

## Atomic data from the Iron Project

### LIX. New radiative transition probabilities for Fe IV including fine structure<sup>\*</sup>

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**Abstract.** We present new calculations for transition probabilities of Fe IV, with much more extensive datasets than heretofore available, for a variety of astrophysical applications. The large-scale close coupling  $R$ -matrix calculations yield 1,798 LS bound states with  $n \leq 11$  and  $l \leq 9$ , and corresponding 138 121 dipole allowed transitions in the form of oscillator strengths  $f$ , line strengths  $S$ , and  $A$ -coefficients. This represents the largest  $R$ -matrix dataset in LS coupling for any ion under either the Opacity Project or the Iron Project. Through algebraic transformation of the LS multiplets, a total of 712 120 dipole allowed fine structure transitions for Fe IV are obtained. Observed transition energies, whenever available, are used together with the energy independent line strengths to derive the  $f$ - and the  $A$ -values for improved accuracy; the adopted algorithm used calculated energies for the remainder. Present results show significantly better accuracy for the important low-lying states than previous calculations. Monochromatic and mean opacities for Fe IV are computed and compared with those obtained using the Opacity Project data. We find differences which could have important consequences for several astrophysical applications involving low ionization stages of iron.

**Key words.** atomic processes – line: formation – radiation mechanisms: thermal – radiative transfer – ISM: HII regions – radio lines: galaxies

#### 1. Introduction

It is well known that low ionization stage of iron are of great interest for astrophysical spectroscopy and models of stellar atmospheres (Hubeny et al. 2003), novae (McKenna et al. 1997), photoionized H II regions (Dopita & Sutherland 2003; Rubin et al. 1997), and active galactic nuclei (Sigut & Pradhan 2003; Sigut et al. 2004). The ion Fe IV is of particular interest since its ionization potential is  $\sim 54.8$  eV, nearly equal that of He II at 54.4 eV. Thus, for example, in a photoionized H II region such as the great diffuse nebula in Orion, stellar ionizing flux is effectively shielded by helium to prevent extensive ionization of Fe ions beyond Fe IV. Whereas hot central stars of high-excitation planetary nebulae may well ionize beyond Fe IV (e.g. Hyung & Aller 1998), ordinary main sequence O, B stars have a 54 eV “cut-off” that attenuates the ionizing flux. Another example is the anomalous Fe II emission from active galactic nuclei. Non-local-Thermodynamic-Equilibrium (NLTE) spectral models need to consider the first four ionization stages, Fe I–IV, with Fe IV as the dominant stage in the fully ionized zone (e.g. Sigut et al. 2004, and

references therein). In previous studies at Ohio State under the Iron Project, we have reported a large amount of radiative and collisional data for the ionization stages Fe I–VI, including fine structure transition probabilities for Fe II and Fe III (references at: [www.astronomy.ohio-state.edu/~pradhan](http://www.astronomy.ohio-state.edu/~pradhan)). The aim of this paper is to report similarly new calculations with improved accuracy for Fe IV including fine structure that is often required for spectral diagnostics and modeling.

However, study of Fe IV is difficult and complexities arise due to its electronic structure with 5 electrons in the half-filled open 3d shell (ground configuration  $1s^2 2s^2 2p^6 3s^2 3p^6 3d^5$ ); electron correlation effects for the many excited states are difficult to represent. Prior to the Opacity Project (OP, 1995, 1996), investigations on radiative processes for Fe IV were carried out through atomic structure calculations. These include radiative decay rates for forbidden transitions by Garstang (1958), which are available from the evaluated compilation by the National Institute for Standards and Technology (NIST: [www.nist.gov](http://www.nist.gov)) and Froese-Fischer & Rubin (2004). Fawcett (1989) has computed the data for many allowed transitions using a semi-empirical method due to Cowan. The energy level data in the NIST compilation is from Ekberg & Edlen (1978).

Ab initio calculations in the close coupling approximation using  $R$ -matrix method for the radiative processes of Fe IV

<sup>\*</sup> Complete electronic data tables of energies and transition probabilities (Tables 3, 4 and 6) are available at the CDS via anonymous ftp to [cdsarc.u-strasbg.fr](http://cdsarc.u-strasbg.fr) (130.79.128.5) or via <http://cdsweb.u-strasbg.fr/cgi-bin/qcat?J/A+A/437/345>

were carried out by Sawey & Berrington (1992) under the Opacity Project (OP, 1995, 1996), and later by Bautista & Pradhan (1997) under the Iron Project (IP, Hummer et al. 1993). Further  $R$ -matrix calculations were reported for the total and state-specific electron-ion recombination rate coefficients using the unified treatment by Nahar et al. (1998). Sawey & Berrington (1992) produced radiative data for photoionization and oscillator strengths for three symmetries: sextets, quartets and doublets; these data are accessible through the OP database, TOPbase (Cunto et al. 1993). Sawey & Berrington employed a very restricted eigenfunction basis sets in their calculations for Fe I–IV, and later works have shown their results for Fe I, II, and III, to be deficient in accuracy and extent (Le Dourneuf et al. 1993; Bautista & Pradhan 1995; Nahar & Pradhan 1994; Nahar 1996; Nahar & Pradhan 1996). Whereas little experimental data on oscillator strengths for these Fe ions are available, the photoionization cross sections computed by Sawey & Berrington almost entirely omitted resonances, which are a prominent effect included in most other OP calculations, owing to their limited wavefunction expansion. For example, for Fe II their effective photoionization cross sections are more than an order of magnitude smaller than those computed later by LeDourneuf et al. (1993) and Nahar & Pradhan (1994); similar discrepancies exists for Fe I and Fe III. The later work of Bautista & Pradhan (1997) took more accurate account of electron-electron correlation effects, showing important resonant features in cross sections missing in the study by Sawey & Berrington (1992). However, owing to computational constraints, Bautista & Pradhan (1997) entirely omitted the doublet symmetry which has the maximum number of bound states. All previous  $R$ -matrix results are in LS coupling that considers the dipole allowed  $LS$  multiplets; no fine structure splitting is taken into account.

The primary motivations for the present study are: (i) the accuracy and completeness of previous calculations for Fe IV are insufficient and/or uncertain; and (ii) fine structure data are needed for many astrophysical applications. Present work reports a more complete set of oscillator strengths and radiative decay rates of Fe IV for both the LS multiplets and allowed fine structure transitions. Similar results on LS multiplets and fine structure transitions were presented earlier for Fe II (Nahar 1994), Fe III (Nahar & Pradhan 1996) in the IP series of publication, and elsewhere for other ions. Present calculations consider correlation effects accurately, as in Bautista & Pradhan (1997), and bound states of all symmetries, sextets, quartets, and doublets. At the present time it is computationally prohibitive to carry out the full Breit-Pauli  $R$ -matrix calculations for fine structure transition probabilities including relativistic effects in an ab initio manner. Among the low ionization stages or iron, Fe I–V, there has been only one such previous effort, for Fe V (Nahar & Pradhan 2000; Nahar et al. 2000). While efforts are under way to resolve the computationally challenging problems in relativistic calculations, which are about an order of magnitude more intensive, there is considerable need for fine structure data. We employ an algebraic recoupling algorithm to obtain the fine structure transition probabilities for Fe IV, using observed energies where available, as in previous IP works on Fe II and Fe III.

Finally, we employ the new radiative dataset to compute monochromatic and mean opacities for Fe IV, both as a test and comparison with the earlier OP work, as well as to investigate possible effect on the astrophysically important problem of iron opacities.

## 2. Theory

The  $R$ -matrix method in close coupling approximation as applied to the OP and IP work enables the consideration of many excited bound states and transitions, typically for all states with  $n \leq 10$ . The methodology for the radiative transitions is discussed in the OP papers by Seaton (1987) and Berrington et al. (1987). General details of the procedures employed for obtaining oscillator strengths ( $f$ ) and radiative decay rates ( $A$ ) for dipole allowed fine structure transitions ( $\Delta J = 0, \pm 1$  with  $\Delta S = 0$ , even parity  $\leftrightarrow$  odd parity) by algebraic transformation of LS multiplets have been described in earlier papers, such as for Fe II (Nahar 1993).

The wavefunction  $\Psi(E)$  for the  $(N+1)$  electron system with total spin and orbital angular momenta symmetry  $SL\pi$  or total angular momentum symmetry  $J\pi$  is expanded in terms of “frozen”  $N$ -electron target (the core) ion functions  $\chi_i$  and vector coupled interacting electron function  $\theta_i$  as

$$\Psi_E(\text{e} + \text{ion}) = \mathcal{A} \sum_i \chi_i(\text{ion})\theta_i + \sum_j c_j \Phi_j(\text{e} + \text{ion}), \quad (1)$$

where the target is in some specific state  $S_i L_i \pi_i$  or level  $J_i \pi_i$ , index  $i$  marking channels  $S_i L_i (J_i) \pi_i$   $k_i^2 \ell_i (S L \pi$  or  $J \pi)$  with energy  $k_i^2$  of the colliding electron described by  $\theta$ .  $\mathcal{A}$  is the anti-symmetrization operator. The second sum expands correlation functions  $\Phi_j$  as products with  $N+1$  bound orbital functions 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  $SL\pi$ .  $c_j$ 's are variational coefficients.

$R$ -matrix solutions of coupled equations to total symmetries  $LS$  states for  $(N+1)$ -electron system,

$$H_{N+1} \Psi = E \Psi, \quad (2)$$

are discrete bound states  $\Psi_B$  for  $E < 0$ . Seaton (1985) describes the matching procedure for inner region and outer region wavefunctions at the  $R$ -matrix boundary which enables calculations of all required energy levels of the Hamiltonian matrix.

For a bound-bound transition from an initial state  $i$  to a final state  $j$ , the line strength ( $S$ ) is defined as

$$S = |\langle \Psi_j || \mathbf{D} || \Psi_i \rangle|^2, \quad (3)$$

in atomic units (au), where the dipole operator  $\mathbf{D}$  is

$$\mathbf{D} = \sum_n \mathbf{r}_n, \quad (4)$$

in the length form, summed over the total number of electrons in the ion, and  $\Psi_i$  and  $\Psi_j$  are the initial and the final

wavefunctions respectively. The oscillator strength  $f_{ij}$  ( $f$ -value) can be obtained from line strength  $S$  in atomic units as

$$f_{ij} = \frac{E_{ij}}{3g_i} S(i, j) \quad (5)$$

and to radiative decay rate or transition probability as

$$A_{ji} = 8.032 \times 10^9 \frac{E_{ij}^3}{3g_i} S(i, j) s^{-1} \quad (6)$$

where  $E_{ij} = E_i - E_j$  is the transition energy in rydbergs and  $g_i$  is the statistical weight factor of the initial state, with  $g_i = (2S_i + 1)(2L_i + 1)$  for a LS multiplet, and  $(2J_i + 1)$  for a fine-structure transition. The radiative transition probability,  $A_{ji}$  (Einstein's A-coefficient or the radiative decay rate), related to the oscillator strength as

$$A_{ji}(\text{au}) = \frac{1}{2} \alpha^3 \frac{g_i}{g_j} E_{ij}^2 f_{ij}, \quad A_{ji}(s^{-1}) = \frac{A_{ji}(\text{au})}{\tau_0}, \quad (7)$$

where  $\alpha$  is the fine-structure constant and  $\tau_0 = 2.4191 \times 10^{-17}$  s is the atomic unit of time.

The fine-structure components of a LS multiplet can be obtained through algebraic transformations of either line strength or directly from the oscillator strength (e.g. Nahar 1995). The line strength, which is independent of the transition energy  $E_{ij}$ , is a better choice. As the observed transition energies are determined more accurately than the calculated ones, use of the former with the line strengths can provide more accurate  $f_{ij}$  and  $A_{ji}$ . Hence, present fine-structure components are obtained from  $S$  values whenever observed energies are available, and from  $f$ -values when calculated  $E_{ij}$  are used.

The fine-structure line strengths,  $S_{JJ}$ , are obtained as

$$S_{JJ} = C(J_i, J_j) S_{LS} / [(2S_i + 1)(2L_i + 1)(2L_j + 1)], \quad (8)$$

for the allowed transitions ( $\Delta J = 0, \pm 1$ ).  $S_j$  is the spin which is the same as  $S_i$ . The values of the coefficients  $C(J_i, J_j)$  can be found in Allen (1976). The  $S_{JJ}$  values satisfy the condition

$$S_{LS} = \sum_J S_{JJ}. \quad (9)$$

The fine-structure  $f$ -values,  $f_{JJ}$ , can be obtained directly from  $f_{LS}$  as (Seaton et al. 1994):

$$f_{JJ}(n_j S_i L_j J_j, n_i S_i L_i J_i) = f_{LS}(n_j S_i L_j, n_i S_i L_i) (2J_j + 1)(2L_i + 1) \times W^2(L_j L_i J_j J_i; 1 S_i), \quad (10)$$

where  $W(L_j L_i J_j J_i; 1 S_i)$  is a Racah coefficient. The above components also satisfy the sum rule

$$\sum_{J_i J_j} (2J_i + 1) f_{JJ}(n_j S_i L_j J_j, n_i S_i L_i J_i) = f_{LS}(n_j S_i L_j, n_i S_i L_i) \times (2S_i + 1)(2L_i + 1). \quad (11)$$

The above form for fine structure components is used when one or both  $LS$  terms of the transition are unobserved, or not all the fine structure levels of an  $LS$  term are observed, and for transitions between high angular momentum states (higher than  $H \leftrightarrow I$ ) for which Allen's coefficients are not available.

The lifetime of a level can be computed as

$$\tau = \frac{1}{\sum_i A_{ki}} \quad (12)$$

where the sum is the total radiative transition probability for level  $k$ .

The opacity is a measure of radiation transport through matter. The monochromatic opacity is a function of the photon frequency and depends mainly on the detailed atomic data: bound-bound oscillator strengths and bound-free photoionization cross sections. The quantity of practical interest in stellar models is the Rosseland mean opacity,  $\kappa_R(T, \rho)$ , defined as (Seaton et al. 1994)

$$\frac{1}{\kappa_R} = \int_0^\infty \frac{1}{\kappa_\nu} g(u) du, \quad g(u) = \frac{15}{4\pi^4} u^4 e^{-u} (1 - e^{-u})^{-2}, \quad (13)$$

where  $g(u)$  is the Planck weighting function and  $u = h\nu/kT$ . Monochromatic opacities  $\kappa_\nu$  depends primarily on oscillator strengths as

$$\kappa_\nu(i \rightarrow j) = \frac{\pi e^2}{mc} N_i f(ij) \phi_\nu \quad (14)$$

where  $N_i$  is ion density in state  $i$ ,  $\phi_\nu$  is a profile factor, and on photoionization cross sections ( $\sigma_{PI}$ ) as

$$\kappa_\nu = N_i \sigma_{PI}(\nu). \quad (15)$$

We compute the monochromatic and the mean opacities as a measure of the differences between the present dataset for the bound-bound transitions and the earlier OP data for Fe IV.

### 3. Computations

The  $R$ -matrix computations for Fe IV are carried out using a wavefunction expansion of 16 terms of target Fe V belonging to the ground configuration,  $3d^4$ , as given in Table 1; the energies used are the measured values available from the NIST compilation at [www.nist.gov](http://www.nist.gov). The orbital wavefunctions of the target were obtained from atomic structure calculations using SUPERSTRUCTURE (Eissner et al. 1974), as in the earlier works of Bautista & Pradhan (1997) and Nahar et al. (1998). The present wavefunction expansion is similar, but smaller than the previous 31 term expansion of Bautista & Pradhan (1997). However, it includes singlet target terms, which were omitted by Bautista and Pradhan, enabling the computation of the large number of  $(N + 1)$ -electron doublet symmetries.

In addition to the target expansion in Table 1, it is necessary to ensure an accurate representation of short range correlation effects that are vital for the bound  $(N + 1)$ -electron states. The second term of the wavefunction expansion, Eq. (1), consists of 61 such "bound channel" correlation functions of Fe IV, as described by Bautista & Pradhan (1997).

The  $R$ -matrix calculations span several stages of computations (Berrington et al. 1987, 1995). The computations were extensive in terms of CPU memory size and time requirement. Hence, they were carried out one or a few symmetries of  $S L \pi$  at a time. The one-electron orbital functions optimised through a configuration-interaction type calculation for

**Table 1.** Target terms and relative energies (in Ry) of Fe V in the wavefunction expansion of Fe IV.

	Term		$E_0/\text{Ry}$
1	3d <sup>4</sup>	<sup>5</sup> D	0.000000
2	3d <sup>4</sup>	<sup>3</sup> H	0.230232
3	3d <sup>4</sup>	<sup>3</sup> P	0.234211
4	3d <sup>4</sup>	<sup>3</sup> F	0.244942
5	3d <sup>4</sup>	<sup>3</sup> G	0.274991
6	3d <sup>4</sup>	<sup>1</sup> G	0.333399
7	3d <sup>4</sup>	<sup>3</sup> D	0.334726
8	3d <sup>4</sup>	<sup>1</sup> I	0.341832
9	3d <sup>4</sup>	<sup>1</sup> S	0.361166
10	3d <sup>4</sup>	<sup>1</sup> D	0.421837
11	3d <sup>4</sup>	<sup>1</sup> F	0.480536
12	3d <sup>4</sup>	<sup>3</sup> F	0.567719
13	3d <sup>4</sup>	<sup>3</sup> P	0.568463
14	3d <sup>4</sup>	<sup>1</sup> G	0.649554
15	3d <sup>4</sup>	<sup>1</sup> D	0.855063
16	3d <sup>4</sup>	<sup>1</sup> S	1.103820

Fe V using SUPERSTRUCTURE are the input to STG1 of the *R*-matrix codes to compute Slater integrals. Radial integrals for the partial wave expansion in Eq. (1) are specified for orbitals  $0 \leq \ell \leq 9$  as a basis of NRANG2 = 12 “continuum” functions – sufficient for bound electrons with  $n < 11$  at a radius of the *R*-matrix box. Computations are carried out for bound symmetries with  $0 \leq L \leq 9$  (both parities) and spin multiplicities,  $2S + 1 = 2, 4, 6$ .

The bound energy eigenvalues are obtained from computer program STGB. All bound states of the Hamiltonian matrix are scanned for up to  $n = 11$  and  $l = 9$  with a fine effective quantum number mesh of  $\Delta\nu = 0.001$ . However, due to the computational complexities stemming from the numerous bound states obtained, the code was unable to generate the standard *R*-matrix energy files. A complementary computer code, PLSRAD, was written to sort out the energies directly from the eigenvalues of the Hamiltonian matrix.

Furthermore, identification of the large number of *LS* bound states was a formidable task for this ion. With the exception of equivalent-electron states, the energies can be identified through quantum defect analysis of Rydberg series:

$$E = E_t - z^2/\nu^2, \quad \nu = n - \mu_l(t) \quad (16)$$

with series limits  $E_t$  at the 16 Fe V “target” (t) states of Table 1, and the weighted percentage contributions of interacting closed channels. An *LS* term is designated according to a possible combination of the configuration of the core and the outer electron, and assigned an appropriate value of  $\nu$  for the outer electron quantum numbers  $n, l$  associated with the maximum channel percentage contribution. A Rydberg series is identified by sorting out the  $\nu$  for terms of same configuration but with increasing  $n$  of the valence electron by unity. Code ELEVID (e.g. Nahar 1995) was used for this analysis. However, uncertainties in assignments of proper configurations are introduced for cases with small differences in  $\nu$  for various terms of the same symmetry, as the quantum defects for these states are almost

the same. There is also some uncertainty in the identification of the adjacent higher or lower terms for such cases.

The code STGBB is used to compute radiative data for the bound-bound transitions; the code exploits methods developed by Seaton (1986) to evaluate the outer region ( $>RA$ ) contributions to the radiative transition matrix elements.

The *f*-, *S*-, and *A*-values for the fine structure transitions are obtained through algebraic transformations of the *LS* multiplet line strengths. Spectroscopically observed transition energies are used whenever available. When the observed energies are not found, the calculated *LS* multiplet energy is used for the fine structure components. The splitting of *LS f*-values is carried out as described above using the code JJTOLS (Nahar 1995).

Using the new bound-bound radiative dataset, but retaining the earlier OP bound-free data (the contribution of bound-free is much smaller), we calculate the monochromatic and Rosseland mean and Planck mean opacities as described by Seaton et al. (1994). Results are compared with those computed using the OP data calculated by Sawey & Berrington (1992).

## 4. Results and discussion

In the subsections below we describe the results for the bound state energies of *LS* terms, *LS* multiplets for dipole allowed transitions, fine structure radiative transitions for Fe IV, and the effect of the new data on opacities. We may note that this entails the calculation and identification of the largest number of *LS* bound terms (1798) computed for any ion under the Opacity or the Iron Projects thus far.

### 4.1. Energy levels

A total of 1798 bound states of Fe IV of sextet, quartet and doublet symmetries with  $n \leq \sim 11$ ,  $l \leq 9$ ,  $0 \leq L \leq 9$ , and both even and odd parities, and spin multiplicities  $2S + 1 = 2, 4, 6$  are obtained. Sawey & Berrington (1992) obtained 1721 bound states, All present energy levels have been identified and a correspondence is established with the observed energies where available.

In Table 2, present bound state energies are compared with the measured values (Ekberg & Edlen 1978, available from the NIST database compiled by Sugar & Corliss 1985), and previously calculated energies from theoretical ab initio calculations by Sawey & Berrington (1992) and by Bautista & Pradhan (1997). Present ground state energy differs from the observed value by 1%, similar to that by Bautista & Pradhan (1997), but improved over that by Sawey & Berrington (1992). The first 44 low-lying energy states of the present dataset agree to less than 5% with the measured values, much improved over those calculated by Sawey & Berrington. All even parity states show consistent improved energies than those by Sawey & Berrington. Present energies are slightly better than or comparable to those by Bautista & Pradhan (1997) for the sextets and quartets (they omitted doublets). However, the higher odd parity states in the present set show larger differences with the measured energies, the highest one being about 18% for the state  $3d^4(^1D)4p(^2D^\circ)$ . A reason for such larger uncertainty for

**Table 2.** Comparison of the present Fe IV energies  $E_c$  with the observed binding energies,  $E_o$ , and earlier computed energies,  $E_{BP}$  of Bautista & Pradhan (1997) and  $E_{SB}$  of Sawey & Berrington (1992). An \* next to a state indicates an incomplete set of observed fine structure levels.

Config.	$SL\pi$	$E_o$ (Ry)	$E_c$ (Ry)	$E_{BP}$ (Ry)	$E_{SB}$ (Ry)
3d <sup>5</sup>	<sup>6</sup> S	4.020000	3.978	3.984	3.96069
3d <sup>5</sup>	<sup>4</sup> G	3.725831	3.658	3.665	3.64011
3d <sup>5</sup>	<sup>4</sup> P	3.698270	3.652	3.660	3.58549
3d <sup>5</sup>	<sup>4</sup> D	3.665794	3.607	3.613	3.56341
3d <sup>5</sup>	<sup>2</sup> I	3.590930	3.502		3.50204
3d <sup>5</sup>	<sup>3</sup> 2D	3.566686	3.509		3.43429
3d <sup>5</sup>	<sup>2</sup> 2F	3.548645	3.494		3.42470
3d <sup>5</sup>	<sup>4</sup> F	3.539584	3.478	3.485	3.42632
3d <sup>5</sup>	<sup>2</sup> H	3.507616	3.434		3.39455
3d <sup>5</sup>	<sup>2</sup> 2G	3.495274	3.421		3.38135
3d <sup>5</sup>	<sup>1</sup> 2F	3.462191	3.392		3.33754
3d <sup>5</sup>	<sup>2</sup> S	3.412002	3.348		3.27170
3d <sup>5</sup>	<sup>2</sup> 2D	3.344582	3.282		3.19871
3d <sup>5</sup>	<sup>1</sup> 2G	3.264596	3.186		3.12545
3d <sup>5</sup>	<sup>2</sup> P	3.107633	3.034		2.94101
3d <sup>5</sup>	<sup>1</sup> 2D	3.033568	2.965		2.85699
3d <sup>4</sup> ( <sup>5</sup> D)4s	<sup>6</sup> D	2.849206	2.872	2.941	2.77361
3d <sup>4</sup> ( <sup>5</sup> D)4s	<sup>4</sup> D	2.758817	2.778	2.795	2.68538
3d <sup>4</sup> ( <sup>3</sup> P2)4s	<sup>4</sup> P	2.607793	2.619	2.648	2.53137
3d <sup>4</sup> ( <sup>3</sup> H)4s	<sup>4</sup> H	2.612277	2.588	2.618	2.53129
3d <sup>4</sup> ( <sup>3</sup> F2)4s	<sup>4</sup> F	2.597263	2.592	2.613	2.51606
3d <sup>4</sup> ( <sup>3</sup> G)4s	<sup>4</sup> G	2.569849	2.549	2.580	2.48781
3d <sup>4</sup> ( <sup>3</sup> P2)4s	<sup>2</sup> P	2.552383	2.561		2.47727
3d <sup>4</sup> ( <sup>3</sup> H)4s	<sup>2</sup> H	2.556817	2.530		2.47708
3d <sup>4</sup> ( <sup>3</sup> F2)4s	<sup>2</sup> F	2.543005	2.536		
3d <sup>4</sup> ( <sup>3</sup> G)4s	<sup>2</sup> G	2.514627	2.492		2.43349
3d <sup>4</sup> ( <sup>3</sup> D)4s	<sup>4</sup> D	2.510927	2.494		2.42780
3d <sup>4</sup> ( <sup>1</sup> G2)4s	<sup>2</sup> G	2.491359	2.476		2.40883
3d <sup>4</sup> ( <sup>1</sup> I)4s	<sup>2</sup> I	2.484110	2.438		
3d <sup>4</sup> ( <sup>1</sup> S2)4s	<sup>2</sup> S	2.464203	2.468		
3d <sup>4</sup> ( <sup>3</sup> D)4s	<sup>2</sup> D	2.458112	2.440		2.37606
3d <sup>4</sup> ( <sup>1</sup> D2)4s	<sup>2</sup> D	2.406789	2.388		2.32291
3d <sup>4</sup> ( <sup>1</sup> F)4s	<sup>2</sup> F	2.350906	2.311		
3d <sup>4</sup> ( <sup>5</sup> D)4p	<sup>6</sup> F <sup>o</sup>	2.295457	2.219		2.25564
3d <sup>4</sup> ( <sup>5</sup> D)4p	<sup>6</sup> P <sup>o</sup>	2.287886	2.213		2.24990
3d <sup>4</sup> ( <sup>3</sup> P1)4s	<sup>4</sup> P	2.284212	2.246		2.19440
3d <sup>4</sup> ( <sup>3</sup> F1)4s	<sup>4</sup> F	2.285076	2.239		2.19842
3d <sup>4</sup> ( <sup>3</sup> D)4p	<sup>4</sup> P <sup>o</sup>	2.265726	2.183		2.22408
3d <sup>4</sup> ( <sup>5</sup> D)4p	<sup>6</sup> D <sup>o</sup>	2.258256	2.174		
3d <sup>4</sup> ( <sup>3</sup> P1)4s	<sup>2</sup> P	2.232085	2.194		2.14451
3d <sup>4</sup> ( <sup>3</sup> F1)4s	<sup>2</sup> F	2.232375	2.186		2.14682
3d <sup>4</sup> ( <sup>3</sup> D)4p	<sup>4</sup> F <sup>o</sup>	2.228839	2.142		2.18918
3d <sup>4</sup> ( <sup>1</sup> G1)4s	<sup>2</sup> G	2.186593	2.125		2.09903
3d <sup>4</sup> ( <sup>5</sup> D)4p	<sup>4</sup> D <sup>o</sup>	2.176046	2.080		2.13458
3d <sup>4</sup> ( <sup>3</sup> H)4p	<sup>4</sup> H <sup>o</sup>	2.081972	1.977		2.03477
3d <sup>4</sup> ( <sup>3</sup> P2)4p	<sup>4</sup> D <sup>o</sup>	2.066669	1.945		2.02440
3d <sup>4</sup> ( <sup>3</sup> F2)4p	<sup>4</sup> G <sup>o</sup>	2.056962	1.940		2.00840
3d <sup>4</sup> ( <sup>3</sup> H)4p	<sup>4</sup> I <sup>o</sup>	2.050188	1.943		2.00550
3d <sup>4</sup> ( <sup>3</sup> P2)4p	<sup>4</sup> P <sup>o</sup>	2.039526	1.911		1.99660
3d <sup>4</sup> ( <sup>3</sup> H)4p	<sup>2</sup> G <sup>o</sup>	2.049047	1.937		
3d <sup>4</sup> ( <sup>3</sup> F2)4p	<sup>4</sup> F <sup>o*</sup>	2.030249	1.907		1.98676
3d <sup>4</sup> ( <sup>3</sup> H)4p	<sup>4</sup> G <sup>o</sup>	2.031609	1.915		1.98801
3d <sup>4</sup> ( <sup>3</sup> F2)4p	<sup>2</sup> D <sup>o*</sup>	2.025500	1.899		
3d <sup>4</sup> ( <sup>3</sup> P2)4p	<sup>2</sup> P <sup>o</sup>	2.015051	1.889		
3d <sup>4</sup> ( <sup>3</sup> H)4p	<sup>2</sup> I <sup>o</sup>	2.018812	1.905		
3d <sup>4</sup> ( <sup>3</sup> F2)4p	<sup>4</sup> D <sup>o</sup>	2.017690	1.887		1.96967

**Table 3.** Sample of energies in the complete table of energies.

Config.	$SL\pi$	$E$ (Ry)
3d <sup>5</sup>	$a^6S$	-4.02000
3d <sup>4</sup> ( <sup>5</sup> D)4d	$b^6S$	-1.39828
3d <sup>4</sup> ( <sup>5</sup> D)5d	$c^6S$	-0.81636
3d <sup>4</sup> ( <sup>5</sup> D)6d	$d^6S$	-0.54091
3d <sup>4</sup> ( <sup>5</sup> D)7d	$e^6S$	-0.38568
3d <sup>4</sup> ( <sup>5</sup> D)8d	$f^6S$	-0.28891
3d <sup>4</sup> ( <sup>5</sup> D)9d	$g^6S$	-0.22449
3d <sup>4</sup> ( <sup>5</sup> D)10d	$h^6S$	-0.17945
3d <sup>4</sup> ( <sup>5</sup> D)11d	$i^6S$	-0.14672
3d <sup>4</sup> ( <sup>5</sup> D)4d	$a^6P$	-1.55722
3d <sup>4</sup> ( <sup>5</sup> D)5d	$b^6P$	-0.87599
3d <sup>4</sup> ( <sup>5</sup> D)6d	$c^6P$	-0.57173
3d <sup>4</sup> ( <sup>5</sup> D)7d	$d^6P$	-0.40367
3d <sup>4</sup> ( <sup>5</sup> D)8d	$e^6P$	-0.30030
3d <sup>4</sup> ( <sup>5</sup> D)9d	$f^6P$	-0.23216
3d <sup>4</sup> ( <sup>5</sup> D)10d	$g^6P$	-0.18486
3d <sup>4</sup> ( <sup>5</sup> D)11d	$h^6P$	-0.15068
...	...	...

higher odd parity states could be the improper balance for inclusion of configurations which can improve the lower states considerably, but introduce some “spectral repulsion” for the higher levels of the ion. Nonetheless, present energies on average are an improvement over the previous ones. The improvement in computed energies for the low-lying states is an important factor in the calculation of opacities, as discussed later.

The 104 observed LS term energies are obtained from statistical averaging of the 269 measured fine structure energies (Ekberg & Edlen 1978, NIST). Compared to the number of observed energy levels, the present 1.798 LS states correspond to 5331 fine structure levels. With the exception of the observed energy levels, the fine structure transition energies are approximated as explained in the Computation section.

The complete table of 1798 bound state energies of Fe IV is available electronically where the energies of 104 observed states have been replaced by measured values as they are used in the transition energies for the atomic transition parameters. Each of first 52 calculated bound state of even parity and of odd parity is assigned with a letter prefix for convenience, as shown in sample Table 3 (these letters may not necessarily match those of the NIST table). For even parity states of a symmetry, an ascending alphabetic order is used, first in the lower case and then in the upper case. The opposite order is chosen for the states of an odd parity symmetry, that is, descending order of alphabet, first in the lower case and then the upper case. However states of the same symmetry lying above the first 52 states do not have any designation; they are recognized by the energies only.

#### 4.2. LS multiplets

The LS coupling oscillator strengths are used in various astrophysical applications, such as calculating plasma opacities. The LS multiplet data for oscillator strengths ( $f$ ) and coefficients of spontaneous decay ( $A$ -values) with 1798 bound states of Fe IV

**Table 4.** Sample data in LS coupling for oscillator strengths,  $f$ ,  $gf$ -values and radiative decay rates,  $A$ -values, for bound-bound transitions in Fe IV [ $Z = 26$ , number of core electrons = 22]. The first transition, [6 0 0 1 6 1 1 1], means  ${}^6S(1) \rightarrow {}^6P^{\circ}(1)$ . The energies are Rydberg and the  $A$ -values are in atomic units.

26 22									
SiLiPi(i)	->	SjLjPj(j)	Ei	Ej	fij	gf	Aji		
138121									
6 0 0 1		6 1 1 1	-4.020000	-2.287886	4.2259E-01	2.536E+00	3.395E+09		
6 0 0 1		6 1 1 2	-4.020000	-1.163950	4.8711E-02	2.923E-01	1.064E+09		
6 0 0 1		6 1 1 3	-4.020000	-1.017630	4.3453E-01	2.607E+00	1.049E+10		
6 0 0 1		6 1 1 4	-4.020000	-0.717120	1.7706E-02	1.062E-01	5.172E+08		
6 0 0 1		6 1 1 5	-4.020000	-0.650580	2.3136E-01	1.388E+00	7.032E+09		
6 0 0 1		6 1 1 6	-4.020000	-0.487200	8.8916E-03	5.335E-02	2.971E+08		
6 0 0 1		6 1 1 7	-4.020000	-0.451150	1.2883E-01	7.730E-01	4.393E+09		
6 0 0 1		6 1 1 8	-4.020000	-0.352670	5.1805E-03	3.108E-02	1.865E+08		
6 0 0 1		6 1 1 9	-4.020000	-0.331080	7.7609E-02	4.657E-01	2.828E+09		
6 0 0 1		6 1 1 10	-4.020000	-0.267150	3.3135E-03	1.988E-02	1.249E+08		
6 0 0 1		6 1 1 11	-4.020000	-0.253220	4.9970E-02	2.998E-01	1.898E+09		
6 0 0 1		6 1 1 12	-4.020000	-0.209400	2.2580E-03	1.355E-02	8.778E+07		
6 0 0 1		6 1 1 13	-4.020000	-0.199880	3.3953E-02	2.037E-01	1.327E+09		
6 0 0 1		6 1 1 14	-4.020000	-0.168560	1.6124E-03	9.675E-03	6.404E+07		
6 0 0 1		6 1 1 15	-4.020000	-0.161760	2.4110E-02	1.447E-01	9.609E+08		
6 0 0 1		6 1 1 16	-4.020000	-0.138610	1.1931E-03	7.159E-03	4.812E+07		
6 0 0 1		6 1 1 17	-4.020000	-0.133580	1.7723E-02	1.063E-01	7.167E+08		
6 1 1 1		6 0 0 2	-2.287886	-1.398280	2.1035E-01	3.786E+00	4.011E+09		
6 0 0 2		6 1 1 2	-1.398280	-1.163950	3.2583E-01	1.955E+00	4.792E+07		
6 0 0 2		6 1 1 3	-1.398280	-1.017630	1.0472E+00	6.283E+00	4.062E+08		
6 0 0 2		6 1 1 4	-1.398280	-0.717120	5.6950E-03	3.417E-02	7.075E+06		
6 0 0 2		6 1 1 5	-1.398280	-0.650580	3.3867E-03	2.032E-02	5.069E+06		
6 0 0 2		6 1 1 6	-1.398280	-0.487200	1.4603E-03	8.762E-03	3.246E+06		
6 0 0 2		6 1 1 7	-1.398280	-0.451150	1.1753E-02	7.052E-02	2.823E+07		
6 0 0 2		6 1 1 8	-1.398280	-0.352670	6.6550E-04	3.993E-03	1.948E+06		
6 0 0 2		6 1 1 9	-1.398280	-0.331080	9.9583E-03	5.975E-02	3.037E+07		
6 0 0 2		6 1 1 10	-1.398280	-0.267150	3.7717E-04	2.263E-03	1.292E+06		
6 0 0 2		6 1 1 11	-1.398280	-0.253220	7.4100E-03	4.446E-02	2.601E+07		
6 0 0 2		6 1 1 12	-1.398280	-0.209400	2.3900E-04	1.434E-03	9.045E+05		
6 0 0 2		6 1 1 13	-1.398280	-0.199880	5.4667E-03	3.280E-02	2.102E+07		
6 0 0 2		6 1 1 14	-1.398280	-0.168560	1.6250E-04	9.750E-04	6.579E+05		
6 0 0 2		6 1 1 15	-1.398280	-0.161760	4.0933E-03	2.456E-02	1.676E+07		
6 0 0 2		6 1 1 16	-1.398280	-0.138610	1.1605E-04	6.963E-04	4.930E+05		
6 0 0 2		6 1 1 17	-1.398280	-0.133580	3.1250E-03	1.875E-02	1.339E+07		

correspond to 138 121 dipole allowed transitions. The complete data table is available electronically. Since the line strength ( $S$ ) does not depend on the transition energy, for improved accuracy the present  $S$  values are used to recompute the  $f$  and  $A$ -values (Eq. (5)) using observed energies whenever available.

Table 4 presents a sample set of the complete electronic file of LS multiplets. The first line of the table provides the ion information, [ $Z = 26$ , number of core electrons = 22], the second line specifies the column heads and the third line gives the total number of transitions. The transitions (138 121 in total) are given next. The first two columns represent the transition, [SiLiPi(i) -> SjLjPj(j)], that is, between  $i$ th and  $j$ th states of the transitional symmetries. The integer designation for a state consists of the spin multiplicity ( $2S + 1$ ), the total angular momentum  $L$ , such as 0 for  $L = S$ , 1 for  $L = P$ , 2 for  $L = D$  etc., the parity  $P_i$ , such as  $P_i = 0$  for an even state

and  $P_i = 1$  for an odd state, and the energy position of the state (the fourth integer). For example, [6 0 0 1 6 1 1 1] means  ${}^6S(1) \rightarrow {}^6P^{\circ}(1)$ , where the numbers within parenthesis are the energy position of the states, the lowest ones in this case. The next two columns are energies in Rydbergs,  $E_i$  and  $E_j$ , of the states. The last three columns are  $f$ ,  $gf$ ,  $A$ -values. The  $A$ -values are in atomic units; they should be divided by atomic unit of time,  $\tau_0 = 2.419 \times 10^{-17}$  to yield  $A s^{-1}$ .

Present results for the Fe IV oscillator strengths are compared with those from earlier works in Table 5. Bautista & Pradhan (1997) considered transitions among sextets and quartets only and hence have relatively smaller set of data compared to the OP data. Under the OP, Sawey & Berrington (1992) produced an extensive set of data, a total of 133 650 transitions among 1721 bound states for all three symmetries, sextets, quartets, and doublets. Hence, OP data contains about

**Table 5.** Comparison of present  $f$ -values for Fe IV with previous works: a – Bautista & Pradhan (1997), b – Sawey & Berrington (1992), c – Fawcett (1989).

Present	Others	$C_i - C_j$	$SL_i - SL_j$	$g_i - g_j$
0.1817	0.2037 <sup>a</sup> , 0.1973 <sup>b</sup> , 0.2037 <sup>c</sup>	$3d^4(^5D)4s-3d^4(^5D)4p$	$^6D-^6P^o$	30–18
0.3085	0.339 <sup>a</sup> , 0.3277 <sup>b</sup> , 0.2830 <sup>c</sup>	$3d^4(^5D)4s-3d^4(^5D)4p$	$^6D-^6D^o$	30–30
0.4142	0.4603 <sup>a</sup> , 0.4433 <sup>b</sup> , 0.4633 <sup>c</sup>	$3d^4(^5D)4s-3d^4(^5D)4p$	$^6D-^6F^o$	30–42
0.1710	0.1883 <sup>a</sup> , 0.1820 <sup>b</sup> , 0.1100 <sup>c</sup>	$3d^4(^5D)4s-3d^4(^5D)4p$	$^4D-^4P^o$	20–12
0.3165	0.351 <sup>a</sup> , 0.3335 <sup>b</sup> , 0.3285 <sup>c</sup>	$3d^4(^5D)4s-3d^4(^5D)4p$	$^4D-^4D^o$	20–20
0.4164	0.4583 <sup>a</sup> , 0.4395 <sup>b</sup> , 0.4375 <sup>c</sup>	$3d^4(^5D)4s-3d^4(^5D)4p$	$^4D-^4F^o$	30–28
0.1599	0.1491 <sup>b</sup> , 0.1073 <sup>c</sup>	$3d^4(^5H)4s-3d^4(^5H)4p$	$^2H-^2G^o$	22–18
0.2679	0.2559 <sup>b</sup> , 0.2018 <sup>c</sup>	$3d^4(^5H)4s-3d^4(^5H)4p$	$^2H-^2H^o$	22–22
0.3472	0.3645 <sup>b</sup> , 0.3136 <sup>c</sup>	$3d^4(^5H)4s-3d^4(^5H)4p$	$^2H-^2I^o$	22–26

4500 transitions less than the present set. Fawcett (1989) employed the semi-empirical Cowan's Hartree-Fock relativistic code with optimized Slater parameters to calculate the transition probabilities of Fe IV. We note that the **current** NIST database of evaluated compilation gives radiative decay rates only for a small number of forbidden transitions, not allowed ones. Comparison in Table 5 of the present  $f$ -values with the previous ones show agreement among all the calculations for sextet and quartet transitions, within 10%. However, for the doublet transitions the present oscillator strengths and those of Sawey & Berrington (1992) show similar values, while Fawcett's values are somewhat smaller.

A fortran code (LIFETIME.f) is provided to read the  $A_{ji}$  values, accessible from higher state  $j$  to lower states  $is$ , from the large electronic file of transitions and to compute the lifetime  $\tau_j$  in sec for any LS state  $j$  ( $a^{(2S+1)L^\pi}$ ). For example, the calculated lifetime of  $z^6P^o$  is  $2.4 \times 10^{-10}$  s, of  $z^6D^o$  is  $1.16 \times 10^{-9}$  s and of  $z^6F^o$  is  $1.37 \times 10^{-9}$  s.

### 4.3. Fine structure transitions

Fine structure  $f$ - and  $A$ -values are presented for 712 120 dipole allowed transitions in Fe IV. As in the case of LS multiplets, observed energies of fine structure transitions are employed whenever available for improved accuracy. As only a limited number of observed levels are available, a smaller set of 2915 fine structure transitions corresponding to 620 LS multiplets has observed transitional energies. Rest of the transitions, 709 205 in total, employ calculated energies. The entire file containing all fine structure transitions is available electronically.

A sample set of  $f$ -,  $S$ -, and  $A$ -values for the dipole allowed fine structure transitions in Fe IV is presented in Table 6. The first line of each subset corresponds to the LS transition followed by the fine structure components. The letter prefix designation of the transitional states in the table corresponds to their energy positions, as explained in Table 3. The energy unit for the individual states and transition for the LS multiplets are in Rydberg. However, for the fine structure transitions, the energies of the initial and final fine structure levels are in unit of  $\text{cm}^{-1}$ , while the transitional energy differences are in  $\text{\AA}$  unit. The  $A$ -values are in  $\text{s}^{-1}$ . An asterisk (\*) below an LS state indicates an incomplete set of observed energy levels, and an

asterisk for the transitional energy indicates that one or both the levels are missing from the observed energy set.

The fortran code (LIFETIME.f) can read the  $A_{ji}$  values, accessible from higher level  $j$  to lower levels  $is$ , from the large electronic file of transitions and compute the lifetime  $\tau_j$  in sec for any fine structure level  $j$  ( $a^{(2S+1)L_j^\pi}$ ). For example, the calculated lifetime of level  $z^4S_{3/2}^o$  is  $1.0 \times 10^{-10}$  s.

Based on the accuracy of the calculated energies and comparison with other works, LS multiplets should be of better accuracy than those in TOPbase and by Bautista & Pradhan (1997). The overall accuracy for most of the present  $f$ -,  $S$ -, and  $A$ -values should be within 30–50% for strong transitions. However, larger uncertainty is expected for the weak transitions and for transitions among highly excited states.

### 4.4. Opacities

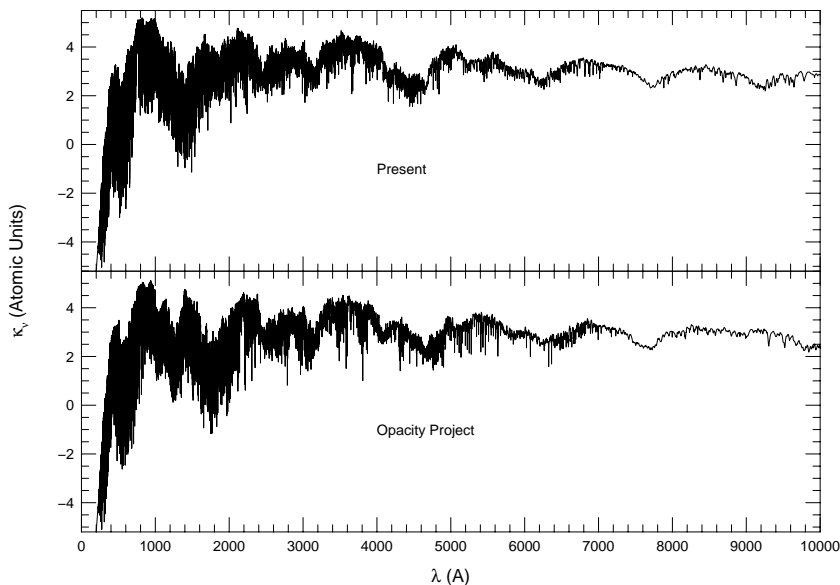
We calculate sample radiative opacities of Fe IV for three reasons. First, as a completeness and consistency check on the huge amount of data computed, second, to gauge the potential impact on iron opacities, and third, spectral models for determination of iron abundances in astrophysical sources. In particular, in the absence of other indicators such as experimental data or large-scale calculations of similar accuracy, we seek to ascertain differences with the results of Sawey & Berrington (1992), such as found for Fe II (Nahar & Pradhan 1994).

Figure 1 shows the monochromatic opacities in most of the wavelength range where Fe IV is a contributor in an astrophysical plasma in local-thermodynamic-equilibrium (LTE). The present results are compared with those using the bound-bound OP data by Sawey & Berrington (1992). In order to compare only the main source of opacity (lines), we have used the same bound-free (photoionization) data in both calculations; the bound-free opacity is less than 10% of the total. We choose the temperature  $\log T(\text{K}) = 4.5$  and the electron density  $\text{Log} N_e(\text{cm}^{-3}) = 17.0$ . The Mihalas-Hummer-Dappen equation-of-state (MHD-EOS; Mihalas et al. 1998) used in the OP work gives relatively large value of the ionization fraction  $\text{Fe IV}/\text{Fe} = 0.57$ ; Fe IV dominates the iron opacity at this temperature and density. Figure 1 shows immediately the reason that Fe IV is the dominant ion in the UV, between 500–4000  $\text{\AA}$ . It is noteworthy that the opacity of Fe IV varies over nearly

**Table 6.** Sample data for allowed fine structure transitions of Fe IV.

$SL_i - SL_j$	$E_i$ Ry/cm <sup>-1</sup>	$E_j$ Ry/cm <sup>-1</sup>	$E_{ij}$ Ry/Å	$g_i$	$g_j$	$f_{ij}$	$S$	$A$ s <sup>-1</sup>
$a^6S^e \rightarrow z^6P^o$	4.0200	2.2879	1.732E+00	6	18	4.226E-01	4.392E+00	3.395E+09
	0.0	190 226.0	525.69	6	8	1.880E-01	1.952E+00	3.403E+09
	0.0	190 008.0	526.29	6	6	1.408E-01	1.464E+00	3.391E+09
	0.0	189 885.0	526.63	6	4	9.381E-02	9.759E-01	3.384E+09
$a^6D^e \rightarrow z^6P^o$	2.8492	2.2879	5.613E-01	30	18	1.827E-01	2.929E+01	7.704E+08
	128 967.0	190 226.0	1632.41	10	8	1.817E-01	9.762E+00	5.684E+08
	128 541.0	190 226.0	1621.14	8	8	6.554E-02	2.798E+00	1.664E+08
	128 191.0	190 226.0	1611.99	6	8	1.461E-02	4.653E-01	2.813E+07
	128 541.0	190 008.0	1626.89	8	6	1.170E-01	5.011E+00	3.930E+08
	128 191.0	190 008.0	1617.68	6	6	1.120E-01	3.579E+00	2.855E+08
	127 929.0	190 008.0	1610.85	4	6	5.523E-02	1.171E+00	9.464E+07
	128 191.0	189 885.0	1620.90	6	4	5.692E-02	1.822E+00	2.167E+08
	127 929.0	189 885.0	1614.05	4	4	1.286E-01	2.733E+00	3.293E+08
	127 766.0	189 885.0	1609.81	2	4	1.842E-01	1.952E+00	2.371E+08
$a^6D^e \rightarrow z^6D^o$	2.8492	2.2583	5.910E-01	30	30	3.085E-01	4.698E+01	8.654E+08
	128 967.0	193 789.0	1542.69	10	10	2.510E-01	1.275E+01	7.035E+08
	128 967.0	193 386.0	1552.34	10	8	5.669E-02	2.897E+00	1.962E+08
	128 541.0	193 789.0	1532.61	8	10	7.178E-02	2.897E+00	1.631E+08
	128 541.0	193 386.0	1542.14	8	8	1.380E-01	5.607E+00	3.872E+08
	128 541.0	192 595.0	1561.18	8	6	9.789E-02	4.025E+00	3.572E+08
	128 191.0	193 386.0	1533.86	6	8	1.328E-01	4.025E+00	2.825E+08
	128 191.0	192 595.0	1552.70	6	6	5.249E-02	1.610E+00	1.452E+08
	128 191.0	193 271.0	1536.57	6	4	1.238E-01	3.759E+00	5.248E+08
	127 929.0	192 595.0	1546.41	4	6	1.846E-01	3.759E+00	3.432E+08
	127 929.0	193 271.0	1530.41	4	4	3.419E-03	6.891E-02	9.738E+06
	127 929.0	193 120.0	1533.95	4	2	1.210E-01	2.443E+00	6.857E+08
	127 766.0	193 271.0	1526.60	2	4	2.431E-01	2.443E+00	3.478E+08
	127 766.0	193 120.0	1530.13	2	2	6.933E-02	6.985E-01	1.975E+08
	$a^6D^e \rightarrow z^6F^o$	2.8492	2.2955	5.537E-01	30	42	4.142E-01	6.731E+01
128 967.0		190 276.0	1631.08	10	12	3.582E-01	1.923E+01	7.483E+08
128 967.0		189 515.0	1651.58	10	10	5.424E-02	2.949E+00	1.326E+08
128 967.0		188 904.0	1668.42	10	8	4.319E-03	2.372E-01	1.293E+07
128 541.0		189 515.0	1640.04	8	10	3.020E-01	1.305E+01	5.992E+08
128 541.0		188 904.0	1656.64	8	8	9.991E-02	4.359E+00	2.428E+08
128 541.0		188 428.0	1669.81	8	6	1.246E-02	5.481E-01	3.975E+07
128 191.0		188 904.0	1647.09	6	8	2.542E-01	8.270E+00	4.687E+08
128 191.0		188 428.0	1660.11	6	6	1.359E-01	4.456E+00	3.288E+08
128 191.0		188 086.0	1669.59	6	4	2.333E-02	7.693E-01	8.373E+07
127 929.0		188 428.0	1652.92	4	6	2.121E-01	4.616E+00	3.451E+08
127 929.0		188 086.0	1662.32	4	4	1.669E-01	3.654E+00	4.029E+08
127 929.0		187 878.0	1668.08	4	2	3.240E-02	7.116E-01	1.553E+08
127 766.0		188 086.0	1657.82	2	4	1.821E-01	1.987E+00	2.209E+08
127 766.0		187 878.0	1663.56	2	2	2.283E-01	2.500E+00	5.502E+08
$a^4P^e \rightarrow z^4S^o$	3.6983	1.6735	2.025E+00	12	4	6.310E-02	1.122E+00	6.233E+09
	35 253.8	257 503.0	449.95	6	4	6.311E-02	5.609E-01	3.119E+09
	35 333.3	257 503.0	450.11	4	4	6.309E-02	3.739E-01	2.077E+09
	35 406.6	257 503.0	450.25	2	4	6.307E-02	1.870E-01	1.038E+09
$a^4P^e \rightarrow z^4P^o$	3.6983	2.2657	1.433E+00	12	12	5.704E-02	1.433E+00	9.402E+08
	35 253.8	193 549.0	631.73	6	6	4.020E-02	5.017E-01	6.720E+08
	35 253.8	191 694.0	639.22	6	4	1.703E-02	2.150E-01	4.170E+08
	35 333.3	193 549.0	632.05	4	6	2.583E-02	2.150E-01	2.875E+08
	35 333.3	191 694.0	639.55	4	4	7.564E-03	6.371E-02	1.234E+08
	35 333.3	191 021.0	642.31	4	2	2.354E-02	1.991E-01	7.611E+08
	35 406.6	191 694.0	639.85	2	4	4.726E-02	1.991E-01	3.849E+08
	35 406.6	191 021.0	642.61	2	2	9.410E-03	3.982E-02	1.520E+08





**Fig. 1.** Monochromatic opacities of Fe IV using the present data (*top panel*) and with the Opacity Project data (*lower panel*) from Sawey & Berrington (1992) at  $\text{Log}T(\text{K}) = 4.5$  and  $\text{Log}N_e (\text{cm}^{-3}) = 17.0$ . The major features show a shift in wavelength on differences in intensities.

10 orders of magnitude, implying that it remains a large contributor over a very wide range of radiation.

The two datasets displayed in Fig. 1 differ considerably. The main features throughout the opacity spectrum appear at different positions. For example, there is relative displacement of nearly 200 Å in the position of the trough which is at  $\sim 1500$  Å in the present results, but at  $\sim 1700$  Å using the OP data. Even more striking are the differences in the present and the OP Rosseland mean opacities, 3.3 and 4.87  $\text{cm}^2/\text{g}$  respectively. The difference implies a systematic shift in groups of energy levels between the two sets of calculations and associated transitions (too numerous to identify in detail). This nearly 50% difference is similar, but in the opposite direction, to the one we found earlier in the Fe II opacities (Nahar & Pradhan 1994) using new IP data as opposed to the OP data by Sawey & Berrington (1997), which has been shown to be inaccurate for low ionization states of iron, Fe I–IV (Nahar & Pradhan 1994; Bautista & Pradhan 1997; Cowley & Bautista 2003). We note that the calculation of latest stellar opacities under the OP has been carried out using the OP data as well as data from other sources (M. J. Seaton, private communication).

Although more extensive investigations are needed to ascertain the full range of differences at all temperatures and densities, we analyze the results somewhat further. The improvement in computed energies in the present calculations for the low-lying states is an important factor in the calculation of opacities, since they account for most of the level population; higher levels are (a) not populated significantly; and (b) smeared out or dissolved due to Stark and electron impact broadening as incorporated in MHD-EOS. An examination of the all level populations of Fe IV at  $T = 3.16 \times 10^5$  K and  $N_e = 10^{17} \text{cm}^{-3}$ , obtained from the MHD-EOS shows that there is nearly a sharp drop in population of levels as one approaches the highest of the 16 states of the ground configuration  $3d^5$ . For example, the population drops by about 2 orders of magnitude from the ground state  $3d^5(^6S)$  at  $\sim -4$  Ryd, to the 17th excited

state  $3d^44s(^6D)$  at  $\sim -2.8$  Ryd. Even higher levels do not contribute to the opacity in any significant way. The decrease is related to the negative exponential functional form in the modified Boltzmann-Saha equations in MHD-EOS.

## 5. Conclusion

Results are presented from a large and extensive calculation for Fe IV. All 1798 states were identified in spectroscopic notation through quantum defect and channel contribution analysis. However, level identifications for highly mixed excited states should be treated with caution since often no definitive assignment is possible, and in any case not needed for practical applications. Present energies agree very well with the observed energies for all low lying terms. However, the uncertainty increases for excited states with higher energies, especially the odd parity states.

An extensive set of  $f$ - and  $A$ -values for 138 121 LS multiplets and 712 120 fine structure transitions are presented. A small subset of the total transitions has been reprocessed with the available observed energies.

The fact that relativistic effects are not considered, and spin-change transitions are not included in this work, implies that there may be additional redistribution of oscillator strengths within LS multiplets, particularly for highly mixed levels. Therefore, specific fine structure data should be treated with care for spectral diagnostics. While it is difficult to ascertain the accuracy of individual transitions for Fe IV in the absence of experimental data, comparison with other theoretical works indicate an accuracy of 30–50% for the strong transitions. Uncertainty is likely to be higher for transitions where relativistic effects are important and deviations from LS coupling are significant.

Although for the relatively few transitions compared the present data show marginal improvement over that of Sawey & Berrington (1992), they are more extensive and the

differences manifest themselves when we compute and compare monochromatic opacities for Fe IV. The present data should therefore be used in astrophysical applications instead of the previous datasets. Moreover, the differences in monochromatic opacities of iron ions are highly significant for stellar models in a variety of ways, but most importantly in the determination of relative element abundances and radiative accelerations (Bahcall et al. 2005; Delahaye & Pinsonneault 2005). Based on this work, and our previous studies on low ionization stages of iron, it may be inferred that more accurate iron opacities than currently available might be needed for specialized applications.

The new Fe IV results should be particularly useful for the analysis and application to ultraviolet to optical spectra from astrophysical and laboratory sources. All data files are electronically available from the CDS or from the first author.

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