particularly useful in the analysis of X-ray and Extreme Ultraviolet spectra from astrophysical and laboratory sources where non-local thermodynamic equilibrium (NLTE) atomic models with many excited levels are needed.

Acknowledgements. This work was partially supported by U.S. National Science Foundation (AST-9870089) and the NASA ADP program. We should like to thank Dr. Gordon Drake and Dr. Ulyana Safronova for communications. The computational work was carried out on the vector machine Cray T94 at the Ohio Supercomputer Center in Columbus, Ohio.

References

Armstrong Jr. L, Fielder W.R., Lin D.L., 1976, Phys. Rev. A 14, 1114

Berrington K.A., Burke P.G., Butler K., et al., 1987, J. Phys. B 20, 6379

Berrington K.A., Eissner W., Norrington P.H., 1995, Comput. Phys. Commun. 92, 290

Buchet J.P., Buchet-Poulizac M.C., Denis A., et al., 1984, Phys. Rev. A 30, 309

Burkhalter P.G., Dozier C.M., Stallings E., Cowan R.D., 1978, J. Appl. Phys. 49, 1092
Cheng K.T., Kim Y.-K., Desclaux J.P., 1979, At. Data Nucl. Data Tab. 24, 111
Cunto W., Mendoza C., Ochsenbein F., Zeippen C.J, 1993, A&A 275, L5 (TOPbase)
Doschek G.A., Meekins J.F., Cowan R.D., 1972, ApJ 177, 261
Drake G.W.F., 1979, Phys. Rev. A 19, 1387
Drake G.W.F., 1988, Can. J. Phys. 66, 586
Eissner W., Jones M., Nussbaumer H., 1974, Comput. Phys. Commun 8, 270
Eissner W., 1991, J. Phys. IV (Paris) C1, 3
Eissner W., 1999, Comput. Phys. Commun. (in preparation)
Fuhr J.R., Martin G.A., Wiese W.L., 1988, J. Phys. Chem. Ref. Data 17, Suppl. No. 4 (NIST)
Galavis M.E., Mendoza C., Zeippen C.J., 1997, A&AS 123, 159 (IP.XXII)
Galavis M.E., Mendoza C., Zeippen C.J., 1998, A&AS 131, 499 (IP.XXIX)
Hayes M.A., 1979, MNRAS 189, 55P
Hummer D.G., Berrington K.A., Eissner W., et al., 1993, A&A 279, 298 (IP)
Johnson W.R., Lin C.D., 1976, Phys. Rev. A 14, 565
Johnson W.R., Plante D.R., Sapirstein J., 1995, Adv. At. Mol. Opt. Phys. 35, 255
Johnson W.R., Liu Z.W., Sapirstein J., 1996, At. Data Nucl. Data 64, 279
Lin C.D., Johnson W.R., Dalgarno A., 1977a, ApJ 217, 1011
Lin C.D., Johnson W.R., Dalgarno A., 1977b, Phys. Rev. A 15, 154
Mendoza C., Zeippen C.J., Storey P.J., 1999, A&AS (IP.XXXIII, in press)
Nahar S.N., 1995, A&A 293, 967 (IP.VII)
Nahar S.N., Pradhan A.K., 1996, A&ASS 119, 509 (IP.XVII)
Nahar S.N., 1998, At. Data Nucl. Data 68, 183
Nahar S.N., 1997, Phys. Scr. 55, 200
Nahar S.N., 1993, Phys. Scr. 48, 297
Quinet P., Le Dourneuf M., Zeippen C.J., 1996, A&AS 120, 361 (IP.XIX)
Scott N.S., Taylor K.T., 1982, Comput. Phys. Commun. 25, 347
Seaton M.J., 1987, J. Phys. B 20, 6363
Seaton M.J., Yan Y., Mihalas D., Pradhan A.K., 1994, MNRAS 266, 805
Shirai T., Funatake Y., Mori K., et al., 1990, J. Phys. Chem. Ref. Data 19, 127
Sugar J., Corliss C., 1985, J. Phys. Chem. Ref. Data 14, Suppl. 2
The Opacity Project 1 & 2, compiled by the Opacity Project team, Institute of Physices, London, UK, 1995, 1996, (OP)
Vainshtein L.A., Safronova U.I., 1985, Phys. Scr. 31, 519
Wiese W.L., Fuhr J.R., Deters T.M., 1996, J. Phys. Chem. Ref. Data 17, Monograph No. 7
Yan Z.-C., Tambasco M., Drake G.W.F., 1998, Phys. Rev. A 57, 1652
Zhang H.L., Sampson D.H., Fontes C.J., 1990, At. Data Nucl. Data Tab. 44, 31