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Atomic data from the Iron Project

VII. Radiative dipole transition probabilities for Fe II*

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Abstract. Oscillator strengths, line strengths and Einstein A-coefficients are obtained for a large number of dipole allowed ($\Delta S = 0$) fine structure transitions in Fe II. Spectroscopic energies of the observed fine structure levels are employed in the transformation from LS coupled multiplet strengths to the individual fine structure lines. The transition probabilities are thus significantly improved in accuracy over those obtained with calculated energies. As part of the second phase of the Iron Project the present work is part of the effort to improve the accuracy and the utility of the Opacity Project data. The calculations correspond to a 83-state close coupling calculations for Fe II described by Nahar & Pradhan (1994). Comparison of present oscillator strengths and lifetimes is made with experimental values, and with those calculated by Kurucz; the present values show an overall better agreement with the experimental data. Radiative data is obtained for 21,589 dipole allowed fine structure transitions in Fe II.

Key words: atomic data – plasmas – ultraviolet: general – infrared: genereal

1. Introduction

The atomic radiative data for energy levels, oscillator strengths, and photoionization cross sections for essentially all astrophysically abundant atoms and ions of the Opacity Project (OP) have been calculated in LS coupling (Seaton et al. 1994). The OP calculations are carried out in an *ab initio* manner using the close coupling (CC) approximation and employing the R-matrix method. The aim of the present work, an extension of the OP (Nahar 1993) and a part of the Iron Project (IP, Hummer et al. 1993), is to provide an extensive dataset for the oscillator strengths (f-values), the line strengths (S) and the spontaneous radiative decay rates (A-values) of fine structure levels for the spectroscopic applications in laboratory and astrophysical plasmas.

While the dominant emphasis of the IP is on collisional processes, it is also envisaged that the accuracy of some of the radiative OP data, particularly for the heavy Iron group elements, would also be improved by the IP effort. Furthermore, the practical utility of the radiative data for a variety of astrophysical and laboratory applications would be enhanced by extending the LS coupling data to include fine structure and using observed spectroscopic energies rather than the calculated ones. With respect to the first criterion, in a recent study we described new OP calculations for Fe II (Nahar & Pradhan 1994, NP) that differ considerably from the earlier work of Sawey & Berrington (1992). The extension of the Fe II calculations to fulfill the second criterion forms the basis of the present report. In principle the fine structure should be considered by a complete treatment of the relativistic effects, in an intermediate coupling scheme, as well as electron-electron correlation effects that manifest themselves as configuration interaction, which for a system as complex as Fe II can be quite extensive. However, at the present time it is beyond the scope of current computational resources to carry through a full Breit-Pauli R-matrix calculation for the 83-state close coupling expansion used by NP (1994), that was necessary to adequately represent the electron correlation effects in Fe II. On the other hand, it is expected that the relativistic effects for Fe II should be relatively less important than an accurate representation of the correlation effects (although for higher ion charges this may not be the case).

In an earlier study of a similar nature (Nahar 1993), we considered the dipole allowed ($\Delta S = 0$) transitions in Si I and Si-like ions and found very good agreement with experimental data (usually within the experimental error bars) for the oscillator strengths of a number of fine structure transitions. Fe II is considerably more complex; however, preliminary work reported by NP (1994) showed that the results obtained appear to be of higher accuracy than the data available from Kurucz (1981, and private communication) for most of the transitions studied, when compared with the experimental data compiled and evaluated by the National Institute of Standards and Technology

* Table for complete data for Fe II transition probabilities are only available from in electronic form: see the editorial in A&A 1992, Vol. 266, No. 2, page E1.

Table 1. Calculated and measured lifetimes, τ, of Fe II levels

State	J	τ(ns) Present	Expt.	Kurucz	State	J	τ(ns) Present	Expt.	Kurucz
z^6P^0	7/2	3.884	3.73(.06)[a],3.8(2)[b], 3.5(3)[c],3.73(5)[d]	3.28	z^6F^0	5/2	3.063	3.3(2)[c],3.33(9)[d]	2.93
					z^6F^0	3/2	3.078	3.3(2)[c],3.34(10)[d]	2.94
z^6P^0	5/2	3.844	3.79(0.12)[a],3.7(2)[b] 3.5(3)[c],3.83(7)[d]	3.26	z^6F^0	1/2	3.081	3.3(3)[c]	2.94
					z^4P^0	5/2	3.250	3.43(.09)[a]	2.97
z^6P^0	3/2	3.819	3.71(.12)[a],3.6(2)[b],3.4(3)[c]	3.25	z^4P^0	3/2	3.241	3.44(.11)[a]	2.96
z^6D^0	9/2	3.460	3.7(.2)[b],3.7(2)[c],3.7(6)[d]	3.41	z^4D^0	7/2	2.476	3.02(.07)[a],3.1(2)[b]	2.43
z^6D^0	7/2	3.487	3.75(20)[b],3.8(3)[c],3.68(7)[d]	3.43	z^4D^0	5/2	2.496	3.1(.08)[a],3.1(2)[b]	2.44
z^6D^0	5/2	3.499	3.7(.2)[b],3.8(3)[c],3.63(8)[d]	3.44	z^4D^0	3/2	2.494	3.0(2)[b]	2.43
z^6D^0	3/2	3.498	3.7(.2)[b],3.7(2)[c],3.83(10)[d]	3.45	z^4D^0	1/2	2.498	2.9(2)[b]	2.42
z^6D^0	1/2	3.492	3.8(.2)[b],3.8(3)[c],3.76(10)[d]	3.45	z^4F^0	9/2	3.471	3.87(.09)[a],3.7(2)[b]	3.34
z^6F^0	11/2	2.982	3.2(.2)[b],3.3(2)[c],3.19(4)[d]	2.83	z^4F^0	7/2	3.435	3.63(.11)[a],3.6(2)[b]	3.22
z^6F^0	9/2	3.024	3.2(.2)[b],3.24(6)[d],3.4(2)[c]	2.89	z^4F^0	5/2	3.417	3.75(.14)[a],3.7(2)[b]	3.26
z^6F^0	7/2	3.034	3.3(2)[c],3.26(10)[d]	2.92	z^4F^0	3/2	3.422	3.7(2)[b]	3.3

[a] Guo et al. (1992), [b] Hannaford et al. (1992), [c] Schade et al. (1988), [d] Biemont et al. (1991).

(NIST; Fuhr et al. 1988). Presently the available data for Fe II derives mainly from two sources: Kurucz (1981) and Fawcett (1988), both of which employ a semi-empirical method due to Cowan (1968). Ekberg & Feldman (1993) also have obtained transition probabilities for 550 transitions based on measured values from various published reports. The present work is a completed account of the work initiated by NP (1994) for a relatively large dataset of Fe II transition probabilities.

The present calculations are carried out through algebraic transformation of the LS multiplet strengths calculated in the close coupling approximation, and observed energies for the fine structure levels which are known to a much higher precision than the calculated energies are used. The dipole allowed transitions ($\Delta S = 0$) are considered for all LS terms for which a partial or complete set of fine structure levels have been observed. The present work employs the level energies of Fe II from Johansson (1978) and 193 (769–576) unpublished levels (Johansson, private communication, 1992). The 265 LS terms observed correspond to 3109 LS multiplets with 21589 fine structure transitions, thus providing a reasonably comprehensive dataset for Fe II for practical applications.

The primary difficulty encountered in the present work is the LS term identification of the large number of computed terms of Fe II, and to establish the correspondence with the measured spectroscopic levels and energies. The theoretical and computational work is described in Sect. 2. A sample of the present extensive data set is provided in Sect. 3, with a discussion of related uncertainties.

2. Summary of theoretical work and computations

The LS multiplet strength, S, which is independent of the energy difference between the transitional states is obtained from the calculated LS oscillator strength, f_{if}, as

$$f_{if} = \frac{E_{fi}}{3g_i}\mathbf{S}\,, \quad (1)$$

where $E_{fi} = E_f - E_i$ is the transition energy and $g_i = (2S_i + 1)(2L_i + 1)$ is the statistical weight of the initial state. Energies are in Rydberg units throughout unless specified otherwise. In terms of dipole length and velocity operators

$$\mathbf{D}_L = \sum_n r_n\,, \quad \mathbf{D}_V = -2\sum_n \nabla_n\,, \quad (2)$$

where the summation is over all atomic electrons, the line strength is given by

$$\mathbf{S}_L = |\langle\psi_f\|\,\mathbf{D}_L\,\|\psi_i\rangle|^2\,, \quad (3a)$$

in the 'length form' and

$$\mathbf{S}_V = E_{fi}^{-2}\,|\langle\psi_f\|\,\mathbf{D}_V\,\|\psi_i\rangle|^2\,, \quad (3b)$$

in the 'velocity form' respectively.

The fine structure line strengths, S_{JJ}, of the LS multiplet strength, S_{LS}, is obtained for the allowed transitions ($\Delta J = 0, \pm 1$) through the algebraic transformation,

$$S_{JJ} = C_{Al}(J_i, J_f)S_{LS}/\left[(2S_i+1)(2L_i+1)(2L_f+1)\right] \quad (4)$$

where values of coefficients $C_{Al}(J_i, J_f)$ are obtained from Allen (1976). The above expression satisfies the conservation condition

$$S_{LS} = \sum_J S_{JJ}\,. \quad (5)$$

The fine structure f-values (oscillator strengths) are then obtained using $E_{J_fJ_i} = E_{J_f} - E_{J_i}$, where E_{J_i} and E_{J_i} are now the *observed* energies, as

Table 2. Calculated and observed (Johansson 1978)[a] energies of Fe II terms. An ∗ next to an energy means the set of observed levels for the term is incomplete. The degeneracy symbol for each state is chosen for convenience as explained in the text

State		E(Ryd) Obs.	E(Ryd) Cal.	State		E(Ryd) Obs.	E(Ryd) Cal.
Octets							
$3d^5\,^6S4s4p\,^3P^0$	z^8P^0	0.70972	0.7783	$3d^54s\,^7S5s$	a^8S	0.25023	0.2457
$3d^54p^2$	a^8P	0.21567	0.2742	$3d^54s\,^7S4d$	a^8D	0.19213	0.2300
Sextets							
$3d^54s^2$	a^6S	0.97721	0.9951	$3d^5\,^5D6d$	c^6G	0.15148∗	0.1550
$3d^5\,^5D4d$	b^6S	0.41061	0.4128	$3d^5\,^5D4p$	z^6P^0	0.79726	0.8111
$3d^5\,^5D5d$	c^6S	0.22638	0.2388	$3d^5\,^6S4s4p$	y^6P^0	0.62392	0.6594
$3d^54s^7S5s$	d^6S	0.21835	0.2117	$3d^5\,^6S4s4p$	x^6P^0	0.46709	0.4785
$3d^5\,^5D4d$	a^6P	0.42130	0.4219	$3d^5\,^4P4s4p$	w^6P^0	0.37553	0.3966
$3d^5\,^5D5d$	b^6P	0.23987	0.2438	$3d^5\,^5D5p$	v^6P^0	0.35631	0.3581
$3d^54p^2$	c^6P	0.14166	0.1834	$3d^5\,^4D4s4p$	u^6P^0	0.32751	0.3443
$3d^6\,^5D4s$	a^6D	1.18591	1.1782	$3d^5\,^5D6p$	t^6P^0	0.21058	0.2126
$3d^5\,^5D5s$	b^6D	0.47640	0.4687	$3d^5\,^5D4p$	z^6D^0	0.83695	0.8466
$3d^5\,^5D4d$	c^6D	0.42604	0.4273	$3d^5\,^4P4s4p$	y^6D^0	0.38557	0.4120
$3d^5\,^5D6s$	d^6D	0.25937	0.2555	$3d^5\,^5D5p$	x^6D^0	0.37896	0.3789
$3d^5\,^5D5d$	e^6D	0.23633	0.2422	$3d^5\,^4D4s4p$	v^6D^0	0.33345	0.3478
$3d^54p^2$	f^6D	0.21862	0.2713	$3d^5\,^5D6p$	u^6D^0	0.21765	0.2197
$3d^5\,^5D7s$	g^6D	0.16227	0.1638	$3d^5\,^4F4s4p$	t^6D^0	0.20451	0.2116
$3d^54s\,^7S4d$	h^6D	0.12955	0.1446	$3d^5\,^5D4p$	z^6F^0	0.80542	0.8177
$3d^5\,^5D4d$	a^6F	0.43250	0.4312	$3d^5\,^4G4s4p$	y^6F^0	0.39240	0.3756
$3d^5\,^5D5d$	b^6F	0.24042∗	0.2454	$3d^5\,^5D5p$	x^6F^0	0.36766	0.3675
$3d^5\,^5D6d$	c^6F	0.15354∗	0.1568	$3d^5\,^4D4s4p$	w^6F^0	0.34940	0.3756
$3d^5\,^5D4d$	a^6G	0.42021	0.4223	$3d^5\,^4F4s4p$	v^6F^0	0.21856	0.2275
$3d^5\,^5D5d$	b^6G	0.23492	0.2417	$3d^5\,^5D6p$	u^6F^0	0.21207	0.2146
Quartets							
$3d^6\,^5D4d$	a^4S	0.40848	0.4142	$3d^6\,^5D5p$	v^4P^0	0.35518	0.3575
$3d^7$	a^4P	1.06566	0.9846	$3d^6\,^3P4p$	u^4P^0	0.35519	0.3348
$3d^6\,^3P4s$	b^4P	0.99450	0.9313	$3d^54s^5P4p$	t^4P^0	0.32856	0.2877
$3d^6\,^3P4s$	c^4P	0.73596	0.6515	$3d^54s^5D4p$	s^4P^0	0.26375	0.2558
$3d^54s^2$	d^4P	0.66603	0.6331	$3d^54s^3D4p$	r^4P^0	0.21916∗	0.2129
$3d^6\,^5D4d$	e^4P	0.38709	0.3747	$3d^6\,^5D6p$	q^4P^0	0.20937	0.2101
$3d^6\,^3P5s$	f^4P	0.29695	0.2832	$3d^6\,^3P5p$	p^4P^0	0.19511	0.1868
$3d^6\,^3P4d$	g^4P	0.23441	0.2206	$3d^6\,^5D4p$	z^4D^0	0.78197	0.7890
$3d^6\,^5D5d$	h^4P	0.21510	0.2267	$3d^6\,^3P4p$	y^4D^0	0.62132	0.5896
$3d^54p^2$	i^4P	0.11286∗	0.1231	$3d^6\,^3F4p$	x^4D^0	0.61370	0.5857
$3d^6\,^5D4s$	a^4D	1.11388	1.1060	$3d^6\,^3D4p$	w^4D^0	0.52817	0.4962
$3d^6\,^3D4s$	b^4D	0.90338	0.8499	$3d^6\,^3P4p$	v^4D^0	0.39918	0.3401
$3d^64s^2$	c^4D	0.63958	0.6191	$3d^6\,^5D5p$	u^4D^0	0.36336	0.3631
$3d^6\,^5D5s$	d^4D	0.46240	0.4555	$3d^6\,^3F4p$	t^4D^0	0.34316	0.3100
$3d^6\,^5D4d$	e^4D	0.41638	0.4225	$3d^54s^5P4p$	s^4D^0	0.31457	0.2952
$3d^6\,^5D6s$	f^4D	0.25338	0.2531	$3d^54s^5D4p$	r^4D^0	0.29153	0.2782
$3d^6\,^3P4d$	g^4D	0.24970∗	0.2206	$3d^54s\,^3F4p$	q^4D^0	0.20248∗	0.1984
$3d^6\,^5D5d$	h^4D	0.23253∗	0.2404	$3d^54s^3D4p$	p^4D^0	0.21354∗	0.2129
$3d^6\,^3F4d$	i^4D	0.23106∗	0.1940	$3d^6\,^5D6p$	o^4D^0	0.21308∗	0.2101
$3d^6\,^3D5s$	j^4D	0.19884	0.1860	$3d^6\,^3P5p$	n^4D^0	0.18767∗	0.1802
$3d^6\,^3G4d$	k^4D	0.20003	0.1808	$3d^6\,^3F5p$	m^4D^0	0.18237∗	0.1537
$3d^6\,^5D7s$	l^4D	0.15833	0.1614	$3d^6\,^5D4p$	z^4F^0	0.78223	0.7968
$3d^7$	a^4F	1.16768	1.081	$3d^6\,^3F4p$	y^4F^0	0.62342	0.5947
$3d^6\,^3F4s$	b^4F	0.98186	0.9327	$3d^6\,^3G4p$	x^4F^0	0.58542	0.5645
$3d^6\,^3F4s$	c^4F	0.73269	0.6462	$3d^6\,^3D4p$	w^4F^0	0.52987	0.5007
$3d^54s^2$	d^4F	0.52031	0.4884	$3d^6\,^5D5p$	v^4F^0	0.36261	0.3654

[a] Observed energies include unpublished level energies of Fe II (Johansson, private communication, 1992).

Table 2. (continued)

State		E(Ryd) Obs.	E(Ryd) Cal.	State		E(Ryd) Obs.	E(Ryd) Cal.
3d^6 ^{5}D4d	e^{4}F	0.40242	0.3933	3d^{5}4s^{5}G4p	u^{4}F^0	0.34810	0.3618
3d^6 ^{3}F5s	f^{4}F	0.28108	0.2401	3d^6 ^{3}F4p	t^{4}F^0	0.33817	0.2981
3d^6 ^{5}D5d	g^{4}F	0.24320	0.2377	3d^{5}4s^{5}D4p	s^{4}F^0	0.29237	0.2822
3d^6 ^{3}P4d	h^{4}F	0.24256	0.2188	3d^{5}4s^{3}D4p	r^{4}F^0	0.23314	0.2367
3d^6 ^{3}H4d	i^{4}F	0.23240*	0.2007	3d^6 ^{5}D6p	q^{4}F^0	0.21278	0.2133
3d^6 ^{3}F4d	j^{4}F	0.21661	0.1875	3d^{5}4s ^{3}F4p	p^{4}F^0	0.20141	0.2022
3d^6 ^{3}G4d	k^{4}F	0.18585	0.1695	3d^6 ^{3}F5p	o^{4}F^0	0.18529	0.1664
3d^6 ^{5}D6d	l^{4}F	0.14940*	0.1396	3d^6 ^{3}G5p	n^{4}F^0	0.16697	0.1575
3d^6 ^{3}D4d	m^{4}F	0.14146*	0.1158	3d^6 ^{3}H4p	z^{4}G^0	0.63548	0.6168
3d^6 ^{3}G4s	a^{4}G	0.95495	0.9168	3d^6 ^{3}F4p	y^{4}G^0	0.60678	0.5844
3d^{5}4s^2	b^{4}G	0.69523	0.6913	3d^6 ^{3}G4p	x^{4}G^0	0.59033	0.5723
3d^6 ^{5}D4d	c^{4}G	0.41310	0.4195	b3d^6 ^{3}F4p	w^{4}G^0	0.36944	0.3475
3d^6 ^{3}G5s	d^{4}G	0.25241	0.2403	3d^{5}4s^{5}G4p	v^{4}G^0	0.33203	0.3085
3d^6 ^{3}H4d	e^{4}G	0.24387	0.2112	3d^{5}4s ^{3}F4p	u^{4}G^0	0.20868*	0.2115
3d^6 ^{5}D5d	f^{4}G	0.23088	0.2389	3d^{5}4s^{3}G4p	t^{4}G^0	0.20038	0.1948
a3d^6 ^{3}F4d	g^{4}G	0.23107	0.1946	3d^6 ^{3}H5p	s^{4}G^0	0.18833	0.1588
3d^6 ^{3}G4d	h^{4}G	0.20197	0.1830	3d^6 ^{3}F5p	r^{4}G^0	0.16926	0.1498
3d^6 ^{5}D6d	i^{4}G	0.14662	0.1538	3d^{5}4s^{5}F4p	q^{4}G^0	0.16594*	0.1777
3d^6 ^{3}H4s	a^{4}H	0.99415	0.9631	3d^6 ^{3}G5p	p^{4}G^0	0.14292*	0.1402
3d^6 ^{3}H5s	b^{4}H	0.29368	0.2404	3d^6 ^{3}H4p	z^{4}H^0	0.63434	0.6193
3d^6 ^{3}H4d	c^{4}H	0.24399	0.2104	3d^6 ^{3}G4p	y^{4}H^0	0.58358	0.5669
3d^6 ^{3}Fa4d	d^{4}H	0.22898	0.1939	3d^{5}4s^{5}G4p	x^{4}H^0	0.34980	0.3693
3d^6 ^{3}G4d	e^{4}H	0.20181	0.1830	3d^{5}4s^{3}I4p	w^{4}H^0	0.23439	0.2606
3d^6 ^{3}H4d	a^{4}I	0.24146	0.2106	3d^{5}4s^{3}G4p	v^{4}H^0	0.19810	0.2010
3d^6 ^{3}G4d	b^{4}I	0.20019	0.1812	3d^{5}4s^{3}G4p	u^{4}H^0	0.18413*	0.1380
3d^6 ^{3}H4d	a^{4}K	0.24407	0.2120	3d^6 ^{3}H5p	t^{4}H^0	0.17227	0.1821
3d^6 ^{3}P4p	z^{4}So	0.64601	0.6075	3d^6 ^{3}G5p	s^{4}H^0	0.14892*	0.1455
3d^6 ^{3}P4p	y^{4}So	0.36382	0.3144	3d^6 ^{3}H4p	z^{4}I^0	0.62942	0.6194
3d^{5}4s^{5}P4p	x^{4}So	0.29358	0.2718	3d^{5}4s^{3}I4p	y^{4}I^0	0.25027	0.2810
3d^6 ^{3}P5p	w^{4}So	0.20214	0.1919	3d^6 ^{3}H5p	x^{4}I^0	0.19004	0.1751
3d^6 ^{5}D4p	z^{4}P^0	0.75942	0.7706	3d^{5}4s^{3}H4p	w^{4}I^0	0.16756*	0.1444
3d^6 ^{3}P4p	y^{4}P^0	0.63549	0.5997	3d^{5}4s^{3}I4p	z^{4}K^0	0.25488*	0.2852
3d^{5}4s5S4p	x^{4}P^0	0.55889	0.5729				
3d^6 ^{3}D4p	w^{4}P^0	0.53329	0.5009				
Doublets							
3d^{6}a^{1}S4s	a^{2}S	0.85046	0.7887	3d^{6}b ^{3}P4p	v^{2}P^0	0.32364*	0.2902
3d^7	a^{2}P	1.02079	0.9148	3d^{5}4s ^{3}P4p	u^{2}P^0	0.30280*	0.2533
3d^{6}a^{3}P4s	b^{2}P	0.95123	0.8763	3d^{5}4s^{3}D4p	t^{2}P^0	0.22047	0.2001
3d^{6}b^{3}P4s	c^{2}P	0.69194	0.5975	3d^{6}a ^{3}P4p	z^{2}D^0	0.62921	0.5944
3d^6 ^{3}P5s	d^{2}P	0.28433	0.2750	3d^{6}a^{3}F4p	y^{2}D^0	0.57815	0.5498
3d^6 ^{3}P4d	e^{2}P	0.23174	0.2095	3d^6 ^{3}D4p	x^{2}D^0	0.51023	0.4747
3d^{6}a^{3}F4d	f^{2}P	0.20457*	0.1648	3d^{6}a^{1}D4p	w^{2}D^0	0.47336	0.4134
3d^7	a^{2}D	0.99985	0.8896	3d^6 ^{1}F4p	v^{2}D^0	0.42364	0.3630
3d^6 ^{3}D4s	b^{2}D	0.85980	0.7966	3d^{6}b^{3}P4p	u^{2}D^0	0.34674	0.2851
3d^{6}a^{1}D4s	c^{2}D	0.84174	0.7565	3d^{6}b^{3}F4p	t^{2}D^0	0.32672*	0.2698
3d^7	d^{2}D	0.75326	0.6128	3d^{5}4s^{3}P4p	s^{2}D^0	0.27478*	0.2521
3d^6 ^{3}P4d	e^{2}D	0.23069*	0.2108	3d^{5}4s^{3}D4p	r^{2}D^0	0.25592	0.2379
3d^{6}a^{3}F4d	f^{2}D	0.21085	0.1754	3d^6 ^{3}P5p	q^{2}D^0	0.19703*	0.1840
3d^6 ^{3}D5s	g^{2}D	0.19066	0.1316	3d^{6}a^{3}F4p	z^{2}F^0	0.60334	0.5794
3d^6 ^{3}G4d	h^{2}D	0.18526	0.1646	3d^6 ^{3}G4p	y^{2}F^0	0.55523	0.5278
3d^{6}a^{3}F4s	a ^{2}F	0.93960	0.8905	3d^{6}a^{1}G4p	x^{2}F^0	0.52418	0.4907
3d^7	b ^{2}F	0.89883	0.7842	3d^6 ^{3}D4p	w^{2}F^0	0.49955	0.4606
3d^6 ^{1}F4s	c ^{2}F	0.78035	0.6907	3d^{6}a^{1}D4p	v^{2}F^0	0.47920	0.4212
3d^{6}b^{3}F4s	d ^{2}F	0.68951	0.5997	3d^6 ^{1}F4p	u^{2}F^0	0.40136	0.3411

Table 2. (continued)

State		E(Ryd)		State		E(Ryd)	
		Obs.	Cal.			Obs.	Cal.
3d^{5}4s^2	e^{2}F	0.44525	0.4881	3d^{6}b^{3}F4p	t^{2}F^0	0.32340	0.3180
3d^{6}a^{3}F5s	f^{2}F	0.27294	0.2314	3d^{5}4s^{3}G4p	s^{2}F^0	0.31193	0.2582
3d^6 ^{3}H4d	g^{2}F	0.23866	0.2066	3d^{6}b^{1}G4p	r^{2}F^0	0.28847*	0.2350
3d^{6}a^{3}F4d	h^{2}F	0.22186*	0.1920	3d^{5}4s^{3}D4p	q^{2}F^0	0.24883	0.2101
3d^6 ^{3}G4d	i^{2}F	0.18195	0.1519	3d^6 ^{3}F5p	p^{2}F^0	0.17192	0.1417
3d^7	a^{2}G	1.04319	0.9380	3d^6 ^{3}H4p	z^{2}G^0	0.62299	0.6072
3d^6 ^{3}G4s	b^{2}G	0.91126	0.8667	3d^{6}a^{3}F4p	y^{2}G^0	0.59778	0.5713
3d^{6}a^{1}G4s	c^{2}G	0.88459	0.8307	3d^6 ^{3}G4p	x^{2}G^0	0.54810	0.5262
3d^{6}b^{1}G4s	d^{2}G	0.65527	0.5513	3d^{6}a^{1}G4p	w^{2}G^0	0.52343	0.4883
3d^{5}4s^2	e^{2}G	0.47524	0.4459	3d^6 ^{1}F4p	v^{2}G^0	0.42770	0.3710
3d^6 ^{3}G5s	f^{2}G	0.24403	0.2310	3d^{6}b^{3}F4p	u^{2}G^0	0.34802	0.2886
3d^6 ^{3}H4d	g^{2}G	0.23335	0.2008	3d^{5}4s^{3}G4p	t^{2}G^0	0.28166	0.2741
3d^{6}a^{3}F4d	h^{2}G	0.21543	0.1849	3d^{6}b^{1}G4p	s^{2}G^0	0.28044	0.2090
3d^6 ^{3}G4d	i^{2}G	0.18960	0.1638	3d^{5}4s^{3}F4p	r^{2}G^0	0.18128*	0.1823
3d^7	a^{2}H	1.00242	0.9222	3d^6 ^{3}H5p	q^{2}G^0	0.18530	0.1452
3d^6 ^{3}H4s	b^{2}H	0.95046	0.8958	3d^6 ^{3}F5p	p^{2}G^0	0.17293	0.1399
3d^{5}4s^2	c^{2}H	0.48592*	0.4588	3d^6 ^{3}G5p	o^{2}G^0	0.14285*	0.1310
3d^6 ^{3}H5s	d^{2}H	0.28571	0.2324	3d^6 ^{3}H4p	z^{2}H^0	0.59326	0.5772
3d^{6}a^{3}F4d	e^{2}H	0.22486	0.1917	3d^6 ^{3}G4p	y^{2}H^0	0.57244	0.5581
3d^6 ^{3}H4d	f^{2}H	0.22313	0.1896	3d^{6}a^{1}G4p	x^{2}H^0	0.53175	0.5012
3d^6 ^{3}G4d	g^{2}H	0.18885	0.1625	3d^6 ^{1}I4p	w^{2}H^0	0.51836	0.4880
3d^6 ^{1}I4s	a^{2}I	0.88997	0.8470	3d^{5}4s^{3}G4p	v^{2}H^0	0.31358	0.3181
3d^6 ^{3}H4d	b^{2}I	0.23571	0.2061	3d^{6}b^{1}G4p	u^{2}H^0	0.29589	0.2394
3d^6 ^{1}I5s	c^{2}I	0.19970	0.1374	3d^{6}4s^{3}I4p	t^{2}H^0	0.21616	0.2158
3d^6 ^{3}G4d	d^{2}I	0.19454	0.1786	3d^6 ^{3}H5p	s^{2}H^0	0.18007	0.1370
3d^6 ^{3}H4d	a^{2}K	0.24006*	0.2092	3d^6 ^{3}G5p	r^{2}H^0	0.14510	0.1415
3d^{6}a^{3}P4p	z^{2}So	0.58600	0.5491	3d^6 ^{3}H4p	z^{2}I^0	0.62049	0.5575
3d^{6}b^{3}P4p	y^{2}So	0.37864	0.3210	3d^6 ^{1}I4p	y^{2}I^0	0.51565	0.4927
3d^{5}4s^{3}P4p	x^{2}So	0.24228	0.2123	3d^{5}4s^{3}I4p	x^{2}I^0	0.19454	0.2054
3d^{6}a^{3}P4p	z^{2}P^0	0.59897	0.5633	3d^6 ^{3}H5p	w^{2}I^0	0.18664	0.1231
3d^6 ^{3}D4p	y^{2}P^0	0.52276	0.4852	3d^6 ^{1}I4p	z^{2}K^0	0.54065	0.5211
3d^{6}a1S4p	x^{2}P^0	0.49460	0.4429	3d^{6}4s^{3}I4p	y^{2}K^0	0.22043	0.2409
3d^{6}a^{1}D4p	w^{2}P^0	0.46880	0.4130				

$$f_{JJ}(J_f, J_i) = S_{JJ} E_{J_f J_i} / [3(2J_i + 1)] \ . \tag{6}$$

The fine structure oscillator strengths, f_{JJ}, can also be obtained directly from the LS oscillator strength, f_{LS}, as (Seaton et al. 1994)

$$\begin{aligned} &f_{JJ}(n_f SL_f J_f, n_i SL_i J_i) \\ &\quad = f_{LS}(n_f SL_f, n_i SL_i)(2J_f + 1)(2L_i + 1) \\ &\quad \times W^2(L_f L_i J_f J_i; 1S) \end{aligned} \tag{7}$$

where $W(L_f L_i J_f J_i; 1S)$ is a Racah coefficient. The above fine structure f-values satisfy the conservation sum

$$\begin{aligned} &\sum_{J_i J_f} (2J_i + 1) f_{JJ}(n_f SL_f J_f, n_i SL_i J_i) \\ &\quad = (2S + 1)(2L_i + 1) f_{LS}(n_f SL_f, n_i SL_i) \ . \end{aligned} \tag{8}$$

The improvement in accuracy through the use of observed energies cannot be achieved by splitting of LS oscillator strengths through Eq. (7), which is used only for transitions between two LS states where one or both states have an incomplete set of observed fine structure levels, and for transitions between high angular momenta states (higher than $\boldsymbol{H} \leftrightarrow \boldsymbol{I}$) for which the values of $C_{Al}(J_i, J_f)$ are not available.

The radiative transition probability, A_{fi}, from higher state f to lower state i can be obtained, in atomic unit, as

$$A_{fi}(\text{a.u.}) = \frac{1}{2} \alpha^3 \frac{g_i}{g_f} E_{fi}^2 f_{if} \ , \tag{9}$$

where α is the fine structure constant and g_f is the statistical weight of the final state, and in c.g.s. unit of time as

$$A_{fi}(\text{s}^{-1}) = \frac{A_{fi}(\text{a.u.})}{\tau_0} \ , \tag{10}$$

where $\tau_0 = 2.419\,10^{-17}$ s is the atomic unit of time. The total radiative probability for the state f is given by

$$A_f = \sum_i A_{fi} \ , \tag{11}$$

Table 3. f-, S-, and A-values for transitions in Fe II. E_i and E_f are the energies in cm^{-1} for the initial and final levels except for the first line where the term energies are Rydberg units. EDIFF is the transition energy in Rydberg

Transition	E_i (cm^{-1})	E_f (cm^{-1})	EDIFF (Ryd)	g_i	g_f	f_{if}	S	a_{ji} (s^{-1})
z8Po → a8Pe	0.7097	0.2157	4.94E-01	24	24	6.697E-01	9.760E+01	1.313E+09
	52965.820	107219.500	4.94E-01	10	10	4.088E-01	2.481E+01	8.026E+08
	52965.820	106836.000	4.91E-01	10	8	2.584E-01	1.579E+01	6.252E+08
	52582.510	107219.500	4.98E-01	8	10	3.276E-01	1.579E+01	5.219E+08
	52582.510	106836.000	4.94E-01	8	8	2.094E-02	1.017E+00	4.112E+07
	52582.510	106404.920	4.90E-01	8	6	3.213E-01	1.572E+01	8.278E+08
	52299.390	106836.000	4.97E-01	6	8	4.341E-01	1.572E+01	6.459E+08
	52299.390	106404.920	4.93E-01	6	6	2.376E-01	8.675E+00	4.640E+08
a6Se → z6Po	0.9772	0.7973	1.80E-01	6	18	4.336E-02	4.337E+00	3.760E+06
	23317.633	42658.224	1.76E-01	6	8	1.887E-02	1.928E+00	3.531E+06
	23317.633	43238.586	1.82E-01	6	6	1.458E-02	1.446E+00	3.859E+06
	23317.633	43620.957	1.85E-01	6	4	9.906E-03	9.638E-01	4.085E+06
a6Se → y6Po	0.9772	0.6239	3.53E-01	6	18	1.610E-02	8.204E-01	5.381E+06
	23317.633	62171.615	3.54E-01	6	8	7.172E-03	3.646E-01	5.416E+06
	23317.633	62049.025	3.53E-01	6	6	5.362E-03	2.735E-01	5.365E+06
	23317.633	61974.933	3.52E-01	6	4	3.568E-03	1.823E-01	5.334E+06
a6Se → x6Po	0.9772	0.4671	5.10E-01	6	18	1.712E+00	6.039E+01	1.192E+09
	23317.633	79331.500	5.10E-01	6	8	7.612E-01	2.684E+01	1.195E+09
	23317.633	79285.110	5.10E-01	6	6	5.704E-01	2.013E+01	1.192E+09
	23317.633	79246.170	5.10E-01	6	4	3.800E-01	1.342E+01	1.189E+09
a6Pe → y6Do	0.4213	0.3856	3.57E-02	18	30	2.768E-06	4.182E-03	1.704E+01
	84266.556	88614.517	3.96E-02	8	10	2.302E-06	1.394E-03	2.323E+01
	84266.556	88209.453	3.59E-02	8	8	5.982E-07	3.996E-04	6.203E+00
	84266.556	88059.381	3.46E-02	8	6	9.571E-08	6.644E-05	1.225E+00
	84326.912	88209.453	3.54E-02	6	8	1.406E-06	7.156E-04	1.061E+01
	84326.912	88059.381	3.40E-02	6	6	9.660E-07	5.111E-04	8.980E+00
	84326.912	87964.650	3.32E-02	6	4	3.081E-07	1.673E-04	4.079E+00
	84424.374	88059.381	3.31E-02	4	6	7.184E-07	2.602E-04	4.222E+00
	84424.374	87964.650	3.23E-02	4	4	1.049E-06	3.903E-04	8.771E+00
	84424.374	87635.920	2.93E-02	4	2	6.800E-07	2.788E-04	9.359E+00
a6De → z6Po	1.1859	0.7973	3.89E-01	30	18	1.263E-01	2.926E+01	2.555E+08
	0.000	42658.224	3.89E-01	10	8	1.264E-01	9.752E+00	1.917E+08
	384.790	42658.224	3.85E-01	8	8	4.487E-02	2.796E+00	5.348E+07
	667.683	42658.224	3.83E-01	6	8	9.882E-03	4.648E-01	8.716E+06
	384.790	43238.586	3.91E-01	8	6	8.145E-02	5.006E+00	1.330E+08
	667.683	43238.586	3.88E-01	6	6	7.706E-02	3.576E+00	9.315E+07
	862.613	43238.586	3.86E-01	4	6	3.766E-02	1.170E+00	3.007E+07
	667.683	43620.957	3.91E-01	6	4	3.958E-02	1.820E+00	7.307E+07
	862.613	43620.957	3.90E-01	4	4	8.866E-02	2.731E+00	1.081E+08
	977.053	43620.957	3.89E-01	2	4	1.263E-01	1.950E+00	7.661E+07

Table 3. (continued)

Transition	E_i (cm^{-1})	E_f (cm^{-1})	EDIFF (Ryd)	g_i	g_f	f_{if}	S	a_{ji} (s^{-1})
a6De → z6Do	1.1859	0.8369	3.49E-01	30	30	2.936E-01	7.572E+01	2.872E+08
	0.000	38458.981	3.50E-01	10	10	2.400E-01	2.055E+01	2.368E+08
	0.000	38660.043	3.52E-01	10	8	5.484E-02	4.670E+00	6.834E+07
	384.790	38458.981	3.47E-01	8	10	6.751E-02	4.670E+00	5.222E+07
	384.790	38660.043	3.49E-01	8	8	1.313E-01	9.036E+00	1.283E+08
	384.790	38858.958	3.51E-01	8	6	9.477E-02	6.487E+00	1.248E+08
	667.683	38660.043	3.46E-01	6	8	1.248E-01	6.487E+00	9.010E+07
	667.683	38858.958	3.48E-01	6	6	5.017E-02	2.595E+00	4.881E+07
	667.683	39013.206	3.49E-01	6	4	1.176E-01	6.058E+00	1.730E+08
	862.613	38858.958	3.46E-01	4	6	1.748E-01	6.058E+00	1.122E+08
	862.613	39013.206	3.48E-01	4	4	3.218E-03	1.111E-01	3.124E+06
	862.613	39109.307	3.49E-01	4	2	1.144E-01	3.938E+00	2.232E+08
	977.053	39013.206	3.47E-01	2	4	2.275E-01	3.938E+00	1.097E+08
	977.053	39109.307	3.47E-01	2	2	6.520E-02	1.126E+00	6.323E+07
a6De → z6Fo	1.1859	0.8054	3.80E-01	30	42	3.976E-01	9.404E+01	3.302E+08
	0.000	41968.046	3.82E-01	10	12	3.425E-01	2.687E+01	3.353E+08
	0.000	42114.818	3.84E-01	10	10	5.270E-02	4.120E+00	6.235E+07
	0.000	42237.033	3.85E-01	10	8	4.251E-03	3.314E-01	6.323E+06
	384.790	42114.818	3.80E-01	8	10	2.888E-01	1.823E+01	2.683E+08
	384.790	42237.033	3.81E-01	8	8	9.678E-02	6.090E+00	1.131E+08
	384.790	42334.822	3.82E-01	8	6	1.220E-02	7.657E-01	1.909E+07
	667.683	42237.033	3.79E-01	6	8	2.431E-01	1.155E+01	2.102E+08
	667.683	42334.822	3.80E-01	6	6	1.313E-01	6.224E+00	1.520E+08
	667.683	42401.302	3.80E-01	6	4	2.271E-02	1.075E+00	3.957E+07
	862.613	42334.822	3.78E-01	4	6	2.031E-01	6.448E+00	1.553E+08
	862.613	42401.302	3.79E-01	4	4	1.610E-01	5.105E+00	1.853E+08
	862.613	42439.822	3.79E-01	4	2	3.139E-02	9.941E-01	7.238E+07
	977.053	42401.302	3.77E-01	2	4	1.747E-01	2.776E+00	9.996E+07
	977.053	42439.822	3.78E-01	2	2	2.200E-01	3.493E+00	2.522E+08
z6Do → a6Pe	0.8369	0.4213	4.16E-01	30	18	6.753E-02	1.462E+01	1.562E+08
	38458.981	84266.556	4.17E-01	10	8	6.782E-02	4.874E+00	1.186E+08
	38660.043	84266.556	4.16E-01	8	8	2.419E-02	1.397E+00	3.356E+07
	38858.958	84266.556	4.14E-01	6	8	5.341E-03	2.323E-01	5.509E+06
	38660.043	84326.912	4.16E-01	8	6	4.338E-02	2.502E+00	8.046E+07
	38858.958	84326.912	4.14E-01	6	6	4.114E-02	1.787E+00	5.672E+07
	39013.206	84326.912	4.13E-01	4	6	2.013E-02	5.849E-01	1.838E+07
	38858.958	84424.374	4.15E-01	6	4	2.099E-02	9.098E-01	4.360E+07
	39013.206	84424.374	4.14E-01	4	4	4.706E-02	1.365E+00	6.473E+07
	39109.307	84424.374	4.13E-01	2	4	6.709E-02	9.748E-01	4.594E+07
z6Do → a6Fe	0.8369	0.4325	4.04E-01	30	42	4.966E-01	1.105E+02	4.660E+08
	38458.981	82853.659	4.05E-01	10	12	4.257E-01	3.157E+01	4.664E+08
	38458.981	82978.677	4.06E-01	10	10	6.546E-02	4.841E+00	8.655E+07
	38458.981	83136.488	4.07E-01	10	8	5.284E-03	3.894E-01	8.795E+06
	38660.043	82978.677	4.04E-01	8	10	3.604E-01	2.142E+01	3.777E+08
	38660.043	83136.488	4.05E-01	8	8	1.208E-01	7.156E+00	1.594E+08
	38660.043	83308.194	4.07E-01	8	6	1.525E-02	8.998E-01	2.704E+07
	38858.958	83136.488	4.03E-01	6	8	3.043E-01	1.358E+01	2.984E+08
	38858.958	83308.194	4.05E-01	6	6	1.646E-01	7.314E+00	2.169E+08

Table 3. (continued)

Transition	E_i (cm^{-1})	E_f (cm^{-1})	EDIFF (Ryd)	g_i	g_f	f_{if}	S	a_{ji} (s^{-1})
	38858.958	83459.675	4.06E-01	6	4	2.851E-02	1.263E+00	5.675E+07
	39013.206	83308.194	4.04E-01	4	6	2.549E-01	7.577E+00	2.224E+08
	39013.206	83459.675	4.05E-01	4	4	2.025E-01	5.998E+00	2.668E+08
	39013.206	83558.543	4.06E-01	4	2	3.951E-02	1.168E+00	1.046E+08
	39109.307	83459.675	4.04E-01	2	4	2.197E-01	3.262E+00	1.441E+08
	39109.307	83558.543	4.05E-01	2	2	2.771E-01	4.104E+00	3.651E+08
a4Pe → z4Po	1.0657	0.7594	3.06E-01	12	12	8.383E-02	9.855E+00	6.315E+07
	13474.411	46967.444	3.05E-01	6	6	5.849E-02	3.449E+00	4.376E+07
	13474.411	47389.779	3.09E-01	6	4	2.538E-02	1.478E+00	2.921E+07
	13673.185	46967.444	3.03E-01	4	6	3.738E-02	1.478E+00	1.842E+07
	13673.185	47389.779	3.07E-01	4	4	1.121E-02	4.380E-01	8.504E+06
	13673.185	47626.076	3.09E-01	4	2	3.529E-02	1.369E+00	5.427E+07
	13904.824	47389.779	3.05E-01	2	4	6.961E-02	1.369E+00	2.603E+07
	13904.824	47626.076	3.07E-01	2	2	1.402E-02	2.738E-01	1.063E+07
a4De → z4Po	1.1139	0.7594	3.54E-01	20	12	1.421E-01	2.406E+01	2.391E+08
	7955.299	46967.444	3.56E-01	8	6	1.426E-01	9.624E+00	1.930E+08
	8391.938	46967.444	3.52E-01	6	6	4.229E-02	2.165E+00	4.198E+07
	8680.454	46967.444	3.49E-01	4	6	6.996E-03	2.406E-01	4.560E+06
	8391.938	47389.779	3.55E-01	6	4	9.976E-02	5.053E+00	1.518E+08
	8680.454	47389.779	3.53E-01	4	4	7.544E-02	2.566E+00	7.540E+07
	8846.768	47389.779	3.51E-01	2	4	2.347E-02	4.010E-01	1.163E+07
	8680.454	47626.076	3.55E-01	4	2	5.930E-02	2.005E+00	1.200E+08
	8846.768	47626.076	3.53E-01	2	2	1.181E-01	2.005E+00	1.185E+08
a4Fe → z4Do	1.1677	0.7820	3.86E-01	28	20	8.545E-02	1.861E+01	1.430E+08
	1872.567	44446.878	3.88E-01	10	8	8.595E-02	6.646E+00	1.299E+08
	2430.097	44446.878	3.83E-01	8	8	1.209E-02	7.576E-01	1.423E+07
	2837.950	44446.878	3.79E-01	6	8	8.120E-04	3.855E-02	7.032E+05
	2430.097	44784.761	3.86E-01	8	6	7.332E-02	4.559E+00	1.170E+08
	2837.950	44784.761	3.82E-01	6	6	2.061E-02	9.703E-01	2.418E+07
	3117.461	44784.761	3.80E-01	4	6	1.682E-03	5.317E-02	1.299E+06
	2837.950	45044.168	3.85E-01	6	4	6.390E-02	2.991E+00	1.139E+08
	3117.461	45044.168	3.82E-01	4	4	2.370E-02	7.443E-01	2.779E+07
	3117.461	45206.450	3.84E-01	4	2	5.948E-02	1.861E+00	1.406E+08
a4Fe → z4Fo	1.1677	0.7822	3.85E-01	28	28	4.314E-02	9.401E+00	5.148E+07
	1872.567	44232.512	3.86E-01	10	10	3.956E-02	3.075E+00	4.735E+07
	1872.567	44753.799	3.91E-01	10	8	3.624E-03	2.782E-01	5.556E+06
	2430.097	44232.512	3.81E-01	8	10	4.416E-03	2.782E-01	4.118E+06
	2430.097	44753.799	3.86E-01	8	8	3.291E-02	2.048E+00	3.933E+07
	2430.097	45079.879	3.89E-01	8	6	5.826E-03	3.598E-01	9.425E+06
	2837.950	44753.799	3.82E-01	6	8	7.634E-03	3.598E-01	6.710E+06
	2837.950	45079.879	3.85E-01	6	6	2.965E-02	1.386E+00	3.528E+07
	2837.950	45289.801	3.87E-01	6	4	5.773E-03	2.686E-01	1.041E+07
	3117.461	45079.879	3.82E-01	4	6	8.560E-03	2.686E-01	6.702E+06
	3117.461	45289.801	3.84E-01	4	4	3.441E-02	1.074E+00	4.082E+07

Table 3. (continued)

Transition	E_i (cm^{-1})	E_f (cm^{-1})	EDIFF (Ryd)	g_i	g_f	f_{if}	S	a_{ji} (s^{-1})
a4Fe → z4Go	1.1677	0.6355	5.32E-01	28	36	8.807E-02	1.390E+01	1.558E+08
	1872.567	60625.449	5.35E-01	10	12	8.269E-02	4.634E+00	1.587E+08
	1872.567	60807.230	5.37E-01	10	10	5.728E-03	3.199E-01	1.327E+07
	1872.567	60956.781	5.38E-01	10	8	1.683E-04	9.378E-03	4.899E+05
	2430.097	60807.230	5.32E-01	8	10	7.838E-02	3.536E+00	1.425E+08
	2430.097	60956.781	5.33E-01	8	8	9.316E-03	4.192E-01	2.129E+07
	2430.097	61041.748	5.34E-01	8	6	2.578E-04	1.158E-02	7.876E+05
	2837.950	60956.781	5.30E-01	6	8	7.823E-02	2.659E+00	1.322E+08
	2837.950	61041.748	5.30E-01	6	6	9.427E-03	3.199E-01	2.130E+07
	3117.461	61041.748	5.28E-01	4	6	8.735E-02	1.986E+00	1.303E+08
a2Se → z2Po	0.8505	0.5990	2.51E-01	2	6	1.317E-02	3.141E-01	2.229E+06
	37227.326	64834.073	2.52E-01	2	4	8.780E-03	2.094E-01	2.232E+06
	37227.326	64806.487	2.51E-01	2	2	4.386E-03	1.047E-01	2.225E+06
a2Se → y2Po	0.8505	0.5228	3.28E-01	2	6	1.123E-01	2.056E+00	3.229E+07
	37227.326	73189.110	3.28E-01	2	4	7.486E-02	1.371E+00	3.229E+07
	37227.326	73187.280	3.28E-01	2	2	3.743E-02	6.853E-01	3.228E+07
a2Pe → z2So	1.0208	0.5860	4.35E-01	6	2	1.706E-01	7.063E+00	7.772E+08
	18360.646	66248.660	4.36E-01	4	2	1.712E-01	4.709E+00	5.239E+08
	18886.780	66248.660	4.32E-01	2	2	1.694E-01	2.354E+00	2.534E+08
a2Pe → z2Do	1.0208	0.6292	3.92E-01	6	10	3.666E-01	1.685E+01	2.709E+08
	18360.646	61093.413	3.89E-01	4	6	3.282E-01	1.011E+01	2.665E+08
	18360.646	62125.600	3.99E-01	4	4	3.734E-02	1.124E+00	4.771E+07
	18886.780	62125.600	3.94E-01	2	4	3.689E-01	5.618E+00	2.300E+08
a2De → z2Po	0.9999	0.5990	4.01E-01	10	6	4.079E-02	3.052E+00	8.775E+07
	20516.960	64834.073	4.04E-01	6	4	4.109E-02	1.831E+00	8.074E+07
	21308.040	64834.073	3.97E-01	4	4	6.726E-03	2.035E-01	8.500E+06
	21308.040	64806.487	3.96E-01	4	2	3.361E-02	1.017E+00	8.483E+07
a2De → z2Do	0.9999	0.6292	3.71E-01	10	10	2.059E-03	1.667E-01	2.272E+06
	20516.960	61093.413	3.70E-01	6	6	1.917E-03	9.333E-02	2.106E+06
	20516.960	62125.600	3.79E-01	6	4	1.404E-04	6.667E-03	2.433E+05
	21308.040	61093.413	3.63E-01	4	6	2.014E-04	6.667E-03	1.418E+05
	21308.040	62125.600	3.72E-01	4	4	1.860E-03	6.000E-02	2.067E+06
a2De → z2Fo	0.9999	0.6033	3.97E-01	10	14	2.723E-02	2.060E+00	2.456E+07
	20516.960	64286.345	3.99E-01	6	8	2.608E-02	1.177E+00	2.500E+07
	20516.960	64425.408	4.00E-01	6	6	1.308E-03	5.886E-02	1.683E+06
	21308.040	64425.408	3.93E-01	4	6	2.698E-02	8.240E-01	2.230E+07

and the lifetime of state f can now be obtained as

$$\tau_f = 1/A_f\,. \qquad (12)$$

Conservation of the total LS multiplet strength, S_{LS}, with the sum of fine structure components, Eq. (5), is checked for each LS transition if splitting is carried out through line strength, Eq. (4), and the discrepancy is found to be usually less than 0.01%. Conservation of the total LS multiplet oscillator strength is checked with the sum of fine structure components, Eq. (8), if splitting is carried out through oscillator strength, Eq. (7), to ensure that there is no discrepancy beween the two values.

The radiative calculations for Fe II for the OP were carried out (NP, 1994) in the close coupling (CC) approximation employing the R-matrix method using a 83 state expansion for the target. The calculations resulted in 743 bound states below the ionization threshold and over 19 000 oscillator strengths in LS multiplet among these states. Present calculations correspond to processing of only 3109 transitions, a small fraction of the total number of bound - bound radiative data computed for Fe II. The major effort in the present work involved in the identification of the calculated states, correlating them with the observed energies, and sorting out the corresponding f-values from a large number of transitions obtained from the close coupling calculations. The calculated energies are not necessarily in the same sequence, because of unobserved levels in between, and are not in the same order as the observed set of LS terms. Being a complex system of 25 electrons with considerable correlations effects, Fe II gives rise to many energy levels that are closely spaced. Identification of these states required consistency checks of the effective quantum numbers of the Rydberg series of states belonging to the Fe III core states and percentage contributions of the contributing channels (NP 1994). A code ELEVID is developed specifically for the identification of states. The code also processes the data for calculated energies and oscillator strengths (that is stored encoded in separate files), and to correlate and sort out the transitions of interest.

The fine structure splitting is carried out from the calculated f-values obtained in the length form only. As explained in the earlier work (Nahar 1993), in the R-matrix calculations the wave functions in the asymptotic region are better represented than in the inner region, and the dipole matrix elements in the length form are weighted more towards the asymptotic region and therefore more accurate than the velocity form. The LS multiplet f-values and A-values presented in this work correspond to observed LS term energies, obtained through statistical average over the fine structure energies.

Some explanation is necessary for transitions between terms having incomplete sets of observed fine structure levels. The measured energies (Johansson 1992) correspond to a large number of levels, 769 in total belonging to 265 LS terms. Not all the LS terms have complete set of observed fine structure levels. Another code JJTOLS carries out a check for completeness of the set of observed fine structure levels which in general is not specified in the observed energy Table (JJTOLS also computes the oscillator strengths and other quantities). For all transitions up to angular momenta $\boldsymbol{H} \leftrightarrow \boldsymbol{I}$, the transition energy between one or both unobserved levels is obtained from the values of f_{JJ}, Eq. (7), and S_{JJ}, Eq. (4), to calculate the transition probability, and for transitions beyond $\boldsymbol{H} \leftrightarrow \boldsymbol{I}$, the transition energy is approximated to ΔE_{LS} for unobserved levels.

3. Results and discussion

As the main aim of the present work is to make available an extensive amount of data for transition probabilities in Fe II, it is necessary to also assess the uncertainties in the theoretical calculations as compared with other reliable measurements and theoretical calculations. Detailed checks and comparison of the f-values obtained from the close coupling calculations are carried out in the earlier work (NP 1994) and it is found that, on the whole, present values are in better agreement with the experimental values in the NIST compilation (Fuhr et al. 1988) than those by Kurucz (1981).

The other check for the f-values is carried out through a comparison with the lifetimes of the atomic levels, τ, which can be measured usually with higher precision than the transition probabilities. The computed lifetimes were compared earlier (NP 1994) with the available experimental data; however, since the work was not complete, some of the contributing A-values from higher levels were not included in the calculated lifetimes. Table 1 presents the revised lifetime values with more contributing levels of Fe II obtained using the additional transition probabilites from the present work, and compares these with the experimental ones (Guo et al. 1992; Hannaford et al. 1992; Schade et al. 1988; Biemont et al. 1991), and with those calculated by Kurucz. Present lifetimes are obtained from allowed transitions only, whereas the Kurucz values consider forbidden transitions as well (though the contribution is small). It can be seen from the Table that the present calculated lifetimes for all the levels agree better with the measured values than the Kurucz data. As the lifetime of a given level involves contributions from several transitions, the good agreement with experiment indicates an improved accuracy in comparison with the earlier works.

It is necessary to designate the multiplet energies in order to tabulate the results. Table 2 presents the observed Fe II LS terms in symmetry order, with even parity terms followed by the odd parity terms and the energies obtained from statistical averaging over the fine structure levels. The degeneracy symbol for each term does not necessarily match the observed one. The notation for degeneracy, in alphabetical order for the even terms and anti-alphabetical order for the odd terms, of the same symmetry is chosen for convenience of identification, and is used throughout for specification of transitions. An asterisk next to the energy of a LS term corresponds to an incomplete set of observed fine structure levels for that term.

Table 3 presents a small sample, taken from the complete table, of the computed f-, S- and A-values for transitions between the lowest few terms of total angular momenta belonging to the four spin symmetries, octet, sextet, quartet and doublet.

The first line of each transition in Table 3 corresponds to LS multiplet f-, S- and A-values, followed by the individual fine structure components. As mentioned earlier, observed energies are used for calculations of the f- and A-values; in the case of unobserved fine structure levels, calculated energies are used. On the first line, the energies of the LS terms are expressed in Rydberg units whereas the level energies are expressed in cm^{-1} units. The transition energy between the levels is given in Rydberg units. The g_i and g_f are the statistical weight factors of the initial and final levels respectively. There are a few transitions in the complete Table for which no f- and A-values are obtained. These correspond to transitions between two closely spaced LS terms where the initial term has a lower energy but a few of its fine structure levels lie high above the dipole allowed levels of the higher term. In addition to the transition probabilities, the Table contains all the LS terms considered with explicit configurations and energies. It also contains a FORTRAN program that can read the transition probabilities and calculate the lifetime of a LS term or a fine structure level.

4. Conclusion

The oscillator strengths, line strengths, and transition probabilites for transitions among dipole allowed fine structure levels of Fe II are obtained as a part of the Iron Project. These values provide an extensive dataset for astrophysical applications involving the analysis of Fe II spectra. A comparison with available experimental values shows better agreement than currently available data. The present transition probabilities are now being utilized in astrophysical models for spectral intensities of Fe II lines.

The radiative work reported herein required about 500 CPU hours on the Cray Y-MP in Columbus, Ohio. Considering the complexity of the work, it is estimated that the relativistic Breit-Pauli calculations with full intermediate coupling would require several times the CPU time and memory used in the present computations.

The complete Table of 3109 LS multiplets and 21 589 fine structure transitions may be obtained electronically via e-mail from nahar@payne.mps.ohio-state.edu.

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