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Atomic structure calculations involving optimization of radial integrals: energy levels and oscillator strengths for Fe XII and Fe XIII $3p$–$3d$ and $3s$–$3p$ transitions

G. E. Bromage, R. D. Cowan* and B. C. Fawcett

Appleton Laboratory, Astrophysics Research Division, Culham Laboratory, Abingdon

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Summary. Energy levels and oscillator strengths are calculated for the $3s^2 3p^q$–$3s^2 3p^{q-1} 3d$ and $3s^2 3p^q$–$3s 3p^{q+1}$ transition arrays of Fe XII and Fe XIII. Strong configuration interactions are explicitly included in the computations, and the method also involves adjustment of radial energy-integrals F^k, G^k, R^k, in order to minimize differences between observed and calculated energy levels, under the least-squares criterion. It is found that F^k, G^k, R^k integrals need to be reduced from *ab init.* values (by over 30 per cent for some of the configuration-mixing integrals for Fe XII) and this substantially affects some oscillator strengths. Several spectral lines are newly classified as a result of this analysis.

The possible use of empirically adjusted radial-integral values in electron–ion collisional–excitation calculations (as a means of improving the accuracy of target wavefunctions) is discussed.

1 Theoretical methods

The energy levels and oscillator strengths presented here for $3s^2 3p^q$–$3s^2 3p^{q-1} 3d$ and $3s^2 3p^q$–$3s 3p^{q+1}$ transitions in Fe XII and XIII, are derived from theoretical calculations which explicitly include configuration mixings among three configurations of the 'lower' parity ($3s^2 3p^q$, $3p^{q+2}$ and $3s 3p^q 3d$) and among four 'upper' configurations ($3s 3p^{q+1}$, $3s^2 3p^{q-1} 3d$, $3p^{q+1} 3d$ and $3s 3p^{q-1} 3d^2$). *Ab init.* values of the Slater radial integrals are first computed with the Hartree-XR program of Cowan (1967) and Cowan & Griffin (1976) including relativistic effects. The relevant quantities computed are: the average energy of each configuration E_{av}; the electrostatic direct and exchange integrals, F^k and G^k, and configuration–interaction integrals, R^k; and the spin–orbit integrals, ζ. A second program (Cowan 1968) then evaluates energy levels and oscillator strengths, using these 'Slater parameters', which in the present investigation were *scaled* empirically as explained below.

Slater parameters F^k, G^k and R^k for the 'upper' configurations were adjusted by means of a non-linear least-squares optimization routine in order to minimize discrepancies between computed energy levels and measured ones. Several calculational models, involving different

*On leave from: The University of California, Los Alamos Scientific Laboratory, Los Alamos, New Mexico 87545, USA.

Table 1. Results of final least-squares calculations for Fe X, XII and XIII, $3s\,3p^{q+1}$ and $3s^2\,3p^{q-1}\,3d$. Configurations included: $A\ 3s\,3p^{q+1}$ (observed), $B\ 3s^2\,3p^{q-1}\,3d$ (observed), $C\ 3s^0\,3p^{q+1}\,3d$ (not observed), $D\ 3s\,3p^{q-1}\,3d^2$ (not observed).

q	Ion	No. of levels in configuration A and B		(Fitted *ab init.*) differential value of $[E_{av}(B) - E_{av}(A)]$		Final scale factors on radial integrals (as percentage of Hartree-XR *ab init.*)				rms deviation of least-squares fit, σ_{LSQ}		$\frac{\sigma_{ab\ init.}}{\sigma_{LSQ}}$
		Known★	(Total)	cm^{-1}	(as percentage of $\overline{E_{av}}$)	F^k	G^k	R^k_i†	R^k_{ii}†	cm^{-1}	(as percentage of total energy range of configurations A and B)	
5	Fe X	18	29	+ 3300 ± 1600	+ 0.8%	93.4 ± 0.3	85.7 ± 0.1	86 ± 1	54 ± 2	261	0.1%	45
4	Fe XI	11	42	‡						‡		
3	Fe XII	20	36	−3600 ± 4000	−0.8	89.8 ± 0.9	88.5 ± 1.1	89 ± 1	68 ± 5	851	0.3	10
2	Fe XIII	16	22	−6800 ± 4300	−1.6	95.9 ± 1.1	91.1 ± 0.8	92 ± 1	80 ± 6	685	0.2	7

★ Includes only established observed energy levels as used for least-squares-fit data; does not include levels identified as a result of the present series of calculations.

† R^k_i are the integrals for mixing between configurations A and B, and between C and D; that is, between a pair of relatively close configurations.
R^k_{ii} are the integrals for mixing between one of the lower configurations (A, B) and one of the higher ones (C, D). (For E_{av} values see Tables 2 and 5).

‡ For Fe XI, the numbers of known levels were insufficient for physically meaningful least-squares runs.

numbers of free parameters to be optimized, were tried for Fe XII and Fe XIII, and also for the corresponding configurations in Fe X already dealt with in an earlier paper (Bromage, Cowan & Fawcett 1977). In all cases, in order to keep the numbers of free parameters to a minimum, ratios of F^k integrals were fixed, as were ratios of G^k integrals. Furthermore, all spin–orbit integrals ζ were fixed at 95 per cent of Hartree-XR values, on the basis of earlier experience for similar ions.

It was found that significantly closer agreement with observation could be obtained by having separate scale factors, one for the F^k and one for the G^k. Moreover, a single scale factor for all R^k integrals could not adequately represent the observations, but introducing a second scale factor (as earlier proposed for Fe X and XI, Bromage *et al.* 1977) substantially reduced the residuals. This latter improvement was particularly marked for Fe X (where there was a factor of eight drop in rms deviation) but was also significant for Fe XII (a factor of two), though *not* for Fe XIII (a factor of 1.2 only). The relevance of these scale factors is discussed further in Section 3 below (see also Bromage *et al.* 1977). The adopted model involved one free F^k scale factor, one G^k factor and the two R^k factors, whilst in addition a differential shift in E_{av} between the two observed configurations was allowed to be free. The results for this model are collected in Table 1. The fitted values of the differential E_{av}

Table 2. Adopted Slater parameter (radial energy-integral) values (cm^{-1}) for Fe XII.

(A) Single-configuration parameters
(Adopted F^k are reduced by 0.90, G^k by 0.89 and ζ by 0.95 from *ab init.* Hartree-XR values.)

Parameter values for the $3s\,3p^4$ configuration

E_{av}	$F^2(3p\,3p)$	$G^1(3s\,3p)$	$\zeta(3p)$
381150	125598	161335	11877

Parameter values for the $3s^2\,3p^2\,3d$ configuration

E_{av}	$F^2(3p\,3p)$	$F^2(3p\,3d)$	$G^1(3p\,3d)$	$G^3(3p\,3d)$	$\zeta(3p)$	$\zeta(3d)$
506530	125456	124864	140997	91526	11830	1151

Parameter values for the $3p^4\,3d$ configuration

E_{av}	$F^2(3p\,3p)$	$F^2(3p\,3d)$	$G^1(3p\,3d)$	$G^3(3p\,3d)$	$\zeta(3p)$	$\zeta(3d)$
1159503	125362	124779	140893	91459	11812	1148

Parameter values for the $3s\,3p^2\,3d^2$ configuration

E_{av}	$F^2(3p\,3p)$	$F^2(3d\,3d)$	$F^4(3d\,3d)$	$F^2(3p\,3d)$	$G^1(3s\,3p)$	$G^2(3s\,3d)$	$G^1(3p\,3d)$
1253997	125246	133700	85993	124364	160928	108923	140789

$G^3(3p\,3d)$	$\zeta(3p)$	$\zeta(3d)$
91265	11770	1136

(B) Configuration–interaction parameters

Parameter values reduced by 0.89 for $3s\,3p^4 \times 3s^2\,3p^2\,3d$
$R^1(3p\,3p, 3s\,3d) = 148234$

Parameter values reduced by 0.68 for $3s\,3p^4 \times 3p^4\,3d$
$R^1(3s\,3p, 3p\,3d) = 114158$, $R^2(3s\,3p, 3d\,3p) = 86724$

Parameter values reduced by 0.68 for $3s\,3p^4 \times 3s\,3p^2\,3d^2$
$R^1(3p\,3p, 3d\,3d) = 108974$, $R^3(3p\,3p, 3d\,3d) = 70694$

Parameter values reduced by 0.68 for $3s^2\,3p^2\,3d \times 3p^4\,3d$
$R^1(3s\,3s, 3p\,3p) = 124520$

Parameter values reduced by 0.68 for $3s^2\,3p^2\,3d \times 3s\,3p^2\,3d^2$
$R^1(3s\,3p, 3p\,3d) = 114054$, $R^2(3s\,3p, 3d\,3p) = 86636$, $R^2(3s\,3d, 3d\,3d) = 87564$

Parameter values reduced by 0.89 for $3p^4\,3d \times 3s\,3p^2\,3d^2$
$R^1(3p\,3p, 3s\,3d) = 148103$

shift were relatively small – about 1 per cent of excitation energies – and within expected errors on *ab init.* calculation of E_{av} values. Scale factors for Fe X derived earlier (Bromage *et al.* 1977) by an *ad hoc* optimization method are very similar to those found in the full least-squares calculation, except that the second R^k factor is found to be somewhat lower than even the previously estimated value 0.65.

Table 3(a). Calculated and observed energy levels for the Fe XII $3s\,3p^4$ configuration (in cm^{-1})

J	Term	Calculated level†	Observed level	Calc – obs†	Percentage composition★
½	^4P	288 500	288 310	200	88%, [9% $(^3P)^4P, s^2p^2d$]
	^2P	392 500	394 120	−1600	27, 41% ^2S, [21% $(^3P)^2P$, 8% $(^1D)^2S, s^2p^2d$]
	^2S	408 100			42, 22% ^2P, [24% $(^3P)^2P$, 8% $(^1D)^2S, s^2p^2d$]
1½	^4P	284 100	284 000	100	89, [9% $(^3P)^4P, s^2p^2d$]
	^2D	340 400	340 010	400	78, [16% $(^1D)^2D, s^2p^2d$]
	^2P	390 000	389 740	300	48, [44% $(^3P)^2P, s^2p^2d$]
2½	^4P	274 300	274 370	−100	89, [9% $(^3P)^4P, s^2p^2d$]
	^2D	342 300	341 740	600	79, [16% $(^1D)^2D, s^2p^2d$]

★ See footnote to Table 3(b).
† In all tables, these quantities are rounded to nearest 100 cm^{-1}.

Table 3(b). Calculated and observed energy levels for the Fe XII $3s^2\,3p^2\,3d$ configuration (in cm^{-1}).

J	Term	Calculated level	Observed level★	Calc – obs	Percentage composition†
½	$(^3P)^4D$	447 400			97%
	$(^3P)^2P$	514 200	513 840	400	21, 32% $(^1D)^2P$, [35% $^2P, sp^4$]
	$(^3P)^4P$	519 400	519 770	−400	80, [8% $^4P, sp^4$]
	$(^1D)^2P$	568 500	(568 930)	(−400)	58, 24% $(^3P)^2P$, [7% $^2P, sp^4$]
	$(^1D)^2S$	578 600	579 620	−1000	72, [14% $^2S, sp^4$]
1½	$(^3P)^4F$	427 400			94
	$(^3P)^4D$	448 600			94
	$(^3P)^2P$	502 200	501 820	400	26, 26% $(^1D)^2P$, [41% $^2P, sp^4$]
	$(^3P)^4P$	516 500	516 770	−300	82, [8% $^4P, sp^4$]
	$(^1S)^2D$	525 500	(526 140)	(−600)	46, 40% $(^3P)^2D$
	$(^1D)^2D$	554 000	553 880	100	78, [14% $^2D, sp^4$]
	$(^1D)^2P$	576 600	577 680	−1100	61, 26% $(^3P)^2P$, [6% $^2P, sp^4$]
	$(^3P)^2D$	606 800	605 540	1300	55, 41% $(^1S)^2D$
2½	$(^3P)^4F$	431 400			92
	$(^1D)^2F$	443 800			45, 31% $(^3P)^2F$, 21% $(^3P)^4D$
	$(^3P)^4D$	453 400			70, 13% $(^1D)^2F$, 10% $(^3P)^2F$
	$(^3P)^4P$	512 700	512 510	200	86, [8% $^4P, sp^4$]
	$(^1S)^2D$	537 300	(538 060)	(−800)	41, 43% $(^3P)^2D$, [6% $^2D, sp^4$]
	$(^1D)^2D$	555 100	554 650	500	71, 17% $(^1S)^2D$, [10% $^2D, sp^4$]
	$(^3P)^2F$	576 100	576 730	−600	49, 35% $(^1D)^2F$
	$(^3P)^2D$	605 000	603 950	1100	47, 31% $(^1S)^2D$
3½	$(^3P)^4F$	437 200			93
	$(^3P)^4D$	448 000			47, 31% $(^1D)^2F$, 18% $(^3P)^2F$
	$(^1D)^2F$	463 300			28, 46% $(^3P)^4D$, 19% $(^3P)^2F$
	$(^1D)^2G$	494 900			96
	$(^3P)^2F$	580 700	581 210	−500	61, 37% $(^1D)^2F$
4½	$(^3P)^4F$	444 300			96
	$(^1D)^2G$	498 200			96

★ Values in parentheses are derived from newly identified lines (see Table 4).
† Percentage contributions from *LS* basis levels are listed when over 10 per cent in same configuration and over 5 per cent for contributions from other configurations.

Table 4(a). Calculated and observed wavelengths (Å) for $3s^2 3p^3$–$3s\,3p^4$ transitions of Fe XII with calculated weighted oscillator strengths $gf \gtrsim 0.05$.

Transition	Calculated wavelength	Observed wavelength	Calc – obs	gf
$^4S-{}^4P$				
1½–2½	364.62	364.468 S	0.15	0.19
1½–1½	352.01	352.107 S	−0.10	0.13
1½–½	346.67	346.852 S	−0.18	0.065
$^2D-{}^2D$				
2½–2½	337.58	338.263 S	−0.68	0.28
1½–1½	334.68	335.06 F	−0.38	0.23
$^2D-{}^2P$				
2½–1½	290.83	291.010 S	−0.18	0.42
1½–½	284.97	283.64 Fb	1.33	0.17
$^2P-{}^2D$				
1½–2½	381.94	382.83 F	−0.89	0.072
$^2P-{}^2P$				
½–½	314.10			0.098
$^2P-{}^2S$				
1½–½	305.23			0.18

Sources for wavelength data:
F ≡ Fawcett (1971) (laboratory λ).
S ≡ Behring *et al.* (1976) (solar λ).
b ≡ blend.
For classification see Fawcett (1971) and references cited in text.

Table 4(b). Calculated and observed wavelengths (Å) for $3s^2 3p^3$–$3s^2 3p^2 3d$ transitions of Fe XII with calculated weighted oscillator strengths (gf) $\gtrsim 0.05$.

Transition	Calculated wavelength	Observed wavelength★	Calc – obs	gf
$^4S-(^3P)^4P$				
1½–2½	195.05	195.119 S	−0.07	3.19
1½–1½	193.60	193.509 S	0.09	2.13
1½–½	192.53	192.394 S	0.14	1.01
$^2D-(^3P)^2F$				
2½–3½	187.04	186.880 S	0.16	4.82
2½–2½	188.68	188.45	0.23	0.22
1½–2½	187.08	186.856	0.22	3.39
$^2D-(^3P)^2D$				
2½–2½	178.92	179.265 N	−0.35	0.13
$^2P-(^3P)^2D$				
1½–2½	190.65	191.045 S	−0.40	3.31
1½–1½	190.00	190.459 N	−0.46	0.50
½–1½	187.71	188.216 S	−0.51	1.69
$^2D-(^3P)^2P$				
2½–1½	219.23	219.438 S	−0.21	1.38
1½–1½	217.07	217.271 S	−0.20	0.54
1½–½	211.59	211.738 S	−0.15	0.61
$^2P-(^3P)^2P$				
1½–1½	237.12			0.13

Table 4 – *continued*

Transition	Calculated wavelength	Observed wavelength*	Calc – obs	*gf*
1½–½	230.60	230.79	−0.19	0.20
½–½	227.24			0.10
$^2D-(^1D)^2D$				
2½–2½	196.47	196.640 S	−0.17	1.69
1½–2½	194.72	194.920 N	−0.20	0.080
2½–1½	196.89	196.923 N	−0.03	0.26
1½–1½	195.14	195.119 Sb	0.02	1.52
$^2P-(^1D)^2D$				
1½–2½	210.70	210.932 N	−0.23	0.23
½–1½	208.38	(208.410) N	(−0.03)	0.15
$^2D-(^1D)^2P$				
1½–½	189.76	189.561 N	0.20	0.049
$^2P-(^1D)^2P$				
1½–1½	201.59	201.121 Sb	0.47	1.54
½–1½	199.02	198.555 Sb	0.46	0.50
1½–½	204.91	204.743 N	0.17	0.071
½–½	202.25	202.090 N	0.16	0.89
$^2P-(^1D)^2S$				
1½–½	200.77	200.356 N	0.41	0.78
$^2D-(^1S)^2D$				
2½–2½	203.58	203.272 N	0.31	1.12
1½–2½	201.71	(201.493) N	(0.22)	0.064
2½–1½	208.61	208.318 N	0.29	0.16
1½–1½	206.65	206.368 N	0.28	0.18
$^2P-(^1S)^2D$				
1½–2½	218.91	218.562 N	0.35	0.038
$^4S-(^3P)^2P$				
1½–½	194.49	194.61 N	−0.12	0.10
$^4S-(^1S)^2D$				
1½–2½	186.11			0.082
1½–1½	190.30	190.06 N	0.24	0.10
$^2D-(^3P)^4P$				
1½–½	209.28			0.083
$^2D-(^1D)^2S$				
1½–½	214.33			0.053

* Sources for wavelength data: see Table 4(a) footnote.
N ≡ New identification (laboratory λ except for λ179.265). (Values in parentheses refer to tentative identifications.)

Throughout the present calculations scaling factors were also applied to radial integrals for the 'lower' configurations; that is, those with the same parity as the ground level. These scale factors were always chosen to give energy levels in close agreement with observational data. However, the electric dipole oscillator strengths presented here are not so critically dependent on these ground configuration scale factors. Moreover, transition wavelengths have always been derived from *observed* $3s^2\,3p^q$ energy levels in conjunction with the newly calculated upper levels.

2 Results

The adopted values of the Slater integrals and E_{av} and ζ for Fe XII are listed in Table 2. The resulting $3s\,3p^4$ and $3s^2\,3p^2\,3d$ energy levels are given in Table 3 along with the principal

percentage compositions of the levels and the observed energies. In this and subsequent tables the calculated energies have been rounded to four significant figures, in keeping with the expected final accuracy of computations. The tabulated composition of the levels indicates the degree of departure from pure *LS* coupling into intermediate coupling: some transitions that are forbidden in *LS* coupling gain appreciable oscillator strength.

The energy levels listed in Table 3 were then used in conjunction with established observational energy levels for the ground configuration, to obtain the wavelengths of $3s^2\,3p^3$–$3s\,3p^4$ and $3s^2\,3p^3$–$3s^2\,3p^2\,3d$ transitions. The strongest of these are listed in Table 4 alongside the observed wavelengths and oscillator strengths. Wavelengths and line identifications are given by Gabriel, Fawcett & Jordan (1965); Fawcett, Gabriel & Saunders (1967); Fawcett (1971) and Behring, Cohen & Feldman (1972) but the improved wavelength measurements of Behring *et al.* (1976) are included wherever possible. It is apparent that the differences between observed and calculated energy levels are typically only a few hundred reciprocal centimetres. This represents an improvement by an order of magnitude over the (*ab init.*) calculations of Flower (1977).

Similar calculations for iso-electronic transitions down the period to Ca VI were also carried out. It was found that adoption of the same scaling factors as those found for Fe XII

Table 5. Adopted Slater parameter (radial energy-integral) values in cm^{-1} for Fe XIII.

(A) Single-configuration parameters
(Adopted F^k values are reduced by 0.96, G^k values by 0.91 and ζ by 0.95 from *ab init.* Hartree-XR values)

Parameter values for the $3s\,3p^3$ configuration

E_{av}	$F^2(3p\,3p)$	$G^1(3s\,3p)$	$\zeta(3p)$
352 359	136 737	168 652	12 444

Parameter values for the $3s^2\,3p\,3d$ configuration

E_{av}	$F^2(3p\,3d)$	$G^1(3p\,3d)$	$G^3(3p\,3d)$	$\zeta(3p)$	$\zeta(3d)$
491 497	136 546	147 008	96 045	12 428	1237

Parameter values for the $3p^3\,3d$ configuration

E_{av}	$F^2(3p\,3p)$	$F^2(3p\,3d)$	$G^1(3p\,3d)$	$G^3(3p\,3d)$	$\zeta(3p)$	$\zeta(3d)$
1 109 901	136 466	136 245	146 795	95 841	12 376	1233

Parameter values for the $3s\,3p\,3d^2$ configuration

E_{av}	$F^2(3d\,3d)$	$F^4(3d\,3d)$	$F^2(3p\,3d)$	$G^1(3s\,3p)$	$G^2(3s\,3d)$	$G^1(3p\,3d)$	$G^3(3p\,3d)$
1 221 185	147 490	95 026	135 979	168 415	113 295	146 776	95 755
	$\zeta(3p)$	$\zeta(3d)$					
	12 358	1222					

(B) Configuration–interaction parameters

Parameter values reduced by 0.92 for $3s\,3p^3 \times 3s\,3p^2\,3d$
$R^1(3p\,3p, 3s\,3d) = 155\,587$

Parameter values reduced by 0.80 for $3s\,3p^3 \times 3p^3\,3d$
$R^1(3s\,3p, 3p\,3d) = 134\,931$, $R^2(3s\,3p, 3d\,3p) = 102\,491$

Parameter values reduced by 0.80 for $3s\,3p^3 \times 3s\,3p\,3d^2$
$R^1(3p\,3p, 3d\,3d) = 128\,816$, $R^3(3p\,3p, 3d\,3d) = 84\,048$

Parameter values reduced by 0.80 for $3s^2\,3p\,3d \times 3p^3\,3d$
$R^1(3s\,3s, 3p\,3p) = 147\,635$

Parameter values reduced by 0.80 for $3s^2\,3p\,3d \times 3s\,3p\,3d^2$
$R^1(3s\,3p, 3p\,3d) = 134\,928$, $R^2(3s\,3p, 3d\,3p) = 102\,522$, $R^2(3s\,3d, 3d\,3d) = 103\,846$

Parameter values reduced by 0.92 for $3p^3\,3d \times 3s\,3p\,3d^2$
$R^1(3p\,3p, 3s\,3d) = 155\,434$

Table 6. Calculated and observed energy levels for the Fe XIII $3s\,3p^3$ and $3s^2\,3p\,3d$ configurations (in cm^{-1}).

	J	Term	Calculated level	Observed level	Calc – obs	Percentage composition*
(A)		$3s\,3p^3$				
	0	^3P	329 000			90%, [9% $^3P\,s^2pd$]
	1	^3D	287 100	287 210	−100	85, [10% $^3D\,s^2pd$]
		^3P	329 800	329 650	200	86, [9% $^3P\,s^2pd$]
		^3S	414 700	415 460	−800	78, 17% ^1P
		^1P	438 400	438 050	400	69, 19% ^3S, [10% $^1P\,s^2pd$]
	2	^5S	212 300			98
		^3D	287 200	287 360	−200	83, [10% $^3D\,s^2pd$]
		^3P	330 300	330 280	0	78, [9% $^3P\,s^2pd$]
		^1D	362 700	362 330	400	54, [39% $^1D\,s^2pd$]
	3	^3D	290 200	290 210	0	89, [10% $^3D\,s^2pd$]
(B)		$3s^2\,3p\,3d$				
	0	^3P	502 100	503 340	−1200	89, [9% $^3P\,sp^3$]
	1	^3P	494 900	494 940	0	49, 38% ^3D, [5% $^3P\,sp^3$]
		^3P	506 300	506 500	−200	48, 39% ^3P, [6% $^3D\,sp^3$]
		^1P	570 500	570 944	−400	86, [10% $^1P\,sp^3$]
	2	^3F	430 700			97
		^3P	487 400	486 360	1000	43, 23% ^1D, [17% $^1D\,sp^3$]
		^1D	499 700	498 880	800	32, 21% ^3P, 18% ^3D, [21% $^1D\,sp$
		^3D	509 200	509 250	−100	61, 24% ^3P, [8% $^3D\,sp^3$]
	3	^3F	437 700			97
		^3D	508 900	509 180	−300	86, [10% $^3D\,sp^3$]
		^1F	557 200	556 910	300	97
	4	^3F	448 200			98

* See footnote to Table 3.

gave the same very good agreement between calculated and observed energy levels, thus emphasizing the usefulness of the computational methods employed.

The $3s\,3p^3$ and $3s^2\,3p\,3d$ levels for Fe XIII derived from the adopted scaled Slater parameters (listed in Table 5) are given in Table 6 and therein compared with those derived from observational data. The percentage compositions of the levels are also included in Table 6. In Table 7 are gathered the calculated and observational wavelength data and calculated weighted oscillator strengths for $3s^2\,3p^2$–$3s\,3p^3$ and $3s^2\,3p^2$–$3s^2\,3p\,3d$ transitions in Fe XIII. Calculations for Fe XIII have also been published by Flower & Nussbaumer (1974), including the same upper configurations as in this study but using *ab init.* radial integrals. Our new values represent a significant improvement especially for $3s\,3p^3$ energy levels.

3 Discussion

Some of the reasons why it becomes expedient to scale Slater parameters so as to achieve consistency between theoretical and observational data in these transition arrays, were discussed earlier (Bromage *et al.* 1977). To summarize, the need was attributed to both the approximations inherent in the theoretical models (e.g. correlation effects) and the restriction on numbers of configurations which can be taken into account in any practicable computation. It was also contended that these calculations can provide improved values of oscillator strengths. It is now worth considering how these computations can be used to improve values of electron–ion collision strengths. It is first necessary to emphasize that the improvements to oscillator strengths are achieved through a more accurate determination of

Table 7(a). Calculated and observed wavelengths (Å) for $3s^2\,3p^2-3s\,3p^3$ Fe XIII transitions with calculated weighted oscillator strengths (gf) $\gtrsim 0.05$.

Transition	Calculated wavelength	Observed wavelength★	Calc − obs	gf
$^3P-{}^3D$				
2–3	368.11	368.12 F	−0.01	0.18
1–2	359.82	359.63 F	0.19	0.15
0–1	348.33			0.07
$^3P-{}^3P$				
2–2	320.76	320.800 S	−0.04	0.26
1–1	312.03	312.164 S	−0.13	0.086
1–0	312.75			0.061
$^3P-{}^3S$				
2–1	252.43	251.953 S	0.48	1.00
1–1	246.67	246.208 S	0.46	0.49
0–1	241.14	240.713 Sb	0.43	0.18
$^1D-{}^1D$				
2–2	317.81	318.21 F	−0.40	0.40
$^1D-{}^1P$				
2–1	256.22	256.42 F	−0.20	0.92
$^1S-{}^1P$				
0–1	288.50			0.15
$^3P-{}^1P$				
1–1	233.07	233.234 N	−0.16	0.13

★ Sources for wavelength data.
F ≡ Fawcett (1971) (laboratory λ).
S ≡ Behring *et al.* (1976) (solar λ).
N ≡ New identification in laboratory and solar spectra (solar λ quoted).
b ≡ blend.
(Classifications are from Fawcett 1971, and references cited in text.)

the composition of levels in terms of the percentage contributions from the chosen basis states. This composition is dependent on the energy separations of levels (of the same J and parity), particularly when these are small. The procedures outlined in this paper ensure that there is a better agreement between observed and calculated energy level separations.

The scale factors applied to the Slater parameters do not have any precise physical meaning but they are needed to improve the accuracy of the transformation from the LS coupling scheme to the empirically determined intermediate coupling situation. Both oscillator strengths and collision strengths are usually computed first in LS coupling and then the effects of level mixings subsequently allowed for by matrix transformations using the state eigenvectors. (Our eigenvectors, of course, are derived from diagonalization of the energy matrices constructed using our *scaled* Slater parameters.) Where computer program suites include atomic structure calculations involving direct diagonalization of energy matrices, scaled Slater parameters such as those listed in the tables here could be used as optional input, where appropriate.

With the better estimates of level-mixing factors, improved calculations of collision strengths should then be possible. The effect on collision strengths is further discussed by Magee *et al.* (1977) who emphasize the importance of using accurate target wavefunctions.

The change in oscillator strength values obtained on using scaled (rather than *ab init.*) Slater parameters, varies from line to line. It is typically between 20 per cent and a factor of two for strong allowed transitions; but may be several orders of magnitude for some inter-

Table 7(b). Calculated and observed wavelengths (Å) for $3s^2\,3p^2$–$3s^2\,3p\,3d$ Fe XIII transitions with calculated weighted oscillator strengths (gf) $\gtrsim 0.05$.

Transition	Calculated wavelength	Observed wavelength★	Calc – obs	gf
$^3P-{}^3D$				
2–3	203.96	203.826 Sb	0.13	2.96
2–2	203.83	203.793 S	0.04	1.14
1–2	200.06	200.021 S	0.04	0.58
2–1	205.05	204.942 S	0.11	0.30
1–1	201.22	201.121 Sb	0.10	0.76
0–1	197.53	197.434 S	0.10	0.08
$^3P-{}^3P$				
2–2	213.30	213.770 S	−0.47	0.62
1–2	209.17	209.617 S	−0.45	0.68
2–1	209.95	209.916 S	0.03	0.12
0–1	202.07	202.044 S	0.03	0.97
1–0	202.94	202.424 N	0.52	0.31
$^1D-{}^1F$				
2–3	196.42	196.525 S	−0.11	2.91
$^1D-{}^1D$				
2–2	221.40	221.822 S	−0.42	1.34
$^1S-{}^1P$				
0–1	208.89	208.679	0.21	1.24
$^3P-{}^1D$				
1–2	203.90	204.263 S	−0.36	0.79
$^1D-{}^3D$				
2–2	216.88			0.34
2–3	217.00			0.12
$^1D-{}^3P$				
2–2	227.63	227.479 N	0.15	0.66

★ Sources of wavelength data: see footnote to Table 7(a).

combination lines. (The residual errors will also be greater for intercombination lines.) This information may serve to indicate the size of changes that may be expected in collision strengths as a result of using scaled Slater parameters such as those presented in this paper.

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