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Inner-shell photoexcitation of Fe xv and Fe xvi

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ABSTRACT

The configuration-interaction method as implemented in the computer code CIV3 is used to determine energy levels, electric dipole radiative transition wavelengths, oscillator strengths and transition probabilities for inner-shell excitation of transitions in Fe xv and Fe xvi. Specifically, transitions are considered of the type $1s^2 2s^2 2p^6 3s^2 - 1s^2 2s^2 2p^5 3l' 3l''$ (l, l' and $l'' = s, p$ or d) in Fe xv and $1s^2 2s^2 2p^6 3s - 1s^2 2s^2 2p^5 3l' l'$ (l and $l' = s, p$ or d) in Fe xvi, using the relativistic Breit–Pauli approach. An assessment of the accuracy of the derived atomic data is performed.

Key words: atomic data – line: formation – X-rays: general.

1 INTRODUCTION

As a result of the launch of the *XMM–Newton* and *Chandra* satellites, new high-resolution X-ray astronomical spectra are becoming widely available. Both emission and absorption X-ray spectra originating from various astrophysical objects, such as accretion disc in active galactic nuclei (AGN), X-ray binary stars, neutron stars, X-ray pulsars, supernova remnants, X-ray emitting shocks and the interstellar ionized medium, have been recorded and studied (see, for example, Kaspi et al. 2000; Yang, Wilson & Ferruit 2001; Ballantyne, Ross & Fabian 2002; Schurch & Warwick 2002). Along with these observations, the X-ray emission and absorption spectra from laboratory sources, such as the Sandia National Laboratory Z-pinch facility, have been reported recently (Foord et al. 2001).

For the reliable interpretation of high-resolution X-ray spectroscopic observations, one needs accurate atomic data describing various fundamental processes that determine the ionization structure, the electron temperature, the level population of excited states and emission/absorption line properties, such as wavelengths or intensities of highly charged ions which are abundant in the observed sources. These atomic data are employed in spectral modelling codes such as GALAXY (Rose 1998), CLOUDY (Ferland et al. 1998), XSTAR (Kallman & Bautista 2001).

A very large number of absorption lines belonging to different charge states of iron ions are present in the X-ray spectra obtained from observed astrophysical objects. Some recent efforts to generate

absorption soft X-ray spectra of the 16 Fe charge states for inner-shell ($n = 2$) photoexcitation was reported by Behar, Sako & Kahn (2001), where a relativistic approach was used to calculate the wavelengths and oscillator strengths for the radiative transitions from the inner 2p and 2s shells, along with autoionization transitions.

In the present work we employ the configuration-interaction (CI) code CIV3 (Hibbert 1975) to determine the wavefunctions of the ions considered. The method of superposition of configurations applied here is capable of producing very accurate data for this type of calculation, which requires high levels of correlation. Relativistic effects are introduced by adding Breit–Pauli operators into the Hamiltonian (Hibbert, Glass & Froese Fischer 1991). Combining these two methods, we can reliably determine LSJ -energy levels, absorption oscillator strengths and emission transition probabilities for the electric dipole (E1) $2p-3l$ transitions between fine-structure levels.

2 METHOD OF CALCULATION

In a CI calculation, the atomic-state wavefunction is represented in the form of a linear superposition of configuration-state functions (CSFs). In the non-relativistic (LS) approximation, this can be expressed as

$$\Psi(LS) = \sum_i a_i \Phi_i(\alpha_i LS), \quad (1)$$

where Φ_i represents a set of CSFs that possess the same total $LS\pi$ symmetry. In the case of the Breit–Pauli approximation, this changes to

$$\Psi(J) = \sum_i a_i \Phi_i(\alpha_i L_i S_i J), \quad (2)$$

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where the CSFs represent several different LS terms, each of which has the same J value and parity π . In each case the set of CSFs $\{\Phi_i\}$ is constructed as normalized antisymmetric products of the one-electron function, the angular momenta of which are coupled in a manner denoted by $\{\alpha_i\}$, such that the resultant is an eigenfunction of the total angular momentum operators $\{L^2, S^2\}$ for the LS -coupling or $\{J^2\}$ for the intermediate LSJ -coupling. The coefficients $\{\alpha_i\}$ correspond to an eigenvector of the Hamiltonian matrix with particular symmetry ($LS\pi$ or $J\pi$).

In order to determine wavefunctions using the LS -coupling scheme of the CI expansion, we use the Hamiltonian constructed solely from the Schrödinger non-relativistic operator, while in the relativistic case we use this operator plus the spin-orbit operator, the spin-other-orbit operator, the spin-spin operator, the mass-correction operator and the Darwin term. The orbit-orbit interaction, although more significant for inner-shell excitation than for outer-shell transitions, remains small compared with the degree of accuracy which can be achieved for E1-transition wavelengths.

The configuration state functions used in equations (1) and (2) are constructed from a set of one-electron orbitals for which the radial part is presented by a linear combination of normalized Slater-type orbitals χ_{jnl} :

$$P_{nl}(r) = \sum_{j=1}^k c_{jnl} \chi_{jnl}(r), \quad (3)$$

where

$$\chi_{jnl}(r) = \frac{(2\xi_{jnl})^{l_{jnl}+1/2}}{[(2l_{jnl}!)^{1/2}]^{1/2}} r^{l_{jnl}} \exp(-\xi_{jnl}r). \quad (4)$$

In our approach radial one-electron orbitals must satisfy the orthonormality conditions

$$\int_0^\infty P_{nl}(r) P_{n'l'}(r) dr = \delta_{nn'}. \quad (5)$$

The parameters c_{jnl} and ξ_{jnl} in equations (3) and (4) are determined by the CIV3 code using an optimization procedure for the eigenvalues of the non-relativistic Hamiltonian.

2.1 Radial functions

We need to obtain wavefunctions of Fe xvi and Fe xv that are as accurate as possible for all states under investigation. Initially, we choose the 1s, 2s, 2p and 3s radial orbitals as the Hartree-Fock functions. Consequently, we can use their parameters given by Clementi & Roetti (1974). With these core orbitals, the radial orbital parameters for 3p and 3d functions were obtained using the CIV3 code.

In Fe xvi we study electric dipole transitions from the ground $1s^2 2s^2 2p^6 3s$ configuration to the configurations $1s^2 2s^2 2p^5 3l 3l'$, where l and l' can be any of the s, p or d orbitals. Consequently, we optimize the 3p orbital functions on the lowest 2P term of the $2p^5 3s 3p$ configuration. Similarly, we optimize 3d orbital functions on the lowest 2P term of the $2p^5 3s 3d$ configuration. In both procedures, we use a single-configuration approach, which gives only two CSF, producing 2P terms.

In addition to valence orbitals $3l$, we use ‘correlation’ orbitals denoted by $\bar{4}l$ in order to improve the accuracy of wavefunctions. The optimization of their parameters was performed in the following way. The $\bar{4}s$ orbital was optimized on the lowest 2P term of the $2p^5 3s 3d$ configuration using the configurations $2p^5 3s 3d$, $2p^5 3d^2$ and $2p^5 3s 4s$. The $\bar{4}p$ orbital was optimized on the lowest 2P term of the $2p^5 3p^2$ configuration using the configurations $2p^5 3p^2$, $2p^5 3s 3d$, $2p^5 3p 4p$ and $2p^5 4p^2$. The $\bar{4}d$ orbital was optimized on the lowest 2P term of the $2p^5 3s 3d$ configuration using the configurations $2p^5 3s 3d$,

Table 1. Parameters of the Fe xvi and Fe xv radial basis orbitals.

| nl | l_{jnl} | Fe xvi | | Fe xv | |
|------------|-----------|-----------|-------------|-----------|-------------|
| | | c_{jnl} | ξ_{jnl} | c_{jnl} | ξ_{jnl} |
| 3p | 2 | 0.323 92 | 13.906 85 | 0.303 51 | 14.168 13 |
| | 3 | 0.404 49 | 10.291 56 | 0.362 21 | 10.720 46 |
| | 3 | -1.269 13 | 5.897 73 | -1.214 07 | 5.722 91 |
| 3d | 3 | 0.094 44 | 10.413 35 | 0.105 33 | 10.185 72 |
| | 3 | 0.928 26 | 5.752 60 | 0.920 12 | 5.596 45 |
| $\bar{4}s$ | 1 | 0.422 14 | 18.299 06 | 0.435 62 | 17.283 47 |
| | 2 | -8.295 09 | 4.744 37 | -9.205 59 | 4.705 63 |
| | 3 | 6.384 04 | 6.009 08 | 9.446 03 | 6.207 82 |
| | 4 | -0.942 33 | 6.389 65 | -2.655 39 | 7.339 90 |
| $\bar{4}p$ | 4 | 3.006 02 | 10.555 76 | 2.488 17 | 10.029 44 |
| | 2 | 0.157 00 | 23.973 02 | 0.548 98 | 13.235 41 |
| | 3 | 2.007 33 | 11.183 12 | 1.215 18 | 8.580 96 |
| | 4 | -2.974 88 | 11.339 20 | -2.782 44 | 9.900 39 |
| $\bar{4}d$ | 4 | 1.164 63 | 5.630 79 | 1.351 55 | 5.708 09 |
| | 3 | 2.655 97 | 6.867 20 | 1.372 02 | 8.376 36 |
| | 4 | -4.348 73 | 6.346 84 | -0.600 14 | 7.791 86 |
| | 4 | 1.715 44 | 5.625 32 | -0.791 22 | 4.751 64 |
| $\bar{4}f$ | 4 | 4.063 87 | 5.017 75 | 1.983 56 | 5.824 60 |
| | 4 | -3.149 69 | 4.652 12 | -1.010 81 | 5.220 16 |

$2p^5 3d^2$, $2p^5 3s \bar{4}d$, $2p^5 3d \bar{4}s$ and $2p^5 \bar{4}d^2$. The $\bar{4}f$ orbital was optimized on the lowest 2P term of the $2p^5 3p^2$ configuration using the configurations $2p^5 3p^2$, $2p^5 3s 3d$, $2p^5 3p \bar{4}f$ and $2p^5 \bar{4}f^2$. The optimized parameters c_{jnl} and ξ_{jnl} and the values of l_{jnl} used in our calculation for each of the orbitals are given in Table 1.

In Fe xv we consider electric dipole transitions from the ground $1s^2 2s^2 2p^6 3s^2$ configuration to the configurations $1s^2 2s^2 2p^5 3l 3l' 3l''$, where l , l' and l'' can be any of the s, p or d orbitals. Consequently, we choose to optimize 3p orbital functions on a single 3P term of the $2p^5 3s^2 3p$ configuration, and 3d orbital functions on a 2P term of the $2p^5 3s^2 3d$ configuration.

The parameters of ‘correlation’ orbitals $\bar{4}s$, $\bar{4}p$, $\bar{4}d$, $\bar{4}f$ were obtained in a procedure similar to that described above. The $\bar{4}s$ orbital was optimized on the $2p^5 3s^2 3d$ 3P term using the configurations $2p^5 3s^2 3d$, $2p^5 3s^2 \bar{4}s$, $2p^5 3s^2 \bar{4}s^2$ and $2p^5 3s 3d \bar{4}s$. The $\bar{4}p$ orbital was optimized on the lowest $2p^5 3s 3p^2$ 3P term using the configurations $2p^5 3s^2 3d$, $2p^5 3p^2 3d$, $2p^5 3s 3p^2$, $2p^5 3s \bar{4}p^2$, $2p^5 3s 3p \bar{4}p$ and $2p^5 3p 3d \bar{4}p$. The $\bar{4}d$ orbital was optimized on the $2p^5 3s^2 3d$ 1P term using the configurations $2p^5 3s^2 3d$, $2p^5 3p^2 3d$, $2p^5 3s^2 \bar{4}d$, $2p^5 3p^2 \bar{4}d$ and $2p^5 3s 3d \bar{4}d$. The $\bar{4}f$ orbital was optimized on the $2p^5 3s^2 3d$ 3P term using the configurations $2p^5 3s^2 3d$, $2p^5 3p^2 3d$ and $2p^5 3p 3d \bar{4}f$. The radial orbital parameters c_{jnl} , ξ_{jnl} and l_{jnl} are presented in Table 1.

2.2 Configuration sets

The ground level of the Fe xvi ion is $1s^2 2s^2 2p^6 3s^2 S_{1/2}^0$. We chose the CI wavefunction expansion for this level such that no more than two electrons are excited from the 2p and 3s shells. As a result, we include configurations $2p^6 3s$, $2p^5 3s 3p$ and $2p^5 3p 3d$ with valence orbitals 3s, 3p and 3d, configurations $2p^6 \bar{4}s$, $2p^5 3s \bar{4}p$, $2p^5 3s \bar{4}f$, $2p^5 3p \bar{4}s$, $2p^5 3p \bar{4}d$, $2p^5 3d \bar{4}p$ and $2p^5 3d \bar{4}f$ with one electron within ‘correlation’ $\bar{4}l$ shell and configurations $2p^5 \bar{4}s \bar{4}p$, $2p^5 \bar{4}s \bar{4}f$, $2p^5 \bar{4}p \bar{4}d$ and $2p^5 \bar{4}d \bar{4}f$ with two valence orbitals. We consider $^2S^e$, $^2P^e$, $^4P^e$ and $^4D^e$ final terms, which can produce levels with the total angular momentum $J = 1/2$. Consequently, we have 94 CSFs in the CI wavefunction expansion of the lower level.

Selection rules for the E1 transition define that we have possible $J = 1/2$ and $3/2$ levels in the upper configuration with the 2p

vacancy. As the configuration itself or LS are not exact quantum numbers in the case of relativistic intermediate coupling, we consider all possible transitions from the 2p to the 3l shells. In order to keep our calculation consistent, we employ the same basic principles for the CI wavefunction expansion as in the lower configuration case. First of all, we include the configurations under consideration for the transition array, namely $2p^53s^2$, $2p^53p^2$, $2p^53p^2$ and $2p^53s3d$. These are supplemented by $2p^63p$, $2p^64p$, $2p^53s4s$, $2p^53s4d$, $2p^53p4p$, $2p^53p4f$, $2p^53d4s$, $2p^53d4d$, $2p^54s^2$, $2p^54p^2$, $2p^54d^2$, $2p^54f^2$, $2p^54s4d$ and $2p^54p4f$ configurations. For the $J = 1/2$ fine-structure levels, we consider the $^2S^o$, $^2P^o$, $^4P^o$ and $^4D^o$ final terms, resulting in 93 configuration state functions. Alternatively for the $J = 3/2$ fine-structure levels, the symmetries considered are $^4S^o$, $^2P^o$, $^4P^o$, $^2D^o$, $^4D^o$ and $^4F^o$ and there are 147 CSFs in a wavefunction expansion.

The ground level of the Fe xv ion is $1s^22s^22p^63s^2\ ^1S_0^o$. We chose all possible configurations with one or no vacancy in the 2p shell and outer electrons distributed in 3l and 4l shells for the inclusion in the CI wavefunction expansion of this state. This means we have one group of the $2p^63s^2$, $2p^63p^2$, $2p^63d^2$, $2p^53s^23p$, $2p^53p^3$, $2p^53p3d^2$, $2p^53s3p3d$ configurations with two or three electrons within the $n = 3$ shell. The configurations $2p^63s4s$, $2p^63p4p$, $2p^63d4d$, $2p^53s^24p$, $2p^53p^24p$, $2p^53d^24p$, $2p^53s3p4s$, $2p^53s3p4d$, $2p^53p3d4s$, $2p^53p3d4d$, $2p^53s3d4p$ and $2p^53s3d4f$ make another group with a single electron excited to the $n = 4$ shell. In addition to that, we include the configurations $2p^64s^2$, $2p^64p^2$, $2p^64d^2$, $2p^64f^2$, $2p^53p^24s^2$, $2p^53p^24p^2$, $2p^53p^24d^2$, $2p^53p^24f^2$, $2p^53s4s4p$, $2p^53s4s4f$, $2p^53s4p4d$, $2p^53s4d4f$, $2p^53p4s4d$, $2p^53p4p4f$, $2p^53d4s4p$, $2p^53d4s4f$, $2p^53d4p4d$ and $2p^53d4d4f$ with two electrons excited to the $n = 4$ shell. We consider the $^1S^e$, $^3P^e$ and $^5D^e$ terms, which produce $J = 0$ fine-structure levels. Construction of such a basis gives us the 401 CSFs in the CI wavefunction expansion for the lower state of the Fe¹⁶⁺ ion.

Because of the electric dipole transition selection rules, we have to consider fine-structure levels with $J = 1$ in the upper state. In the same way as for the lower even state, we make three groups of configurations for the upper (odd) state. The first group consists of the $2p^63s3p$, $2p^63p3d$, $2p^53s^23d$, $2p^53s3p^2$, $2p^53s3d^2$, $2p^53p^23d$, $2p^53d^3$ configurations, which have one or two electrons excited to $n = 3$ shells. The next group is made of the configurations $2p^63s4p$, $2p^63p4s$, $2p^63p4d$, $2p^63d4p$, $2p^63d4f$, $2p^53s^24s$, $2p^53s^24d$, $2p^53p^24s$, $2p^53p^24d$, $2p^53d^24s$, $2p^53d^24d$, $2p^53s3d4s$, $2p^53s3d4d$, $2p^53s3p4p$, $2p^53p3d4f$, $2p^53p3d4p$ and $2p^53p3d4f$ with all possible electron distributions having a single electron excited to the $n = 4$ shell. The third group is made of the $2p^64s4p$, $2p^64p4d$, $2p^64d4f$, $2p^53s4s^2$, $2p^53s4p^2$, $2p^53s4d^2$, $2p^53s4f^2$, $2p^53d4s^2$, $2p^53d4p^2$, $2p^53d4d^2$, $2p^53d4f^2$, $2p^53s4s4d$, $2p^53s4p4f$, $2p^53d4s4d$, $2p^53d4p4f$, $2p^53p4s4p$, $2p^53p4s4f$, $2p^53p4p4d$ and $2p^53p4d4f$ configurations, which have two electrons in the open $n = 4$ shells. We restricted our set where there could be no more than two electrons in the excited $n = 4$ shell. Here we consider the $^3S^o$, $^1P^o$, $^3P^o$, $^5P^o$, $^3D^o$, $^5D^o$, $^5F^o$ terms, which can produce fine-structure levels with $J = 1$. As a result of this, we have the CI wavefunction expansion with 1065 CSFs for the upper states of the Fe¹⁶⁺ ion.

3 RESULTS

3.1 Energy levels

In Table 2 we present the energy levels for the Fe xv ion calculated using the Breit–Pauli approximation. The energy levels are given in cm^{-1} relative to the ground state $1s^22s^22p^63s^2\ ^1S_{1/2}$ along with

the leading percentage compositions a_i from equation (2) for the 18 excited-state fine-structure levels with $J = 1/2$ and 27 levels with $J = 3/2$. We present only contributions with $a_i^2 \geq 0.1$ for this ion.

The leading percentage compositions in Table 2 indicate the strong level of mixing between different LS states of the excited upper state, which has a vacancy in the 2p shell. In general, the mixing could be so strong that it would not be possible to make a definite identification of levels represented by that wavefunction. For this reason we do not try to assign fine-structure levels to any LSJ quantum numbers. Instead we use a level index to indicate the parity (o for odd or e for even) and J to represent the level and E_J the level energy. The leading contributions of wavefunctions depend on the model used, and hence they can differ depending on the calculations or radial orbitals used.

In Table 3 we present the fine-structure energy levels for the Fe xv ion. The energy level values relative to the ground state $1s^22s^22p^63s^2\ ^1S_0$ are given in cm^{-1} for the 87 levels of the excited state with 2p vacancy. The leading percentage compositions are limited to those with $a_i^2 \geq 0.07$.

One can note an even stronger configuration mixing for the levels of the Fe xv ion compared with Fe xvi. For the 35_1^o level, the two largest contributions are as low as 10 per cent. Similarly to the Fe xvi ion case, we cannot assign fine-structure levels in any other way than using a level index with parity and J and an energy value.

3.2 Electric dipole transition probabilities and oscillator strengths

After determining the CI wavefunctions Ψ_i for the ground-state fine-structure levels and the wavefunctions Ψ_j for the excited-state fine-structure levels, one can determine the electric dipole transition probabilities (A -values) and oscillator strengths (f -values). Oscillator strengths can be calculated using both the length (L) and velocity (V) forms of the E1-transition operator.

The E1 absorption length-form oscillator strength f_L is given by

$$f_L = \frac{2}{3g_i} \Delta E_{ij} \left| \left\langle \Psi_i \left| \sum_{k=1}^N \mathbf{r}_k \right| \Psi_j \right\rangle \right|^2, \quad (6)$$

and the velocity-form oscillator strength f_V by

$$f_V = \frac{2}{3g_i} (\Delta E_{ij})^{-1} \left| \left\langle \Psi_i \left| \sum_{k=1}^N \nabla_k \right| \Psi_j \right\rangle \right|^2, \quad (7)$$

where $g_i = 2J_i + 1$ is the statistical weight of the initial (ground) level and ΔE_{ij} is the transition energy in atomic units. The sum in the transition operator runs over all N electrons.

The difference between the results obtained from the length and velocity forms can serve as an indicator of the accuracy of the calculation. Usually, the velocity-form results are more sensitive to the accuracy of the wavefunctions Ψ compared with the length-form data. Hence, although we have performed atomic data calculations for both forms of the transition operator, only the length-form results are presented in our final tables. We use the velocity-form f -values for establishing the accuracy of our results, as discussed in the next section.

The length-form electric dipole line emission transition probability A_L (in s^{-1}) is given by

$$A_L = \frac{2.142 \times 10^{10}}{g_j} (\Delta E_{ij})^3 \left| \left\langle \Psi_i \left| \sum_{k=1}^N \mathbf{r}_k \right| \Psi_j \right\rangle \right|^2, \quad (8)$$

Table 2. Energy level indices, their values (in cm^{-1}) relative to the $1^6_{1/2}$ level and configuration contributions of the Fe_{XVI} ion levels with $J = 1/2$ and $3/2$.

| Level index | Energy (cm^{-1}) | Contributions (in per cent) | | |
|--------------|-----------------------------|-----------------------------|------------------------|------------------------|
| $1^6_{1/2}$ | 0.00 | 100, $2p^6 3s^2 S$ | | |
| $1^0_{1/2}$ | 5894 438.26 | 97, $2p^5 3s^2 2P$ | | |
| $2^0_{1/2}$ | 6314 191.40 | 50, $2p^5(3p^2 1D) 2P$ | 20, $2p^5(3p^2 3P) 2P$ | 12, $2p^5(3p^2 3P) 4P$ |
| $3^0_{1/2}$ | 6350 003.23 | 60, $2p^5(3p^2 3P) 4P$ | 20, $2p^5(3p^2 3P) 2S$ | 12, $2p^5(3p^2 1D) 2P$ |
| $4^0_{1/2}$ | 6399 342.30 | 66, $2p^5(3p^2 3P) 4D$ | 18, $2p^5(3p^2 3P) 2S$ | |
| $5^0_{1/2}$ | 6415 639.99 | 97, $2p^5 3s(3P)3d 4P$ | | |
| $6^0_{1/2}$ | 6435 168.96 | 56, $2p^5(3p^2 3P) 2S$ | 25, $2p^5(3p^2 3P) 4P$ | 17, $2p^5(3p^2 3P) 4D$ |
| $7^0_{1/2}$ | 6469 208.84 | 40, $2p^5 3s(1P)3d 2P$ | 23, $2p^5(3p^2 3P) 2P$ | 22, $2p^5 3s(3P)3d 4D$ |
| $8^0_{1/2}$ | 6500 188.48 | 53, $2p^5 3s(3P)3d 4D$ | 23, $2p^5(3p^2 3P) 2P$ | 13, $2p^5 3s(3P)3d 2P$ |
| $9^0_{1/2}$ | 6547 551.37 | 79, $2p^5(3p^2 1S) 2P$ | | |
| $10^0_{1/2}$ | 6560 344.42 | 24, $2p^5(3p^2 3P) 2P$ | 23, $2p^5(3p^2 1D) 2P$ | 23, $2p^5 3s(1P)3d 2P$ |
| | | 12, $2p^5(3p^2 1S) 2P$ | | |
| $11^0_{1/2}$ | 6629 844.75 | 63, $2p^5 3s(3P)3d 2P$ | 21, $2p^5 3s(1P)3d 2P$ | |
| $12^0_{1/2}$ | 7086 001.87 | 93, $2p^5(3d^2 3F) 4D$ | | |
| $13^0_{1/2}$ | 7143 845.04 | 37, $2p^5(3d^2 3P) 4P$ | 35, $2p^5(3d^2 1D) 2P$ | 14, $2p^5(3d^2 3P) 2P$ |
| $14^0_{1/2}$ | 7155 468.37 | 37, $2p^5(3d^2 3P) 4P$ | 37, $2p^5(3d^2 1D) 2P$ | 17, $2p^5(3d^2 3P) 2S$ |
| $15^0_{1/2}$ | 7215 108.75 | 49, $2p^5(3d^2 3P) 4D$ | 16, $2p^5(3d^2 3P) 2S$ | 16, $2p^5(3d^2 1D) 2P$ |
| | | 15, $2p^5(3d^2 3P) 2P$ | | |
| $16^0_{1/2}$ | 7250 448.25 | 52, $2p^5(3d^2 3P) 2S$ | 23, $2p^5(3d^2 3P) 4D$ | 22, $2p^5(3d^2 3P) 4P$ |
| $17^0_{1/2}$ | 7289 757.84 | 57, $2p^5(3d^2 3P) 2P$ | 17, $2p^5(3d^2 3P) 4D$ | 10, $2p^5(3d^2 1D) 2P$ |
| $18^0_{1/2}$ | 7355 951.26 | 91, $2p^5(3d^2 1S) 2P$ | | |
| $1^0_{3/2}$ | 5798 374.25 | 97, $2p^5 3s^2 2P$ | | |
| $2^0_{3/2}$ | 6311 725.79 | 39, $2p^5(3p^2 3P) 4P$ | 19, $2p^5(3p^2 1D) 2P$ | 14, $2p^5(3p^2 3P) 2P$ |
| | | 11, $2p^5(3p^2 3P) 4D$ | | |
| $3^0_{3/2}$ | 6331 877.23 | 23, $2p^5(3p^2 3P) 4P$ | 22, $2p^5(3p^2 1D) 2P$ | 15, $2p^5(3p^2 3P) 4S$ |
| | | 13, $2p^5(3p^2 1D) 2D$ | | |
| $4^0_{3/2}$ | 6349 533.49 | 60, $2p^5(3p^2 3P) 2D$ | 19, $2p^5(3p^2 3P) 4D$ | 11, $2p^5(3p^2 3P) 4P$ |
| $5^0_{3/2}$ | 6408 720.63 | 38, $2p^5(3p^2 3P) 4S$ | 22, $2p^5(3p^2 1D) 2D$ | 10, $2p^5(3p^2 3P) 2D$ |
| | | 9, $2p^5(3p^2 3P) 2P$ | | |
| $6^0_{3/2}$ | 6422 948.02 | 86, $2p^5 3s(3P)3d 4P$ | | |
| $7^0_{3/2}$ | 6427 301.06 | 44, $2p^5(3p^2 3P) 4D$ | 15, $2p^5(3p^2 1D) 2D$ | 12, $2p^5(3p^2 3P) 2D$ |
| $8^0_{3/2}$ | 6446 426.41 | 48, $2p^5(3p^2 1S) 2P$ | 17, $2p^5(3p^2 3P) 4P$ | 17, $2p^5(3p^2 3P) 4S$ |
| $9^0_{3/2}$ | 6457 919.22 | 19, $2p^5(3p^2 1S) 2P$ | 14, $2p^5(3p^2 1D) 2D$ | 11, $2p^5(3p^2 3P) 4S$ |
| | | 9, $2p^5(3p^2 1D) 2P$ | | |
| $10^0_{3/2}$ | 6463 757.39 | 37, $2p^5 3s(3P)3d 4F$ | 27, $2p^5 3s(1P)3d 2D$ | 12, $2p^5 3s(3P)3d 4D$ |
| $11^0_{3/2}$ | 6489 949.57 | 41, $2p^5 3s(1P)3d 2P$ | 24, $2p^5 3s(3P)3d 4D$ | |
| $12^0_{3/2}$ | 6526 905.54 | 33, $2p^5 3s(3P)3d 4D$ | 18, $2p^5(3p^2 3P) 2P$ | 18, $2p^5 3s(3P)3d 2P$ |
| $13^0_{3/2}$ | 6543 424.40 | 49, $2p^5 3s(3P)3d 4F$ | 31, $2p^5 3s(1P)3d 2D$ | 13, $2p^5 3s(3P)3d 2D$ |
| $14^0_{3/2}$ | 6577 045.85 | 34, $2p^5(3p^2 3P) 2P$ | 21, $2p^5(3p^2 1D) 2P$ | 17, $2p^5 3s(1P)3d 2D$ |
| | | 10, $2p^5 3s(3P)3d 2D$ | | |
| $15^0_{3/2}$ | 6599 042.88 | 31, $2p^5 3s(1P)3d 2P$ | 24, $2p^5 3s(3P)3d 2D$ | 20, $2p^5 3s(3P)3d 2P$ |
| | | 10, $2p^5 3s(3P)3d 4D$ | | |
| $16^0_{3/2}$ | 6668 318.00 | 49, $2p^5 3s(3P)3d 2P$ | 15, $2p^5 3s(3P)3d 2D$ | 14, $2p^5(3p^2 1D) 2P$ |
| | | 10, $2p^5 3s(1P)3d 2D$ | | |
| $17^0_{3/2}$ | 7088 331.50 | 83, $2p^5(3d^2 3F) 4D$ | | |
| $18^0_{3/2}$ | 7128 904.15 | 30, $2p^5(3d^2 3F) 4F$ | 25, $2p^5(3d^2 1D) 2D$ | 18, $2p^5(3d^2 3F) 2D$ |
| | | 14, $2p^5(3d^2 1D) 2P$ | | |
| $19^0_{3/2}$ | 7136 445.93 | 65, $2p^5(3d^2 3P) 4P$ | 13, $2p^5(3d^2 3F) 4F$ | |
| $20^0_{3/2}$ | 7154 574.60 | 27, $2p^5(3d^2 3F) 4F$ | 21, $2p^5(3d^2 1D) 2P$ | 15, $2p^5(3d^2 1D) 2D$ |
| | | 10, $2p^5(3d^2 3P) 4P$ | | |
| $21^0_{3/2}$ | 7180 867.40 | 61, $2p^5(3d^2 3P) 2D$ | 20, $2p^5(3d^2 3P) 4D$ | |
| $22^0_{3/2}$ | 7199 579.44 | 29, $2p^5(3d^2 3P) 4S$ | 25, $2p^5(3d^2 1D) 2D$ | 21, $2p^5(3d^2 3P) 2P$ |
| $23^0_{3/2}$ | 7232 577.26 | 19, $2p^5(3d^2 3P) 4D$ | 19, $2p^5(3d^2 3P) 4S$ | 17, $2p^5(3d^2 1D) 2P$ |
| | | 15, $2p^5(3d^2 1S) 2P$ | 12, $2p^5(3d^2 3F) 2D$ | |
| $24^0_{3/2}$ | 7250 659.74 | 29, $2p^5(3d^2 3P) 4D$ | 27, $2p^5(3d^2 3P) 4S$ | 15, $2p^5(3d^2 3P) 4P$ |
| | | 12, $2p^5(3d^2 3P) 2D$ | 11, $2p^5(3d^2 1S) 2P$ | |
| $25^0_{3/2}$ | 7265 182.81 | 54, $2p^5(3d^2 1S) 2P$ | 23, $2p^5(3d^2 1D) 2P$ | |
| $26^0_{3/2}$ | 7311 405.96 | 49, $2p^5(3d^2 3F) 2D$ | 18, $2p^5(3d^2 1D) 2D$ | 10, $2p^5(3d^2 3P) 2P$ |
| $27^0_{3/2}$ | 7321 430.69 | 52, $2p^5(3d^2 3P) 2P$ | 18, $2p^5(3d^2 1D) 2P$ | |

Table 3. Energy level indices, their values (in cm^{-1}) relative to 1_0^e level and configuration contributions of the Fe xv ion levels with $J = 1$.

| Level index | Energy (cm^{-1}) | Contributions (in per cent) | | |
|-------------|-----------------------------|--|---|---|
| 1_0^e | 0.00 | 97, $2p^6 3s^2 1S$ | | |
| 1_1^o | 6147 739.62 | 58, $2p^5 3s(3P)(3p^2 3P) 5P$ | 14, $2p^5 3s(3P)(3p^2 3P) 5D$ | 7, $2p^5 3s(1P)(3p^2 3P) 3P$ |
| 2_1^o | 6174 676.75 | 44, $2p^5 3s(1P)(3p^2 3P) 3D$ 9, $2p^5 3s(3P)(3p^2 3P) 5P$ | 23, $2p^5 3s(3P)(3p^2 3P) 3D$ | 18, $2p^5 3s(3P)(3p^2 3P) 5D$ |
| 3_1^o | 6191 267.43 | 30, $2p^5 3s(3P)(3p^2 1D) 3P$ 9, $2p^5 3s(3P)(3p^2 3P) 3P$ | 19, $2p^5 3s(1P)(3p^2 3P) 3P$ 7, $2p^5 3s(1P)(3p^2 3P) 3S$ | 11, $2p^5 3s(3P)(3p^2 3P) 5P$ |
| 4_1^o | 6231 893.67 | 40, $2p^5 3s(3P)(3p^2 3P) 5D$ 7, $2p^5 3s(1P)(3p^2 1D) 1P$ | 19, $2p^5 3s(3P)(3p^2 1D) 3P$ | 10, $2p^5 3s(1P)(3p^2 3P) 3D$ |
| 5_1^o | 6246 529.03 | 43, $2p^5 3s(1P)(3p^2 1D) 1P$ 8, $2p^5 3s(3P)(3p^2 3P) 5D$ | 24, $2p^5 3s(3P)(3p^2 1D) 3D$ | 10, $2p^5 3s(3P)(3p^2 3P) 1P$ |
| 6_1^o | 6258 293.40 | 32, $2p^5 3s(1P)(3p^2 3P) 3S$ 12, $2p^5 3s(3P)(3p^2 3P) 5D$ | 28, $2p^5 3s(3P)(3p^2 3P) 3S$ | 17, $2p^5 3s(3P)(3p^2 3P) 5P$ |
| 7_1^o | 6288 597.95 | 39, $2p^5 3s(1P)(3p^2 3P) 3P$ 9, $2p^5 3s(1P)(3p^2 1S) 1P$ | 15, $2p^5 3s(3P)(3p^2 1D) 3D$ | 10, $2p^5 3s(1P)(3p^2 3P) 3S$ |
| 8_1^o | 6329 178.78 | 20, $2p^5 3s(3P)(3p^2 1S) 3P$ 10, $2p^5 3s(3P)(3p^2 3P) 3P$ | 20, $2p^5 3s(1P)(3p^2 1S) 1P$ 9, $2p^5 3s(3P)(3p^2 1D) 3D$ | 17, $2p^5 3s(1P)(3p^2 3P) 3P$ |
| 9_1^o | 6337 249.68 | 21, $2p^5 3s(1P)(3p^2 1S) 1P$ 16, $2p^5 3s(3P)(3p^2 1S) 3P$ | 17, $2p^5 3s(1P)(3p^2 1D) 1P$ 8, $2p^5 3s(3P)(3p^2 3P) 3P$ | 16, $2p^5 3s(3P)(3p^2 1D) 3D$ 7, $2p^5 3s(3P)(3p^2 3P) 3S$ |
| 10_1^o | 6350 857.59 | 36, $2p^5 3s^2 3d 3P$ | 22, $2p^5 3s(3P)(3p^2 3P) 3P$ | 12, $2p^5 3s(3P)(3p^2 1D) 3D$ |
| 11_1^o | 6387 516.45 | 29, $2p^5 3s(3P)(3p^2 3P) 3D$ 10, $2p^5 3s(1P)(3p^2 3P) 3S$ | 14, $2p^5 3s(1P)(3p^2 3P) 3D$ 7, $2p^5 3s(3P)(3p^2 1S) 3P$ | 11, $2p^5 3s(3P)(3p^2 3P) 3S$ 7, $2p^5 3s^2 3d 3P$ |
| 12_1^o | 6406 899.00 | 29, $2p^5 3s^2 3d 3P$ 10, $2p^5 3s^2 3d 3D$ | 23, $2p^5 3s(3P)(3p^2 1D) 3P$ 8, $2p^5 3s(1P)(3p^2 3P) 3S$ | 15, $2p^5 3s(3P)(3p^2 3P) 3S$ 7, $2p^5 3s(1P)(3p^2 3P) 3P$ |
| 13_1^o | 6421 423.44 | 44, $2p^5 3s(3P)(3p^2 1S) 3P$ | 37, $2p^5 3s(1P)(3p^2 1S) 1P$ | 9, $2p^5 3s(3P)(3p^2 3P) 3D$ |
| 14_1^o | 6435 776.92 | 31, $2p^5 3s(3P)(3p^2 3P) 3P$ 9, $2p^5 3s(1P)(3p^2 3P) 3D$ | 17, $2p^5 3s(3P)(3p^2 3P) 3D$ 8, $2p^5 3s(1P)(3p^2 3P) 3S$ | 10, $2p^5 3s(3P)(3p^2 3P) 3S$ |
| 15_1^o | 6459 950.72 | 54, $2p^5 3s^2 3d 3D$ | 21, $2p^5 3s^2 3d 1P$ | 9, $2p^5 3s(3P)(3p^2 1D) 3D$ |
| 16_1^o | 6504 115.15 | 63, $2p^5 3s(3P)(3p^2 3P) 1P$ | 7, $2p^5 3s(1P)(3p^2 1D) 1P$ | |
| 17_1^o | 6566 910.79 | 63, $2p^5 3s^2 3d 1P$ | 14, $2p^5 3s^2 3d 3D$ | 9, $2p^5 3s(1P)(3p^2 1D) 1P$ |
| 18_1^o | 6840 706.65 | 59, $2p^5(3p^2 3P)(4P)3d 5D$ | 19, $2p^5(3p^2 3P)(4D)3d 5D$ | 15, $2p^5(3p^2 3P)(4S)3d 5D$ |
| 19_1^o | 6844 631.26 | 33, $2p^5(3p^2 1D)(2P)3d 3P$ 9, $2p^5(3p^2 3P)(4P)3d 3D$ | 15, $2p^5(3p^2 3P)(2P)3d 3D$ | 12, $2p^5(3p^2 1D)(2D)3d 3D$ |
| 20_1^o | 6862 886.91 | 59, $2p^5(3p^2 3P)(4P)3d 5P$ | 34, $2p^5(3p^2 3P)(4D)3d 5P$ | |
| 21_1^o | 6889 714.99 | 69, $2p^5(3p^2 3P)(4P)3d 5F$ | | |
| 22_1^o | 6901 127.27 | 15, $2p^5(3p^2 3P)(4D)3d 3P$ 7, $2p^5(3p^2 1D)(2F)3d 3P$ | 8, $2p^5(3p^2 3P)(2D)3d 3P$ | 8, $2p^5(3p^2 1D)(2P)3d 1P$ |
| 23_1^o | 6902 205.00 | 22, $2p^5(3p^2 3P)(4D)3d 3S$ 9, $2p^5(3p^2 1D)(2D)3d 1P$ | 18, $2p^5(3p^2 3P)(2D)3d 3S$ 9, $2p^5(3p^2 1S)(2P)3d 3D$ | 17, $2p^5(3p^2 3P)(2D)3d 1P$ |
| 24_1^o | 6927 478.71 | 42, $2p^5(3p^2 3P)(4D)3d 5F$ | 29, $2p^5(3p^2 3P)(2D)3d 3D$ | |
| 25_1^o | 6941 493.09 | 16, $2p^5(3p^2 3P)(4S)3d 5D$ 11, $2p^5(3p^2 1D)(2F)3d 3P$ | 15, $2p^5(3p^2 1D)(2P)3d 1P$ 11, $2p^5(3p^2 1D)(2D)3d 3S$ | 13, $2p^5(3p^2 3P)(2P)3d 3P$ |
| 26_1^o | 6945 122.56 | 10, $2p^5(3p^2 1D)(2D)3d 3D$ | 9, $2p^5(3p^2 1S)(2P)3d 3D$ | 7, $2p^5(3p^2 3P)(2D)3d 3S$ |
| 27_1^o | 6959 918.90 | 19, $2p^5(3p^2 3P)(2D)3d 3P$ | 18, $2p^5(3p^2 3P)(4D)3d 5D$ | 9, $2p^5(3p^2 3P)(4P)3d 5D$ |
| 28_1^o | 6967 028.92 | 13, $2p^5(3p^2 1D)(2F)3d 3P$ 8, $2p^5(3p^2 3P)(4P)3d 5P$ | 11, $2p^5(3p^2 3P)(4D)3d 5P$ 8, $2p^5(3p^2 3P)(2D)3d 1P$ | 10, $2p^5(3p^2 3P)(2D)3d 3S$ 7, $2p^5(3p^2 3P)(4D)3d 3D$ |
| 29_1^o | 6974 896.38 | 28, $2p^5(3p^2 3P)(2S)3d 3D$ 7, $2p^5(3p^2 3P)(4P)3d 3P$ | 17, $2p^5(3p^2 3P)(2D)3d 3D$ | 8, $2p^5(3p^2 3P)(4P)3d 3D$ |
| 30_1^o | 6979 899.50 | 22, $2p^5(3p^2 1S)(2P)3d 1P$ 8, $2p^5(3p^2 3P)(4P)3d 3D$ 7, $2p^5(3p^2 1D)(2P)3d 1P$ | 14, $2p^5(3p^2 3P)(4S)3d 5D$ 8, $2p^5(3p^2 3P)(4P)3d 3P$ | 12, $2p^5(3p^2 3P)(4D)3d 5D$ 7, $2p^5(3p^2 3P)(2D)3d 3D$ |
| 31_1^o | 6988 099.03 | 22, $2p^5(3p^2 3P)(2S)3d 3D$ 9, $2p^5(3p^2 3P)(4P)3d 5F$ | 14, $2p^5(3p^2 3P)(4D)3d 5F$ 8, $2p^5(3p^2 3P)(4P)3d 3D$ | 11, $2p^5(3p^2 3P)(4D)3d 3D$ |
| 32_1^o | 6993 174.84 | 15, $2p^5(3p^2 3P)(4S)3d 5D$ 7, $2p^5(3p^2 3P)(2D)3d 3P$ | 11, $2p^5(3p^2 1S)(2P)3d 3D$ 7, $2p^5(3p^2 3P)(2S)3d 3D$ | 7, $2p^5(3p^2 3P)(4D)3d 3P$ |
| 33_1^o | 6996 219.63 | 18, $2p^5(3p^2 3P)(4D)3d 5P$ 8, $2p^5(3p^2 3P)(4D)3d 3P$ | 11, $2p^5(3p^2 3P)(4P)3d 5P$ 7, $2p^5(3p^2 1D)(2F)3d 3P$ | 9, $2p^5(3p^2 3P)(4D)3d 3S$ 7, $2p^5(3p^2 1D)(2P)3d 1P$ |
| 34_1^o | 6999 955.71 | 88, $2p^5 3s(3P)(3d^2 3F) 3D$ | | |
| 35_1^o | 7009 064.96 | 10, $2p^5(3p^2 3P)(4P)3d 3D$ 7, $2p^5(3p^2 3P)(4D)3d 5F$ | 10, $2p^5(3p^2 3P)(2S)3d 3D$ 7, $2p^5(3p^2 1D)(2D)3d 1P$ | 8, $2p^5(3p^2 1D)(2D)3d 3D$ |
| 36_1^o | 7015 007.38 | 11, $2p^5(3p^2 3P)(4S)3d 5D$ 7, $2p^5(3p^2 1D)(2F)3d 3D$ | 11, $2p^5(3p^2 1D)(2P)3d 3D$ 7, $2p^5(3p^2 1S)(2P)3d 1P$ | 8, $2p^5(3p^2 3P)(2D)3d 1P$ |

Table 3 – continued

| Level index | Energy (cm ⁻¹) | Contributions (in per cent) | | |
|------------------------------|----------------------------|---|---|---|
| 37 ₁ ^o | 7018 904.13 | 24, 2p ⁵ (3p ² 3P)(² D)3d ¹ P 7, 2p ⁵ (3p ² 3P)(⁴ D)3d ³ P | 16, 2p ⁵ (3p ² 1D)(² D)3d ¹ P 7, 2p ⁵ (3p ² 3P)(² D)3d ³ D | 9, 2p ⁵ (3p ² 3P)(⁴ S)3d ³ D |
| 38 ₁ ^o | 7038 548.12 | 14, 2p ⁵ (3p ² 3P)(² D)3d ³ P 8, 2p ⁵ (3p ² 1S)(² P)3d ¹ P | 14, 2p ⁵ 3s(³ P)(3d ² 3P) ⁵ D 7, 2p ⁵ (3p ² 3P)(² P)3d ³ D | 12, 2p ⁵ 3s(³ P)(3d ² 3F) ⁵ D |
| 39 ₁ ^o | 7040 724.02 | 13, 2p ⁵ (3p ² 1D)(² F)3d ¹ P | 12, 2p ⁵ (3p ² 1D)(² D)3d ³ S | 7, 2p ⁵ (3p ² 1D)(² D)3d ¹ P |
| 40 ₁ ^o | 7046 813.82 | 49, 2p ⁵ 3s(³ P)(3d ² 3F) ⁵ D | 9, 2p ⁵ 3s(³ P)(3d ² 3P) ⁵ D | |
| 41 ₁ ^o | 7050 112.33 | 19, 2p ⁵ (3p ² 3P)(⁴ P)3d ³ D | 8, 2p ⁵ (3p ² 3P)(² P)3d ³ D | 7, 2p ⁵ (3p ² 3P)(⁴ S)3d ³ D |
| 42 ₁ ^o | 7059 660.35 | 71, 2p ⁵ 3s(³ P)(3d ² 3P) ³ D | 7, 2p ⁵ 3s(¹ P)(3d ² 3P) ³ S | |
| 43 ₁ ^o | 7064 022.85 | 13, 2p ⁵ (3p ² 3P)(⁴ S)3d ³ D 8, 2p ⁵ 3s(¹ P)(3d ² 3F) ³ D | 10, 2p ⁵ (3p ² 3P)(⁴ P)3d ³ P | 8, 2p ⁵ 3s(³ P)(3d ² 3F) ⁵ D |
| 44 ₁ ^o | 7069 206.33 | 20, 2p ⁵ (3p ² 1S)(² P)3d ³ P 7, 2p ⁵ 3s(³ P)(3d ² 3F) ⁵ D | 8, 2p ⁵ (3p ² 3P)(⁴ D)3d ³ D | 8, 2p ⁵ (3p ² 3P)(⁴ S)3d ³ D |
| 45 ₁ ^o | 7081 975.89 | 18, 2p ⁵ (3p ² 1D)(² P)3d ³ D 7, 2p ⁵ 3s(¹ P)(3d ² 3P) ³ P | 13, 2p ⁵ 3s(³ P)(3d ² 1D) ³ P | 12, 2p ⁵ (3p ² 3P)(² P)3d ³ P |
| 46 ₁ ^o | 7088 323.63 | 12, 2p ⁵ (3p ² 3P)(² D)3d ³ S | 9, 2p ⁵ (3p ² 1D)(² F)3d ³ D | 7, 2p ⁵ 3s(³ P)(3d ² 1D) ³ P |
| 47 ₁ ^o | 7096 320.01 | 18, 2p ⁵ (3p ² 3P)(⁴ D)3d ³ P 7, 2p ⁵ 3s(³ P)(3d ² 1D) ³ P | 10, 2p ⁵ (3p ² 3P)(⁴ D)3d ³ S | 7, 2p ⁵ (3p ² 3P)(⁴ P)3d ³ P |
| 48 ₁ ^o | 7097 641.29 | 16, 2p ⁵ 3s(¹ P)(3d ² 3P) ³ D 9, 2p ⁵ (3p ² 1D)(² D)3d ³ S | 13, 2p ⁵ 3s(³ P)(3d ² 3P) ⁵ P | 10, 2p ⁵ (3p ² 1D)(² P)3d ³ D |
| 49 ₁ ^o | 7102 194.62 | 30, 2p ⁵ 3s(¹ P)(3d ² 3P) ³ D 7, 2p ⁵ (3p ² 1D)(² D)3d ³ S | 10, 2p ⁵ (3p ² 3P)(⁴ D)3d ³ P | 8, 2p ⁵ 3s(¹ P)(3d ² 3P) ³ P |
| 50 ₁ ^o | 7108 998.97 | 15, 2p ⁵ (3p ² 3P)(⁴ D)3d ³ D | 15, 2p ⁵ (3p ² 3P)(² P)3d ³ D | 7, 2p ⁵ (3p ² 3P)(⁴ D)3d ³ S |
| 51 ₁ ^o | 7118 590.36 | 15, 2p ⁵ (3p ² 3P)(⁴ D)3d ³ S 8, 2p ⁵ (3p ² 3P)(² D)3d ³ P | 11, 2p ⁵ (3p ² 3P)(² D)3d ³ S 7, 2p ⁵ (3p ² 3P)(⁴ D)3d ³ P | 11, 2p ⁵ (3p ² 1S)(² P)3d ³ P |
| 52 ₁ ^o | 7121 107.39 | 21, 2p ⁵ 3s(¹ P)(3d ² 1D) ¹ P 7, 2p ⁵ (3p ² 1D)(² D)3d ³ D | 20, 2p ⁵ 3s(³ P)(3d ² 1D) ³ D 7, 2p ⁵ 3s(¹ P)(3d ² 3F) ³ D | 8, 2p ⁵ (3p ² 1S)(² P)3d ³ P |
| 53 ₁ ^o | 7134 194.37 | 17, 2p ⁵ 3s(³ P)(3d ² 1D) ³ P 7, 2p ⁵ 3s(³ P)(3d ² 3P) ³ S | 13, 2p ⁵ 3s(³ P)(3d ² 3P) ⁵ P 7, 2p ⁵ 3s(¹ P)(3d ² 1D) ¹ P | 8, 2p ⁵ (3p ² 1D)(² D)3d ³ S |
| 54 ₁ ^o | 7138 272.28 | 18, 2p ⁵ (3p ² 1D)(² F)3d ¹ P | 13, 2p ⁵ (3p ² 3P)(² P)3d ³ P | |
| 55 ₁ ^o | 7140 630.62 | 25, 2p ⁵ (3p ² 1D)(² F)3d ¹ P 8, 2p ⁵ (3p ² 1D)(² F)3d ³ P | 11, 2p ⁵ (3p ² 3P)(² P)3d ³ P | 9, 2p ⁵ 3s(³ P)(3d ² 3P) ¹ P |
| 56 ₁ ^o | 7144 478.01 | 19, 2p ⁵ (3p ² 3P)(⁴ S)3d ³ D | 13, 2p ⁵ 3s(³ P)(3d ² 3F) ⁵ F | 8, 2p ⁵ (3p ² 3P)(⁴ D)3d ³ D |
| 57 ₁ ^o | 7164 762.25 | 25, 2p ⁵ 3s(³ P)(3d ² 3P) ⁵ P | 11, 2p ⁵ 3s(¹ P)(3d ² 3P) ³ S | 8, 2p ⁵ 3s(¹ P)(3d ² 3F) ³ D |
| 58 ₁ ^o | 7170 702.77 | 29, 2p ⁵ 3s(³ P)(3d ² 3P) ⁵ D 7, 2p ⁵ 3s(¹ P)(3d ² 3P) ³ S | 22, 2p ⁵ (3p ² 1D)(² P)3d ³ P | 16, 2p ⁵ (3p ² 3P)(² P)3d ³ D |
| 59 ₁ ^o | 7171 829.48 | 14, 2p ⁵ 3s(³ P)(3d ² 3P) ³ S 8, 2p ⁵ 3s(³ P)(3d ² 3P) ³ D | 10, 2p ⁵ 3s(¹ P)(3d ² 3P) ³ S | 9, 2p ⁵ 3s(³ P)(3d ² 3F) ⁵ F |
| 60 ₁ ^o | 7196 956.72 | 36, 2p ⁵ 3s(¹ P)(3d ² 3P) ³ P | 17, 2p ⁵ 3s(¹ P)(3d ² 3P) ³ S | 9, 2p ⁵ (3p ² 1D)(² P)3d ¹ P |
| 61 ₁ ^o | 7208 809.42 | 44, 2p ⁵ 3s(³ P)(3d ² 3F) ⁵ F | 13, 2p ⁵ (3p ² 1S)(² P)3d ³ P | |
| 62 ₁ ^o | 7217 798.64 | 22, 2p ⁵ 3s(¹ P)(3d ² 3F) ³ D 8, 2p ⁵ 3s(¹ P)(3d ² 1D) ¹ P | 20, 2p ⁵ 3s(¹ P)(3d ² 1S) ¹ P 7, 2p ⁵ 3s(³ P)(3d ² 3P) ⁵ D | 16, 2p ⁵ 3s(³ P)(3d ² 1S) ³ P |
| 63 ₁ ^o | 7222 757.56 | 29, 2p ⁵ 3s(³ P)(3d ² 3P) ³ P | 9, 2p ⁵ 3s(³ P)(3d ² 1D) ³ P | |
| 64 ₁ ^o | 7236 310.32 | 17, 2p ⁵ 3s(³ P)(3d ² 1S) ³ P 9, 2p ⁵ 3s(¹ P)(3d ² 3F) ³ D | 12, 2p ⁵ (3p ² 3P)(² P)3d ¹ P | 11, 2p ⁵ 3s(¹ P)(3d ² 1S) ¹ P |
| 65 ₁ ^o | 7251 963.66 | 25, 2p ⁵ (3p ² 3P)(² P)3d ¹ P 7, 2p ⁵ 3s(¹ P)(3d ² 3P) ³ S | 14, 2p ⁵ (3p ² 1S)(² P)3d ³ D | 7, 2p ⁵ 3s(³ P)(3d ² 3P) ³ S |
| 66 ₁ ^o | 7261 771.50 | 19, 2p ⁵ 3s(¹ P)(3d ² 1D) ¹ P 8, 2p ⁵ 3s(³ P)(3d ² 3P) ³ S | 16, 2p ⁵ 3s(³ P)(3d ² 1D) ³ D | 8, 2p ⁵ 3s(¹ P)(3d ² 3F) ³ D |
| 67 ₁ ^o | 7297 507.81 | 12, 2p ⁵ 3s(¹ P)(3d ² 3P) ³ D | 9, 2p ⁵ 3s(³ P)(3d ² 3P) ³ P | 7, 2p ⁵ (3p ² 1D)(² D)3d ³ D |
| 68 ₁ ^o | 7311 658.30 | 40, 2p ⁵ 3s(³ P)(3d ² 1S) ³ P | 31, 2p ⁵ 3s(¹ P)(3d ² 1S) ¹ P | |
| 69 ₁ ^o | 7344 267.16 | 42, 2p ⁵ 3s(³ P)(3d ² 3P) ¹ P | 11, 2p ⁵ (3p ² 1D)(² F)3d ¹ P | |
| 70 ₁ ^o | 7714 655.12 | 72, 2p ⁵ (3d ³ 4F) ⁵ D | 19, 2p ⁵ (3d ³ 4F) ⁵ F | 8, 2p ⁵ (3d ³ 4P) ⁵ D |
| 71 ₁ ^o | 7733 634.82 | 58, 2p ⁵ (3d ³ 4F) ⁵ F | 16, 2p ⁵ (3d ³ 4F) ³ D | 13, 2p ⁵ (3d ³ 4F) ⁵ D |
| 72 ₁ ^o | 7770 067.00 | 28, 2p ⁵ (3d ³ 2P) ³ P 9, 2p ⁵ (3d ³ 2D) ³ D | 27, 2p ⁵ (3d ³ 2D) ³ P 8, 2p ⁵ (3d ³ 2D) ³ P | 11, 2p ⁵ (3d ³ 2P) ³ S |
| 73 ₁ ^o | 7782 871.89 | 16, 2p ⁵ (3d ³ 4P) ⁵ D 11, 2p ⁵ (3d ³ 4P) ³ D | 14, 2p ⁵ (3d ³ 2D) ³ D 8, 2p ⁵ (3d ³ 4P) ³ P | 13, 2p ⁵ (3d ³ 3D) ¹ P |
| 74 ₁ ^o | 7784 674.79 | 17, 2p ⁵ (3d ³ 4P) ⁵ P 11, 2p ⁵ (3d ³ 2P) ³ P | 15, 2p ⁵ (3d ³ 4P) ³ P 10, 2p ⁵ (3d ³ 2P) ³ S | 11, 2p ⁵ (3d ³ 2D) ³ D 8, 2p ⁵ (3d ³ 2D) ³ P |
| 75 ₁ ^o | 7794 765.11 | 37, 2p ⁵ (3d ³ 4P) ³ D | 32, 2p ⁵ (3d ³ 2F) ³ D | |
| 76 ₁ ^o | 7806 306.82 | 17, 2p ⁵ (3d ³ 2P) ³ S 11, 2p ⁵ (3d ³ 4P) ⁵ D | 16, 2p ⁵ (3d ³ 4P) ³ S 10, 2p ⁵ (3d ³ 2P) ¹ P | 15, 2p ⁵ (3d ³ 4P) ³ P |

Table 3 – *continued*

| Level index | Energy (cm ⁻¹) | | Contributions (in per cent) | |
|------------------------------|----------------------------|--|--|---|
| 77 ₁ ^o | 7823 526.67 | 34, 2p ⁵ (3d ³ 4P) ⁵ P 13, 2p ⁵ (3d ³ ² D) ¹ P | 16, 2p ⁵ (3d ³ ² P) ³ P | 13, 2p ⁵ (3d ³ ² D) ³ P |
| 78 ₁ ^o | 7841 169.07 | 39, 2p ⁵ (3d ³ ³ D) ³ P 7, 2p ⁵ (3d ³ 4P) ³ P | 13, 2p ⁵ (3d ³ ² F) ³ D | 10, 2p ⁵ (3d ³ 4P) ³ D |
| 79 ₁ ^o | 7851 139.10 | 20, 2p ⁵ (3d ³ 4P) ⁵ D 8, 2p ⁵ (3d ³ ² D) ³ D | 19, 2p ⁵ (3d ³ ² P) ³ D 7, 2p ⁵ (3d ³ ² P) ³ S | 17, 2p ⁵ (3d ³ 4P) ⁵ P |
| 80 ₁ ^o | 7860 735.41 | 18, 2p ⁵ (3d ³ ² D) ¹ P 11, 2p ⁵ (3d ³ ⁴ F) ³ D | 16, 2p ⁵ (3d ³ 4P) ⁵ D 10, 2p ⁵ (3d ³ ² D) ³ P | 15, 2p ⁵ (3d ³ ² P) ³ D |
| 81 ₁ ^o | 7874 067.28 | 26, 2p ⁵ (3d ³ ² D) ³ P 8, 2p ⁵ (3d ³ ⁴ F) ³ D | 18, 2p ⁵ (3d ³ ² F) ³ D 7, 2p ⁵ (3d ³ 4P) ³ D | 13, 2p ⁵ (3d ³ ² P) ³ P 7, 2p ⁵ (3d ³ ² P) ³ D |
| 82 ₁ ^o | 7888 117.15 | 15, 2p ⁵ (3d ³ ² P) ³ P 10, 2p ⁵ (3d ³ ² P) ³ S 7, 2p ⁵ (3d ³ 4P) ⁵ P | 10, 2p ⁵ (3d ³ ² F) ³ D 10, 2p ⁵ (3d ³ ² D) ³ D 7, 2p ⁵ (3d ³ ² P) ³ D | 10, 2p ⁵ (3d ³ ² D) ³ D 9, 2p ⁵ (3d ³ 4P) ³ D |
| 83 ₁ ^o | 7902 900.41 | 32, 2p ⁵ (3d ³ 4P) ³ P 9, 2p ⁵ (3d ³ ² D) ³ P | 15, 2p ⁵ (3d ³ ² D) ³ P 7, 2p ⁵ (3d ³ ⁴ F) ³ D | 9, 2p ⁵ (3d ³ 4P) ⁵ D |
| 84 ₁ ^o | 7928 082.97 | 38, 2p ⁵ (3d ³ ² D) ³ D 7, 2p ⁵ (3d ³ ⁴ F) ³ D | 18, 2p ⁵ (3d ³ ² D) ¹ P | 11, 2p ⁵ (3d ³ ² P) ¹ P |
| 85 ₁ ^o | 7943 443.25 | 36, 2p ⁵ (3d ³ ⁴ F) ³ D | 26, 2p ⁵ (3d ³ ² P) ³ D | 12, 2p ⁵ (3d ³ ² D) ³ D |
| 86 ₁ ^o | 7957 251.08 | 40, 2p ⁵ (3d ³ 4P) ³ S 8, 2p ⁵ (3d ³ ² D) ¹ P | 12, 2p ⁵ (3d ³ ² P) ³ S 7, 2p ⁵ (3d ³ 4P) ³ P | 8, 2p ⁵ (3d ³ ² D) ³ D |
| 87 ₁ ^o | 7971 441.35 | 38, 2p ⁵ (3d ³ ² P) ¹ P 9, 2p ⁵ (3d ³ 4P) ³ S | 21, 2p ⁵ (3d ³ ² D) ¹ P | 12, 2p ⁵ (3d ³ ² P) ³ S |
| 88 ₁ ^o | 8015 934.65 | 65, 2p ⁵ (3d ³ ² D) ¹ P | 24, 2p ⁵ (3d ³ ² D) ³ D | |

where $g_j = 2J_j + 1$ is the statistical weight of the excited-state level.

We present the electric-dipole transition array 2p–3l wavelengths λ_{ij} and the absorption oscillator strengths f_{ij} from the ground-state $2p^6 3s^2 S_{1/2}$ level to the individual levels of the upper state of Fe xvi in Table 4. In addition, we provide the associated emission transition probabilities A_{ji} from the excited $2p^5 3l$ configuration fine-structure levels $J = 1/2$ and $3/2$ to the ground state in the same table. The electric dipole transition probabilities presented here were calculated in the length form. Results sorted for the transition arrays between different total J values and listed in ascending wavelength.

The 2p–3l transition atomic data for Fe xv are presented in Table 5. In this case the selection rules allow only the transitions from the ground level $2p^6 3s^2 S_0$ to the fine-structure levels with $J = 1$ of the upper state having a vacancy in the 2p shell. The absorption oscillator strengths f_{ij} and emission transition probabilities A_{ji} were calculated in both the length and velocity form, although we choose to present only the data obtained in the length form. Data are once again presented in ascending wavelength.

4 DISCUSSION

To the best of our knowledge, there are no publicly available detailed atomic data (either theoretical or experimental) for electric dipole transitions involving the inner-shell 2p electrons in Fe xv and Fe xvi. The situation is similar for the lower ionization stages of iron ions.

In this context, the work of Behar et al. (2001) should be mentioned, where the calculation of atomic data and their use for the modelling of Fe⁰⁺–Fe¹⁵⁺ absorption spectra was reported. As a result of the need to obtain large quantities of atomic data, and for the sake of simplifying the computations, the approximation used in their work was very limited in choosing the CI wavefunc-

tion expansion. When considering 2p excited states, the configuration mixing was restricted to $2s^2 2p^5 [3s^2 3d + 3p^2]$ in the case of Fe xvi and to $2s^2 2p^5 [3s^2 3d + 3s 3p^2]$ for Fe xv. Unfortunately, we cannot make a comparison of our atomic data with those of Behar et al. (2001), because detailed results on electric dipole transitions (line wavelengths, oscillator strengths) were not presented in their paper. Instead, we examine internal indicators of the accuracy of our calculated atomic data, as discussed by Hibbert (1996).

One of the possible ways to evaluate the accuracy of the calculated E1-transition atomic data is to compare f -values estimated using the length form (equation 6) against those obtained using the velocity form (equation 7). Good agreement would provide support for the accuracy of the wavefunctions used in the calculation, and indicate that they should lead to reliable atomic data. A traditional way to do this is to plot $\log(f_v)$ against $\log(f_L)$.

In Fig. 1 the velocity-form oscillator strengths $\log(f_v)$ are plotted against the length-form oscillator strengths $\log(f_L)$ for all lines from the 2p–3l transition array in Fe xvi. We present a comparison for the three different wavefunction expansions. The first set of data (*set 1*) was calculated using a truncated CI wavefunction expansion consisting only of the configurations with $n = 3$ electrons from the configuration set described in Section 2.2. The next set of data (*set 2*) was calculated by adding configurations having one $n = 4$ electron, whereas the last set (*set 3*) was calculated with the wavefunction expansion including all configurations listed in Section 2.2.

One can see from Fig. 1 that there is good agreement between the length- and velocity-form transition data in general, and that the best agreement is achieved including all described configurations in the wavefunction expansion. In this case agreement is within 10 per cent, with the exception of a few transitions that have oscillator strengths $f_{if} < 5 \times 10^{-5}$. These lines represent transitions to the levels of the $2p^5 3d^2$ configurations, which would be forbidden in non-relativistic LS -coupling.

Table 4. Electric dipole transition 2p–3l wavelengths λ (in Å), absorption oscillator strengths f_{ij} (in au) and corresponding emission transition probabilities A_{ji} (in s⁻¹) for the Fe xv 6 ions.

| Level index lower | upper | λ (Å) | f_{ij} | A_{ji} (s ⁻¹) |
|-------------------------------|--------------------------------|---------------|------------|-----------------------------|
| 1/2–1/2 | | | | |
| 1 ^e _{1/2} | 18 ^o _{1/2} | 13.594 43 | 1.987 (–5) | 7.173 (+8) |
| 1 ^e _{1/2} | 17 ^o _{1/2} | 13.717 88 | 5.537 (–4) | 1.963 (+10) |
| 1 ^e _{1/2} | 16 ^o _{1/2} | 13.792 25 | 7.443 (–6) | 2.610 (+8) |
| 1 ^e _{1/2} | 15 ^o _{1/2} | 13.859 80 | 5.289 (–4) | 1.837 (+10) |
| 1 ^e _{1/2} | 14 ^o _{1/2} | 13.975 32 | 4.119 (–4) | 1.407 (+10) |
| 1 ^e _{1/2} | 13 ^o _{1/2} | 13.998 06 | 3.010 (–4) | 1.025 (+10) |
| 1 ^e _{1/2} | 12 ^o _{1/2} | 14.112 33 | 3.466 (–8) | 1.161 (+6) |
| 1 ^e _{1/2} | 11 ^o _{1/2} | 15.083 31 | 7.956 (–1) | 2.333 (+13) |
| 1 ^e _{1/2} | 10 ^o _{1/2} | 15.243 10 | 4.390 (–4) | 1.260 (+10) |
| 1 ^e _{1/2} | 9 ^o _{1/2} | 15.272 88 | 7.625 (–4) | 2.180 (+10) |
| 1 ^e _{1/2} | 8 ^o _{1/2} | 15.384 17 | 1.129 (–1) | 3.183 (+12) |
| 1 ^e _{1/2} | 7 ^o _{1/2} | 15.457 84 | 1.275 (–2) | 3.560 (+11) |
| 1 ^e _{1/2} | 6 ^o _{1/2} | 15.539 61 | 2.693 (–6) | 7.440 (+7) |
| 1 ^e _{1/2} | 5 ^o _{1/2} | 15.586 91 | 1.261 (–3) | 3.463 (+10) |
| 1 ^e _{1/2} | 4 ^o _{1/2} | 15.626 60 | 1.592 (–3) | 4.348 (+10) |
| 1 ^e _{1/2} | 3 ^o _{1/2} | 15.748 02 | 3.106 (–3) | 8.353 (+10) |
| 1 ^e _{1/2} | 2 ^o _{1/2} | 15.837 34 | 9.166 (–3) | 2.438 (+11) |
| 1 ^e _{1/2} | 1 ^o _{1/2} | 16.965 14 | 3.091 (–2) | 7.163 (+11) |
| 1/2–1/3 | | | | |
| 1 ^e _{1/2} | 27 ^o _{3/2} | 13.658 53 | 1.454 (–3) | 2.599 (+10) |
| 1 ^e _{1/2} | 26 ^o _{3/2} | 13.677 26 | 4.204 (–7) | 7.495 (+6) |
| 1 ^e _{1/2} | 25 ^o _{3/2} | 13.764 28 | 5.341 (–4) | 9.402 (+9) |
| 1 ^e _{1/2} | 24 ^o _{3/2} | 13.791 85 | 1.127 (–9) | 1.977 (+4) |
| 1 ^e _{1/2} | 23 ^o _{3/2} | 13.826 33 | 5.497 (–4) | 9.590 (+9) |
| 1 ^e _{1/2} | 22 ^o _{3/2} | 13.889 70 | 3.987 (–5) | 6.892 (+8) |
| 1 ^e _{1/2} | 21 ^o _{3/2} | 13.925 89 | 4.573 (–5) | 7.864 (+8) |
| 1 ^e _{1/2} | 20 ^o _{3/2} | 13.977 07 | 3.999 (–4) | 6.827 (+9) |
| 1 ^e _{1/2} | 19 ^o _{3/2} | 14.012 58 | 2.020 (–7) | 3.430 (+6) |
| 1 ^e _{1/2} | 18 ^o _{3/2} | 14.027 40 | 2.638 (–4) | 4.472 (+9) |
| 1 ^e _{1/2} | 17 ^o _{3/2} | 14.107 69 | 2.463 (–7) | 4.127 (+6) |
| 1 ^e _{1/2} | 16 ^o _{3/2} | 14.996 28 | 6.975 (–1) | 1.034 (+13) |
| 1 ^e _{1/2} | 15 ^o _{3/2} | 15.153 71 | 8.419 (–1) | 1.223 (+13) |
| 1 ^e _{1/2} | 14 ^o _{3/2} | 15.204 39 | 1.666 (–2) | 2.403 (+11) |
| 1 ^e _{1/2} | 13 ^o _{3/2} | 15.282 52 | 1.362 (–2) | 1.945 (+11) |
| 1 ^e _{1/2} | 12 ^o _{3/2} | 15.321 19 | 1.190 (–1) | 1.691 (+12) |
| 1 ^e _{1/2} | 11 ^o _{3/2} | 15.408 44 | 1.587 (–1) | 2.230 (+12) |
| 1 ^e _{1/2} | 10 ^o _{3/2} | 15.470 88 | 5.816 (–3) | 8.104 (+10) |
| 1 ^e _{1/2} | 9 ^o _{3/2} | 15.484 86 | 2.295 (–4) | 3.192 (+9) |
| 1 ^e _{1/2} | 8 ^o _{3/2} | 15.512 47 | 3.322 (–3) | 4.605 (+10) |
| 1 ^e _{1/2} | 7 ^o _{3/2} | 15.558 63 | 6.313 (–4) | 8.698 (+9) |
| 1 ^e _{1/2} | 6 ^o _{3/2} | 15.569 17 | 5.667 (–3) | 7.797 (+10) |
| 1 ^e _{1/2} | 5 ^o _{3/2} | 15.603 74 | 1.235 (–3) | 1.691 (+10) |
| 1 ^e _{1/2} | 4 ^o _{3/2} | 15.749 19 | 9.991 (–6) | 1.343 (+8) |
| 1 ^e _{1/2} | 3 ^o _{3/2} | 15.793 10 | 8.938 (–3) | 1.195 (+11) |
| 1 ^e _{1/2} | 2 ^o _{3/2} | 15.843 53 | 4.425 (–3) | 5.880 (+10) |
| 1 ^e _{1/2} | 1 ^o _{3/2} | 17.246 21 | 6.272 (–2) | 7.033 (+11) |

Another trend evident from Fig. 1 is that inclusion of the configurations with the $\bar{4}l$ correlation orbitals significantly changes some f -values (compare *set 1* and *set 2*). A more detailed analysis of data reveals that electric dipole transition oscillator strengths change by up to 30 per cent, even for stronger ($f_L > 10^{-2}$) lines. Consequently, it allows us to conclude that use of a limited CI wavefunction expansion with only $n = 3$ shell configurations included (as

Table 5. Electric dipole transition 2p–3l wavelengths λ (in Å), absorption oscillator strengths f_{ij} (in au) and corresponding emission transition probabilities A_{ji} (in s⁻¹) for the Fe xv 6 ions.

| Level index lower | upper | λ (Å) | f_{ij} | A_{ji} (s ⁻¹) |
|-----------------------------|------------------------------|---------------|-------------|-----------------------------|
| 1 ^e ₀ | 88 ^o ₁ | 12.475 15 | 3.446 (–6) | 4.923 (+7) |
| 1 ^e ₀ | 87 ^o ₁ | 12.544 78 | 5.546 (–6) | 7.836 (+7) |
| 1 ^e ₀ | 86 ^o ₁ | 12.567 15 | 2.883 (–7) | 4.058 (+6) |
| 1 ^e ₀ | 85 ^o ₁ | 12.589 00 | 5.302 (–7) | 7.438 (+6) |
| 1 ^e ₀ | 84 ^o ₁ | 12.613 39 | 4.057 (–6) | 5.670 (+7) |
| 1 ^e ₀ | 83 ^o ₁ | 12.653 58 | 1.046 (–6) | 1.453 (+7) |
| 1 ^e ₀ | 82 ^o ₁ | 12.677 30 | 5.240 (–7) | 7.249 (+6) |
| 1 ^e ₀ | 81 ^o ₁ | 12.699 92 | 5.884 (–9) | 8.111 (+4) |
| 1 ^e ₀ | 80 ^o ₁ | 12.721 45 | 5.535 (–7) | 7.604 (+6) |
| 1 ^e ₀ | 79 ^o ₁ | 12.737 00 | 1.050 (–6) | 1.439 (+7) |
| 1 ^e ₀ | 78 ^o ₁ | 12.753 20 | 3.090 (–8) | 4.225 (+5) |
| 1 ^e ₀ | 77 ^o ₁ | 12.781 96 | 3.705 (–7) | 5.043 (+6) |
| 1 ^e ₀ | 76 ^o ₁ | 12.810 15 | 1.750 (–7) | 2.371 (+6) |
| 1 ^e ₀ | 75 ^o ₁ | 12.829 12 | 1.294 (–7) | 1.749 (+6) |
| 1 ^e ₀ | 74 ^o ₁ | 12.845 75 | 3.456 (–9) | 4.657 (+4) |
| 1 ^e ₀ | 73 ^o ₁ | 12.848 73 | 6.551 (–8) | 8.823 (+5) |
| 1 ^e ₀ | 72 ^o ₁ | 12.869 90 | 2.546 (–8) | 3.418 (+5) |
| 1 ^e ₀ | 71 ^o ₁ | 12.930 53 | 5.309 (–9) | 7.059 (+4) |
| 1 ^e ₀ | 70 ^o ₁ | 12.962 34 | 2.689 (–10) | 3.558 (+3) |
| 1 ^e ₀ | 69 ^o ₁ | 13.616 06 | 1.162 (–3) | 1.394 (+10) |
| 1 ^e ₀ | 68 ^o ₁ | 13.676 79 | 1.857 (–6) | 2.207 (+7) |
| 1 ^e ₀ | 67 ^o ₁ | 13.703 31 | 1.472 (–5) | 1.743 (+8) |
| 1 ^e ₀ | 66 ^o ₁ | 13.770 74 | 1.837 (–3) | 2.154 (+10) |
| 1 ^e ₀ | 65 ^o ₁ | 13.789 37 | 3.250 (–7) | 3.801 (+6) |
| 1 ^e ₀ | 64 ^o ₁ | 13.819 20 | 4.788 (–6) | 5.574 (+7) |
| 1 ^e ₀ | 63 ^o ₁ | 13.845 13 | 2.414 (–4) | 2.800 (+9) |
| 1 ^e ₀ | 62 ^o ₁ | 13.854 64 | 4.200 (–4) | 4.865 (+9) |
| 1 ^e ₀ | 61 ^o ₁ | 13.871 91 | 3.087 (–4) | 3.566 (+9) |
| 1 ^e ₀ | 60 ^o ₁ | 13.894 76 | 1.149 (–5) | 1.324 (+8) |
| 1 ^e ₀ | 59 ^o ₁ | 13.943 44 | 5.158 (–5) | 5.899 (+8) |
| 1 ^e ₀ | 58 ^o ₁ | 13.945 63 | 1.952 (–5) | 2.232 (+8) |
| 1 ^e ₀ | 57 ^o ₁ | 13.957 20 | 1.174 (–4) | 1.340 (+9) |
| 1 ^e ₀ | 56 ^o ₁ | 13.996 82 | 1.189 (–4) | 1.349 (+9) |
| 1 ^e ₀ | 55 ^o ₁ | 14.004 36 | 9.948 (–5) | 1.128 (+9) |
| 1 ^e ₀ | 54 ^o ₁ | 14.008 99 | 2.818 (–4) | 3.193 (+9) |
| 1 ^e ₀ | 53 ^o ₁ | 14.017 00 | 3.365 (–4) | 3.808 (+9) |
| 1 ^e ₀ | 52 ^o ₁ | 14.042 76 | 1.320 (–3) | 1.489 (+10) |
| 1 ^e ₀ | 51 ^o ₁ | 14.047 72 | 1.004 (–4) | 1.131 (+9) |
| 1 ^e ₀ | 50 ^o ₁ | 14.066 68 | 1.317 (–5) | 1.480 (+8) |
| 1 ^e ₀ | 49 ^o ₁ | 14.080 15 | 8.581 (–5) | 9.624 (+8) |
| 1 ^e ₀ | 48 ^o ₁ | 14.089 19 | 3.071 (–4) | 3.440 (+9) |
| 1 ^e ₀ | 47 ^o ₁ | 14.091 81 | 1.991 (–6) | 2.229 (+7) |
| 1 ^e ₀ | 46 ^o ₁ | 14.107 71 | 4.439 (–5) | 4.958 (+8) |
| 1 ^e ₀ | 45 ^o ₁ | 14.120 35 | 4.482 (–4) | 4.998 (+9) |
| 1 ^e ₀ | 44 ^o ₁ | 14.145 86 | 1.285 (–5) | 1.428 (+8) |
| 1 ^e ₀ | 43 ^o ₁ | 14.156 24 | 2.574 (–4) | 2.855 (+9) |
| 1 ^e ₀ | 42 ^o ₁ | 14.164 99 | 4.758 (–6) | 5.273 (+7) |
| 1 ^e ₀ | 41 ^o ₁ | 14.184 17 | 7.814 (–5) | 8.635 (+8) |
| 1 ^e ₀ | 40 ^o ₁ | 14.190 81 | 1.252 (–6) | 1.382 (+7) |
| 1 ^e ₀ | 39 ^o ₁ | 14.203 08 | 1.630 (–6) | 1.796 (+7) |
| 1 ^e ₀ | 38 ^o ₁ | 14.207 47 | 5.930 (–5) | 6.532 (+8) |
| 1 ^e ₀ | 37 ^o ₁ | 14.247 24 | 6.640 (–6) | 5.082 (+7) |
| 1 ^e ₀ | 36 ^o ₁ | 14.255 15 | 7.714 (–5) | 8.440 (+8) |
| 1 ^e ₀ | 35 ^o ₁ | 14.267 24 | 4.627 (–6) | 5.054 (+7) |
| 1 ^e ₀ | 34 ^o ₁ | 14.285 80 | 5.342 (–8) | 5.820 (+5) |
| 1 ^e ₀ | 33 ^o ₁ | 14.293 43 | 1.647 (–5) | 1.792 (+8) |
| 1 ^e ₀ | 32 ^o ₁ | 14.299 66 | 2.027 (–5) | 2.204 (+8) |
| 1 ^e ₀ | 31 ^o ₁ | 14.310 04 | 7.542 (–6) | 8.189 (+7) |
| 1 ^e ₀ | 30 ^o ₁ | 14.326 85 | 5.127 (–6) | 5.554 (+7) |
| 1 ^e ₀ | 29 ^o ₁ | 14.337 13 | 6.547 (–6) | 7.081 (+7) |

Table 5 – *continued*

| Level index lower | Level index upper | λ (Å) | f_{ij} | A_{ji} (s ⁻¹) |
|----------------------|------------------------------|---------------|------------|-----------------------------|
| 1e ₀ | 28 ₁ ^o | 14.353 32 | 7.163 (−5) | 7.731 (+8) |
| 1e ₀ | 27 ₁ ^o | 14.367 98 | 9.178 (−5) | 9.885 (+8) |
| 1e ₀ | 26 ₁ ^o | 14.398 59 | 1.657 (−6) | 1.777 (+7) |
| 1e ₀ | 25 ₁ ^o | 14.406 12 | 8.682 (−6) | 9.301 (+7) |
| 1e ₀ | 24 ₁ ^o | 14.435 26 | 1.757 (−6) | 1.875 (+7) |
| 1e ₀ | 23 ₁ ^o | 14.488 12 | 3.125 (−5) | 3.310 (+8) |
| 1e ₀ | 22 ₁ ^o | 14.490 38 | 3.117 (−5) | 3.301 (+8) |
| 1e ₀ | 21 ₁ ^o | 14.514 39 | 8.704 (−7) | 9.186 (+6) |
| 1e ₀ | 20 ₁ ^o | 14.571 13 | 1.469 (−6) | 1.538 (+7) |
| 1e ₀ | 19 ₁ ^o | 14.609 99 | 1.157 (−5) | 1.205 (+8) |
| 1e ₀ | 18 ₁ ^o | 14.618 37 | 8.970 (−7) | 9.333 (+6) |
| 1e ₀ | 17 ₁ ^o | 15.227 86 | 1.795 (+0) | 1.721 (+13) |
| 1e ₀ | 16 ₁ ^o | 15.374 88 | 1.383 (−1) | 1.301 (+12) |
| 1e ₀ | 15 ₁ ^o | 15.479 99 | 6.003 (−1) | 5.570 (+12) |
| 1e ₀ | 14 ₁ ^o | 15.538 14 | 1.701 (−2) | 1.567 (+11) |
| 1e ₀ | 13 ₁ ^o | 15.572 87 | 6.211 (−3) | 5.694 (+10) |
| 1e ₀ | 12 ₁ ^o | 15.608 17 | 7.247 (−3) | 6.615 (+10) |
| 1e ₀ | 11 ₁ ^o | 15.655 54 | 2.533 (−2) | 2.298 (+11) |
| 1e ₀ | 10 ₁ ^o | 15.745 90 | 2.410 (−3) | 2.161 (+10) |
| 1e ₀ | 9 ₁ ^o | 15.779 71 | 4.131 (−2) | 3.689 (+11) |
| 1e ₀ | 8 ₁ ^o | 15.799 84 | 1.287 (−4) | 1.146 (+9) |
| 1e ₀ | 7 ₁ ^o | 15.901 79 | 1.991 (−4) | 1.751 (+9) |
| 1e ₀ | 6 ₁ ^o | 15.978 80 | 1.256 (−3) | 1.093 (+10) |
| 1e ₀ | 5 ₁ ^o | 16.008 89 | 5.987 (−2) | 5.194 (+11) |
| 1e ₀ | 4 ₁ ^o | 16.046 49 | 1.058 (−2) | 9.138 (+10) |
| 1e ₀ | 3 ₁ ^o | 16.151 78 | 1.277 (−5) | 1.088 (+8) |
| 1e ₀ | 2 ₁ ^o | 16.195 18 | 4.040 (−5) | 3.425 (+8) |
| 1e ₀ | 1 ₁ ^o | 16.266 14 | 1.669 (−4) | 1.403 (+9) |

in *set 1*) is not sufficient to achieve a reasonable accuracy for f values.

While comparing the *set 2* and *set 3* figures, one can see that agreement between f_L and f_V is much better in the case of wavefunction expansion having configurations with one and two electrons in the $n = 4$ shell. Nevertheless, while considering the differences between f_L values from these two sets, we note that they change by only a few per cent for the stronger lines (having $f_L > 10^{-3}$) and by no more than 10 per cent for the lines with $10^{-6} < f_L < 10^{-3}$. Therefore, we conclude that using the full set of configurations described in Section 2.2 allows us to achieve convergence for 2p–3l transition oscillator strengths, and to determine reliable atomic data. The addition of more excited configurations into the wavefunction expansion, such as $n = 5$ shell configurations or configurations with two electrons excited from the 2p shell, should not change the derived values of oscillator strengths significantly.

In Fig. 2 the velocity-form oscillator strengths $\log(f_V)$ are plotted against the length-form oscillator strengths $\log(f_L)$ for all lines from the 2p–3l transition array in Fe xv. Here we have two different arrays: transitions to the excited-state $J = 1/2$ levels (circles) and those to the $J = 3/2$ levels (triangles). Similarly to the previous figure, a comparison is made for the three different sets of CSFs for Fe xv, arranged using the same rules as for Fe xvi.

The pattern of f -value changes here is similar to the earlier case; the introduction of configurations with $n = 4$ electrons significantly changes the oscillator strength data from *set 1* to *set 2*. The agreement between f_L and f_V is better when a full set of configurations with one and two electrons in the $n = 4$ shell is included, as described in Section 2.2. Very good agreement between f_L and f_V can be achieved for all lines with $f_L > 5 \times 10^{-5}$, and for most of the weaker lines. There are some exceptions to this rule where

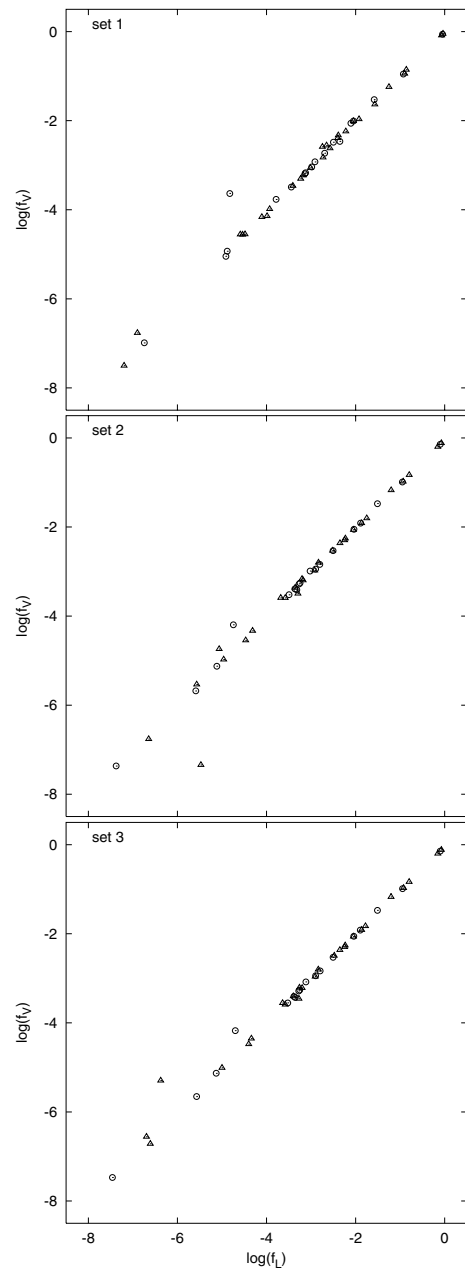


Figure 1. Comparison of the oscillator strengths in the length and velocity forms of the E1 transition operator for the Fe xvi ion calculated with different sets of CSFs.

the differences between the two forms is more evident, but these lines are comparatively weak and correspond to the transitions to the levels marked 39₁^o, 40₁^o, 42₁^o, 64₁^o, 65₁^o, 67₁^o, 68₁^o and 74₁^o. As one can see from Table 3, the leading contributions to these levels come from the ³L or ⁵L terms of the 3p²3d, 3s3d² and 3d³ configurations, and therefore the E1 transitions to these terms are forbidden in pure LS coupling.

One of the possible ways to improve the accuracy of the calculated oscillator strengths would be a further increase of the CSF numbers in a wavefunction expansion. Although we can make only a very general quantitative estimate, we do not think that this extension will change the calculated f -values by more than 10 per cent. Therefore, we conclude that the atomic data presented here are of high

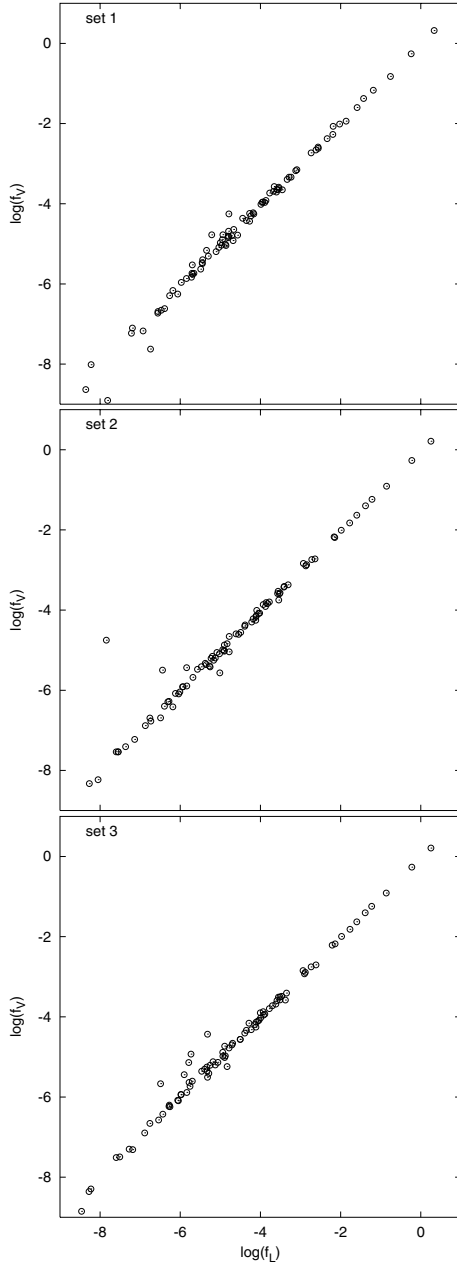


Figure 2. Comparison of the oscillator strengths in the length and velocity forms of the E1 transition operator for the Fe xv ion calculated with different sets of CSFs. Circles denote the 1/2–1/2 transitions and triangles denote the 1/2–3/2 transitions.

accuracy, and may be employed for the modelling of plasma X-ray spectra.

As in the case of oscillator strengths, we can perform convergence tests for the E1-transition wavelengths. In Table 6, we present transition wavelengths λ for the strongest lines ($f_L \geq 10^{-3}$) in Fe xvi and Fe xv obtained using all configurations described earlier (*set 3*) in the CSF expansion for wavefunction. Alongside, we present the percentage deviations $\delta\lambda_i(\%) = 100 \times (\lambda_i - \lambda)\lambda^{-1}$ for the wavelengths, obtained using truncated wavefunction expansions of *set 1* for the $\delta\lambda_1$ and *set 2* for $\delta\lambda_2$. It is quite evident from Table 6 that expansion of CSF basis leads to the convergence of the calculated transition wavelengths. In the case of Fe xvi, the average absolute value of $\delta\lambda_1 = 0.070\%$, whereas $\delta\lambda_2 = 0.015\%$ for the

Table 6. Electric dipole transition wavelengths λ (in Å) for selected lines of the Fe xvi and Fe xv ions and the deviations $\delta\lambda_i$ (in per cents) from the corresponding line wavelengths calculated with different sets of CSFs.

| Level index | | $\lambda(\text{Å})$ | $\delta\lambda_1(\%)$ | $\delta\lambda_2(\%)$ |
|-------------|--------------|---------------------|-----------------------|-----------------------|
| lower | upper | | | |
| Fe xvi | | | | |
| $1^e_{1/2}$ | $1^o_{1/2}$ | 16.965 14 | −0.187 | 0.004 |
| $1^e_{1/2}$ | $2^o_{1/2}$ | 15.837 34 | 0.027 | 0.002 |
| $1^e_{1/2}$ | $3^o_{1/2}$ | 15.748 02 | 0.050 | 0.002 |
| $1^e_{1/2}$ | $4^o_{1/2}$ | 15.626 60 | 0.034 | 0.001 |
| $1^e_{1/2}$ | $5^o_{1/2}$ | 15.586 91 | −0.064 | 0.003 |
| $1^e_{1/2}$ | $7^o_{1/2}$ | 15.457 84 | −0.042 | 0.001 |
| $1^e_{1/2}$ | $8^o_{1/2}$ | 15.384 17 | −0.082 | 0.001 |
| $1^e_{1/2}$ | $11^o_{1/2}$ | 15.083 31 | −0.258 | −0.002 |
| $1^e_{1/2}$ | $1^o_{3/2}$ | 17.246 21 | −0.190 | 0.004 |
| $1^e_{1/2}$ | $2^o_{3/2}$ | 15.843 53 | 0.029 | 0.001 |
| $1^e_{1/2}$ | $3^o_{3/2}$ | 15.793 10 | 0.034 | 0.002 |
| $1^e_{1/2}$ | $5^o_{3/2}$ | 15.603 74 | 0.048 | 0.002 |
| $1^e_{1/2}$ | $6^o_{3/2}$ | 15.569 17 | −0.022 | 0.003 |
| $1^e_{1/2}$ | $8^o_{3/2}$ | 15.512 47 | 0.047 | −0.010 |
| $1^e_{1/2}$ | $10^o_{3/2}$ | 15.470 88 | −0.049 | 0.002 |
| $1^e_{1/2}$ | $11^o_{3/2}$ | 15.408 44 | −0.067 | 0.000 |
| $1^e_{1/2}$ | $12^o_{3/2}$ | 15.321 19 | −0.074 | 0.000 |
| $1^e_{1/2}$ | $13^o_{3/2}$ | 15.282 52 | −0.057 | 0.003 |
| $1^e_{1/2}$ | $14^o_{3/2}$ | 15.204 39 | −0.097 | −0.002 |
| $1^e_{1/2}$ | $15^o_{3/2}$ | 15.153 71 | −0.159 | −0.001 |
| $1^e_{1/2}$ | $16^o_{3/2}$ | 14.996 28 | −0.181 | −0.004 |
| $1^e_{1/2}$ | $27^o_{3/2}$ | 13.658 53 | −0.162 | −0.027 |
| Fe xv | | | | |
| 1^e_0 | 4^o_1 | 16.046 49 | −0.064 | 0.008 |
| 1^e_0 | 5^o_1 | 16.008 89 | −0.069 | 0.005 |
| 1^e_0 | 6^o_1 | 15.978 80 | −0.035 | 0.009 |
| 1^e_0 | 9^o_1 | 15.779 71 | −0.070 | −0.004 |
| 1^e_0 | 10^o_1 | 15.745 90 | −0.118 | 0.004 |
| 1^e_0 | 11^o_1 | 15.655 54 | −0.058 | −0.001 |
| 1^e_0 | 12^o_1 | 15.608 17 | −0.131 | 0.000 |
| 1^e_0 | 13^o_1 | 15.572 87 | −0.067 | −0.013 |
| 1^e_0 | 14^o_1 | 15.538 14 | −0.105 | 0.000 |
| 1^e_0 | 15^o_1 | 15.479 99 | −0.210 | −0.001 |
| 1^e_0 | 16^o_1 | 15.374 88 | −0.165 | −0.002 |
| 1^e_0 | 17^o_1 | 15.227 86 | −0.314 | −0.005 |
| 1^e_0 | 52^o_1 | 14.042 76 | −0.122 | −0.023 |
| 1^e_0 | 66^o_1 | 13.770 74 | −0.235 | −0.023 |
| 1^e_0 | 69^o_1 | 13.616 06 | −0.305 | −0.030 |

$J = 1/2 - 1/2$ transitions and $\delta\lambda_1 = 0.063\%$, $\delta\lambda_2 = 0.012\%$ for the $J = 1/2 - 3/2$ transitions. In case of Fe xv, the corresponding values are $\delta\lambda_1 = 0.099\%$, $\delta\lambda_2 = 0.022\%$. The maximum value of difference between *set 2* and *set 3* results is 0.1% for both Fe xvi and Fe xv ions.

It is not possible to determine an absolute value of the transition wavelength λ accuracy obtained in our ab initio calculation. We can only estimate that calculated energy differences ΔE are accurate to about 0.05–0.06 au. For the $2p - 3l$ transitions considered here, it would give an estimated wavelength accuracy of 0.2%, twice the actual deviation between sets 2 and 3.

5 CONCLUSIONS

We have presented extensive calculations of energy levels, transition wavelengths, absorption oscillator strengths and emission transition probabilities for Fe xvi and Fe xv. Atomic data for the

electric dipole transitions representing the inner-shell transition array $2p-3l$ were determined using the configuration-interaction method implemented in the CIV3 code. As a result of the lack of available previous atomic data, it was not possible to make a comparison of our calculations with experimental values or with the results of other calculations. However, our results indicate satisfactory agreement between length and velocity oscillator strength forms. Therefore, we conclude that the data are generally of high accuracy, and suitable for applications in plasma X-ray spectral modelling.

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REFERENCES

Ballantyne D.R., Ross R.R., Fabian A.C., 2002, MNRAS, 336, 867
Behar E., Sako M., Kahn S.M., 2001, ApJ, 563, 497

Clementi E., Roetti C., 1974, At. Data Nucl. Data Tables, 14, 177
Ferland G.J., Korista K.T., Verner D.A., Ferguson J.W., Kingdon J.B., Verner E.M., 1998, PASP, 110, 761
Foord M.E. et al., 2001, in Ferland G., Savin D.W., eds, ASP Conf. Ser., Vol. 247, Spectroscopic Challenges of Photoionized Plasmas. Astron. Soc. Pac., San Francisco, p. 117
Hibbert A., 1975, Comput. Phys. Commun., 9, 141
Hibbert A., 1996, Physica Scripta, T65, 104
Hibbert A., Glass R., Froese Fischer C., 1991, Comput. Phys. Commun., 64, 455
Kallman T., Bautista M., 2001, ApJSS, 133, 221
Kaspi S., Brandt W.N., Netzer H., Sambruna R., Chartas G., Garmire G.P., Nousek J.A., 2000, ApJ, 535, L17
Rose S.J., 1998, J. Phys. B: At. Mol. Opt. Phys., 31, 2129
Schurch N.J., Warwick R.S., 2002, MNRAS, 334, 811
Yang Y., Wilson A.S., Ferruit P., 2001, ApJ, 563, 124

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