Energy levels and radiative rates for transitions in Fe V, Co VI and Ni VII

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Abstract
Energy levels, Landé g-factors and radiative lifetimes are reported for the lowest 182 levels of the 3d^1, 3d^34s and 3d^34p configurations of Fe V, Co VI and Ni VII. Additionally, radiative rates (A-values) have been calculated for the E1, E2 and M1 transitions among these levels. The calculations have been performed in a quasi-relativistic approach (QR) with a very large configuration interaction (CI) wavefunction expansion, which has been found to be necessary for these ions. Our calculated energies for all ions are in excellent agreement with the available measurements, for most levels. Discrepancies among various calculations for the radiative rates of E1 transitions in Fe V are up to a factor of two for stronger transitions (f ≥ 0.1), and larger (over an order of magnitude) for weaker ones. The reasons for these discrepancies have been discussed and mainly are due to the differing amount of CI and methodologies adopted. However, there are no appreciable discrepancies in similar data for M1 and E2 transitions, or the g-factors for the levels of Fe V, the only ion for which comparisons are feasible.

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Emission lines of iron group elements, particularly of Fe and Ni, show rich spectra covering a wide wavelength range in a variety of solar and astrophysical plasmas. Their lines are observed from almost all ionisation stages as may be noted from the Atomic Line List (v2.04) of Peter van Hoof (http://www.pa.uky.edu/~peter/atomic/), CHIANTI database [1, 2] at http://www.chiantidatabase.org and the atomic and molecular database Stout [3]. Similarly, many of these elements are also useful for studies of fusion plasmas. However, to reliably model the spectral lines in plasmas, atomic data are required for several parameters, such as energy levels and radiative rates (A-values). Therefore, over the past few decades several workers have reported data for many such ions, including ourselves – see for example [4–6]. However, (in general) most of the work has been performed for highly ionised systems and comparatively less attention has been paid to the lowly ionised species. This is because such ions are more problematic and usually require much larger calculations to achieve a reasonably satisfactory level of accuracy.

Iron is a very important element for both astrophysical and fusion plasma studies, and emission and absorption lines of Fe V have been observed in many hot stars and nebulae – see for example, Kramida [7] and references therein. Its lines have also been observed in white dwarfs [8] and are useful for the study of the fine-structure constant in a gravitational field. The first investigation of the Fe V spectrum was undertaken as early as 1937 by Bowen [9], who identified 57 levels of the 3d^4, 3d^34s and 3d^34p configurations. This study was subsequently extended by other workers, such as [10, 11]. Therefore, a very rich experimental spectrum of high accuracy, involving as many as 982 lines, is available for this ion [11]. A critical compilation of all measured lines of several ions with 19 \leq Z \leq 28 was undertaken by Sugar and Corliss [12], and their recommended energy levels are also available on the NIST (National Institute of Standards and Technology) website http://www.nist.gov/pml/data/asd.cfm[13]. Later, Azarov et al. [14] also measured many lines of the 3d^34d and 3d^35s configurations of Fe V. A similar situation exists for Co VI [12], and as for Fe V, its lines were studied as early as 1938 [15, 16]. However, the observed spectrum of Ni VII is not as rich as for the other Ti-like ions Fe V and Co VI, because many levels are missing for the 3d^4 and 3d^4p configurations and none has been measured for 3d^34s – see Table ?? or the NIST website. Additionally, the situation regarding radiative data (A-values) is even worse, particularly for Co VI and Ni VII, although some results are available for Fe V [14, 17–20]. Therefore, in this paper we calculate energy levels and A-values for three Ti-like ions, namely Fe V, Co VI and Ni VII.

As noted above, calculations for lowly ionised ions are generally not straightforward, and hence require a significant amount of effort. This also applies to Ti-like species. Early calculations for energy levels were performed by Ekberg [11], who adopted a
least-square fit to the observed values, apart from applying a few corrections. In spite of this, differences between the observed and calculated energies are between $+299$ and $-470 \text{ cm}^{-1}$ (see tables III–V of [11]), although they equate to less than 0.2%. Later, O’Malley et al. [20] performed relativistic configuration interaction (RCI) calculations with $\sim 15000$ vectors, and determined energies for 5 ($J = 0$) levels of the $3d^4$ and 19 ($J = 1$) of $3d^34p$ configurations. They achieved a good accuracy within $\sim 3\%$ of the measurements – see their table III. The largest ab initio calculation available so far is by Nahar and Pradhan [18], who adopted the Breit-Pauli $R$-matrix method to calculate energies for 3865 levels of Fe V. However, the main problem with their work is that differences with measurements are up to 10%, for several levels and of all configurations – see their table III or table III of [20] for a shorter version. The most difficult to determine are the energy levels of the $3d^4$ configuration, as may also be noted from table 1 of Ballance et al. [21], who adopted the general-purpose relativistic atomic structure package (GRASP) to calculate energies for 359 levels of the $3d^4$, $3d^34s$, $3d^14p$, $3d^34d$, and $3d24s^2$ configurations. Since their focus was on the calculation of collisional data, they could only include a limited CI (configuration interaction), but differences between their energies and those of NIST are up to 16% for several levels, particularly those belonging to $3d^4$.

Adopting the same GRASP code as by [21], we have performed our calculations with much more extensive CI, but differences with the NIST compilation remain significant, both in magnitude and orderings, particularly for the lowest 34 levels of the $3d^4$ configuration. Therefore, we employed the flexible atomic code (FAC) of Gu [22] which (generally) provides results of comparable accuracy with other atomic structure codes, but is much more efficient to run and hence saves both computational and human time. Unfortunately, the results obtained with this code are as unsatisfactory as with GRASP. To be specific, we included CI with up to 100915 levels ($n \leq 5$), but differences in energy for the levels of the $3d^4$ configuration of Fe V are up to 15%, as shown in Table A. Therefore, it became clear that we either have to extend the CI to a much higher order, or have to apply another approach, such as the use of non-orthogonal orbitals. However, having recently gained experience from our work on Cr-like ions [6, 23], we have employed the quasi-relativistic approximation (QR) [24].

### 2. Details of calculations

In this work we investigate the lowest two even-parity configurations $3d^4$ and $3d^34s$ with 72 energy levels and one odd-parity configuration $3d^34p$ with 110 levels. We utilise the quasi-relativistic (QR) approach [24] as it was done in our previous studies [6, 23] of spectroscopic parameters for iron peak elements. At the start of the calculations we solve quasi-relativistic Hartree-Fock equations (QRHF) [25] for the ground configuration, and determine all one-electron radial orbitals (RO) for electrons with principal quantum number $N \leq 3$. Next we solve QRHF equations in the frozen-core potential for all $4\ell$ electrons ($\ell \leq 3$) for the configurations $3d^4 4\ell$. Subsequently the determined RO basis is extended by including transformed radial orbitals (TRO) [24] to effectively account for correlation effects [26]. TROs are determined for electrons with principal quantum number $5 \leq n \leq 10$ and all allowed values of the orbital quantum number $\ell < n$. Using this methodology, our basis consists of 55 ROs. The same ROs are utilised both for even and odd configurations. This way we avoid issues with RO non-orthogonality, important in the calculation of radiative transitions. Inaccuracies in level energies arising from that approximation are minimised by the adoption of a large CI basis.

The correlation effects are included using the CI method. Therefore a list of admixed configurations (AC) is constructed for each investigated configuration (adjusted configuration). This AC list is composed by including one- and two-electron promotions from the active shells ($3\ell$ and $4\ell$) of the investigated configuration to all those of the same parity, which can be described by the RO basis generated earlier. The presence of various admixed configurations in the CI basis dictates what kind of additional symmetries
are included in the eigen-functions of the investigated configurations. Thus the number of ACs can be considered as the main
criterion for the inclusion of electron correlation effects.

The adopted RO basis includes one-electron radial orbitals having orbital momenta from $\ell = 0$ to $\ell = 9$. Their combinations in
the admixed configurations enable us to construct nearly all necessary symmetries of momenta. Therefore the method of TRO con-
struction [24, 26] and extensive set of the principal quantum numbers $n$ ensures a very effective inclusion of the radial correlations.

Parameters of the calculation for the Ti-like ions under consideration are presented in Table B. The large maximum numbers of
AC for the even $M_e$AC and odd $M_o$AC configurations, together with possible configuration state function (CSF) numbers ($M_{CSF}$ and
$M_{CSF}^o$) given in this table, indicate that it is impossible to include into the CI wavefunction expansion all CSFs originating from
the arranged AC sets. Therefore one needs to select the admixed configurations according to their average contributions into
the eigen-functions of the investigated configurations. The contributions are determined in the second order of the perturbation theory
 – see [27]. We apply the selection criteria $w = 10^{-6}$, i.e. all ACs with the average contribution $\bar{w} < w$ are excluded from the
calculations.

The two even-parity configurations, namely 3d$^3$4d and 3d$^2$4s$^2$, are close to the investigated configurations in their energies,
and hence strongly affect these. To correctly determine their influence and to account more consistently for the 3- and 4-electron
correlation corrections, the set of selected ACs is extended by adding the admixed configurations that interact strongly with above
mentioned (3d$^3$4d and 3d$^2$4s$^2$) configurations. The selection criteria for these configurations is much larger ($w = 10^{-3}$). In the case
of odd-parity configurations, the additional admixed configurations are generated for the 3s$^2$3p$^5$3d$^5$, 3s$^2$3p$^6$3d$^4$f, 3s$^2$3p$^6$3d$^2$4s4p,
and 3s$^2$3p$^3$3d4s$^2$4p set of AC. The numbers $S$ in Table B represent the reduced (even and odd) configurations included in the CI
basis, which are about 4 to 5 times smaller than the initial ones.

A comparison of $S$ values for the three ions considered here demonstrates that, for the same configuration selection criteria
$w$, the number of selected configurations (slightly) decreases as the degree of ionisation increases. Such behaviour confirms the
well-known fact that the importance of correlation effects decreases with increase of the electrostatic potential affecting moving
electrons.

While performing actual CI calculations, the value of the $S$ parameter is not so important compared to the number of CSF ($C$)
generated by the configurations included in the CI basis. Corresponding C-values for the even and odd configurations are also given
in Table B. We note that their values are quite large (e.g. $C^o \sim 10^7$), and it becomes time consuming to perform calculations for
Hamiltonian matrices of such sizes.

At the next step we reduce the number of CSF, a procedure which relies on the relocation of the virtually excited electrons to
the front of the active shells of AC. We further discard those CSFs which have off-diagonal matrix elements of operator, describing
electrostatic interaction with the investigated configurations, equal to zero [28]. The numbers of CSF after these reductions are
given as $R^e$ and $R^o$ in Table B. One can see that this step reduces the basis of CSFs by almost an order of magnitude. We note
that this type of significant CSF reduction does not affect the effectiveness of the CI wavefunction expansion. Interestingly, while
the ionisation degree increases and consequently the number of selected configurations $S$ decreases, the number $R$ of produced
CSFs increases. This behaviour demonstrates that the above described AC reduction procedure leads to the inclusion of different
configurations for different degrees of ionisation in the isoelectronic sequence. Therefore the values of $R$ can increase.

In our computational method, the most important factor limiting the calculation is the number of CSFs with the same total $LS$
momenta. For the Fe V, Co VI, and Ni VII Ti-like ions considered here, the largest number $T$ of same $LS$ momenta is attributed to
the $^3F$ term, both for even and odd configurations, given in Table B. It is clear that their values are proportional to $R^e$ and $R^o$.  

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Correlation effects are very important for medium ionisation stage ions with an open 3d shell. When we implement the CI model, we include a huge number of admixed interacting configurations, but our limited computing resources necessitate some compromises – see Table B. Although each separate configuration cannot significantly affect the calculated results, the combined influence of such (omitted) configurations is comparatively appreciable, and hence causes some discrepancies between the calculated and experimental level energies. Therefore, we reduce integrals of the electrostatic interaction for all investigated configurations by 1.3%, as in [23]. Such a minimal change of integral values noticeably reduces discrepancies in the theoretical level energies, leading to more accurate transition wavelengths. This in turn reduces the influence of errors in transition energies, and subsequently on transition parameters.

Relativistic effects are included in the Breit-Pauli approximation as described in [24]. The level energies of the investigated configurations and their eigen-functions are determined by diagonalising the Hamiltonian matrix. These data are utilised to determine radiative transition parameters for electric dipole (E1), electric octupole (E3), and magnetic dipole (M2) transitions among the levels of even- and odd-parity configurations, and for magnetic dipole (M1) and electric quadrupole (E2) transitions among the levels of the same parity configurations – see section 4. These parameters are further used to determine the total radiative lifetimes $\tau$ of the excited levels. By utilising the determined CI wavefunctions, we also compute electron-impact excitation cross-sections and rates in the plane-wave Born approximation. These parameters are not discussed in the present paper but they are freely available from the database ADAMANT (http://www.adamant.tfai.vu.lt/database).

Apart from our own computer codes developed specifically for the calculation of spectroscopic parameters and electron-impact excitation cross-sections in the QR approximation, we adapt the codes from the MCHF package [29–31] for use of the quasi-relativistic radial orbitals.

3. Energy levels and Landé $g$-factors

Level energies obtained in the QR approximation are listed in Table A for all 34 levels of the 3d$^4$ configuration of Fe V, and agreement with the corresponding experimental data of NIST is highly satisfactory. The ordering of the levels is also the same in both theory and measurements. Generally, our calculated energies are slightly higher, but the discrepancies for most of the levels are less than 1.0%, except for seven which deviate by up to 1.24%. The largest relative discrepancy of 1.48% is for level 23 ($\frac{1}{2}S_0$). On the other hand, the highest level $\frac{1}{2}S_0$ of the ground configuration 3d$^4$ shows the largest absolute discrepancy of 818 cm$^{-1}$ (0.83%). The averaged relative disagreement for the levels of the 3d$^4$ configuration is only 0.83%. More importantly, agreement between our calculations and the NIST compilations is much better (within 0.5%) for levels of the 3d$^3$4s and 3d$^3$4p configurations – see Table ?? in which energies for all 182 levels of Fe V are listed. The averaged relative discrepancy for the excited configuration levels is only 0.16%, and is 0.12% for levels of the even-parity configuration 3d$^3$4s and 0.17% for the odd-parity 3d$^3$4p. This good agreement for a larger number of levels is highly satisfactory and encouraging. However, we note that the $LSJ$ designations listed in the table are not always definitive, because we have performed just a formal identification based on the maximum percentage contribution of a particular CSF in the CI wavefunction expansion, and some levels are highly affected by CSF mixing. For this reason their description using just a simple $LSJ$ notation is not definitive in all cases, and other, more sophisticated level identification schemes have to be applied instead of an $LS$ designation. All such levels are shown by a superscript “a” – see e.g., levels 83, 87, 89, and 104 in Table ???. However, this is a rather general atomic structure problem, as also noted in our earlier papers [6, 23].

In Table ?? we compare our calculated energies with the NIST compilations for all 182 levels of Co VI. As for Fe V, measurements are available for most levels, and discrepancies with these are slightly lower. The averaged relative discrepancy for the
ground configuration is 0.75%. Similar to Fe V, the largest relative disagreement is for level $^1S_0$. The averaged relative discrepancy for the excited configurations is only 0.12%, with 0.16% for the 3d$^3$4s configuration and only 0.048% for 3d$^4$4p.

Unfortunately, as it has been stated in Section 1, the number of levels for which measurements are available is very limited for Ni VII. Therefore it is not used to calculate and compare the averaged relative discrepancies. Nevertheless, in Table ?? we list our calculated energies for all the 182 levels of Ni VII along with those of NIST. The differences between the theoretical and experimental energies are smaller than 0.8%, excluding level 2 where it is 1.4% (4 cm$^{-1}$). The discrepancies are no greater than 301 cm$^{-1}$, and below 0.1% for common levels of the 3d$^4$4p configuration. Therefore, for all three Ti-like ions Fe V, Co VI and Ni VII there are no significant discrepancies for energy levels between theory and measurements, and therefore our results listed in Tables ??, ??, ?? can be confidently applied to the modelling of plasmas.

For all three ions investigated the QR calculations are performed in the same approximation. Consequently, a comparison of the discrepancies for specific level energies in Fe V and Co VI enables us to draw conclusions about the accuracy of the theoretical energies for those Ni VII levels which have no experimental data.

Finally, we note that data in the Tables ??, ??, ?? are provided for only the lowest 182 levels of the 3d$^4$, 3d$^3$4s and 3d$^3$4p configurations. Inclusion of similar results for levels of the 3d$^4$4d or 3d$^4$4f configurations is not feasible, because these cover a much wider energy range (and number over 1000) and intermix with many levels from other configurations (such as 3p$^5$3d$^3$ and 3d$^5$5$^l$), whereas there is no such intermixing among the lowest 182.

Also listed in Tables ??, ??, ?? are the Landé $g$-factors (dimensionless) that show the splitting of energy levels in a magnetic field, and represent the Zeeman effect for a particular LSJ level. It is given by

$$g = 1 + \sum_{CLS} \alpha_{CLSJ} \frac{J(J+1) - L(L+1) + S(S+1)}{2J(J+1)}$$

(1)

where the sum is over all CSFs for that level, $C$ is the configuration, $LSJ$ are total moments of the level, and $\alpha_{CLSJ}$ is a weight (a square of the expansion coefficient) of a particular CSF for the level eigen-function. Sometimes measurement of $g$ are available and hence may help in assessing the accuracy of the calculations. Unfortunately, for the ions considered here no experimental results are available with which to compare our data, but O’Malley et al. [20] have reported $g$-factors for 19 ($J = 1$) levels of the 3d$^4$4p configuration of Fe V calculated in the relativistic configuration interaction (RCI) approximation. Therefore, in Table C we have included their and our $g$-factors for ready comparison. For most levels there are no discrepancies between the two independent calculations, but our results are lower by $\sim 40\%$ for two, namely 89 ($^5P_1$) and 138 ($^3D_0$). The $g$-factors are sensitive to primarily those levels which have low LS-purity, and hence the differences between the two calculations.

4. Radiative rates and lifetimes

Apart from spectral modelling (including diagnostics) and the determination of the total radiative lifetimes ($\tau$), $A$-values are required for calculations of local thermodynamic equilibrium (LTE) in stellar opacities, and radiative levitation and acceleration of heavy elements – see for example, [18] and references therein. For this reason, Nahar and Pradhan [18] performed very large calculations of energy levels and E1 $A$-values for transitions in Fe V, as already stated in Section 1. However, for more sophisticated modelling applications, and particularly the determination of $\tau$, corresponding results for the electric quadrupole E2, magnetic dipole M1, and magnetic quadrupole M2 transitions are also desirable. Therefore, in a separate paper [19] they reported $A$-values for the M1 and E2 transitions of Fe V.
In Tables ??,??,?? we list transition energies ($\Delta E$, cm$^{-1}$), wavelengths ($\lambda$, Å), emission radiative rates ($A$-values, s$^{-1}$), weighted oscillator strengths ($gf$, dimensionless), and transition line strengths ($S$-values in atomic units) for the E1, E2 and M1 transitions of Fe V, Cu VI and Ni VII, respectively. These results are among the 182 levels listed in Tables ??,??,??, but we only include those transitions with $A$-values (and other parameters) which are $\geq 10\%$ of the largest value for an emission transition probability from the upper level $j$. Hence to save on space data for very weak transitions are not provided, as their impact on plasma modelling should be insignificant. For the same reason, $A$-values for the M2 and E3 transitions are also not included in Tables ??,??,??, except for some E1 transitions of Fe V with those of [10, 18, 20]. In general, the $A$-values (and other related parameters) for all (including much weaker) transitions, along with electron-impact excitation data determined in the plane-wave Born approximation, are freely available in ASCII format from the ADAMANT database at Vilnius University (http://www.adamant.tfai.vu.lt/database).

Additionally, we list $\lambda$ (Å) and $f$-values (dimensionless) for all absorption E1 transitions with $f \geq 0.1$ in Tables ??,??,??, except for some weaker ($f \geq 0.001$) absorption lines originating from the lowest 5 levels of the ground configuration term 3d$^4$5D. These lines may have applications in the modelling of the absorption spectra of low-temperature plasmas.

$A$-values for E1 transitions of Fe V are available in the literature, mainly by [18, 20]. Additionally, Garstang [32] has reported $A$-values for the M1 and E2 transitions, but only among levels of the lowest 3d$^4$ configuration. In Table D we compare our results for some E1 transitions of Fe V with those of [10, 18, 20]. In general, the $f$-values of Fawcett [10] and O’Malley et al. [20] show good agreement with our results, although differences for a few are up to a factor of two, which include some (comparatively) strong transitions, such as 23 – 132 and 34 – 182. Similarly, our data agree closely with those of [20], particularly for strong transitions, although differences are up to a factor of two for some weaker ones, such as: 1 – 89, 6 – 133 and 23 – 138. However, the maximum discrepancies for any set of $f$-values listed in Table D are with the BPRM results of Nahar and Pradhan [18], and this includes both the strong (1 – 80 and 23 – 132) and weak (1 – 82 and 6 – 133) transitions. For these (and other) transitions the $f$-values of [18] differ by over an order of magnitude with other results. Differences in $f$-values between any two calculations can often be large (i.e. a factor of two or more for some strong transitions) as seen in Table D or in table VI of [18]. Such differences mainly arise with the varying amount of CI adopted in a calculation as well as the methodology applied, as discussed and demonstrated earlier by Aggarwal et al. [5] for three Mg-like ions. However, based on the comparisons shown in Table D and noting the large discrepancies in the energy levels of Nahar and Pradhan [18] in section 3, their radiative data appear to be comparatively less accurate.

In Table E we compare our $A$-values with those of Garstang [32] for the M1 transitions among the levels of the 3d$^4$ configuration. These transitions are comparatively stronger than the corresponding E2 ones among these levels, also reported in [32]. Similar results of [19] for these transitions are not included in this table, because there are no discrepancies with the data of [32] – see table 6 of [19]. Considering the low strengths of these transitions, the agreement among three independent calculations is highly satisfactory. The only exceptions are the 4 – 7 and 5 – 7 transitions for which the $A$-values of [32] appear to be interchanged. For these two transitions (as for others) there are no significant discrepancies between our $A$-values ($1.18 \times 10^{-3}$ and $6.24 \times 10^{-3}$ s$^{-1}$) and those from [19] ($8.34 \times 10^{-4}$ and $4.34 \times 10^{-3}$ s$^{-1}$). Since [19] have also reported $A$-values for the E2 transitions, in Table F we show comparisons for a few, particularly those with larger strengths. As for M1 transitions, for these E2 also there are no discrepancies between the two calculations, except that there is a difference of about a factor of two, and our results are lower. This is because there is a difference of a factor of 2/3 in the definitions of $A$-values for the E2 transitions – see Eq. (4) of [33] and Eq. (11) of [19]. A similar problem was noted earlier for the E2 transitions of Fe XVII [33], and our definitions of $A$-values and
transition strengths $S$ correspond to those adopted by the NIST.

As for other ions, we have also calculated lifetimes ($\tau = 1.0/\sum_i A_{ji}$, s), where the sum is over all calculated radiative decay channels with $i < j$. For the calculations we include $A$-values for all E1, E2 and M1 transitions, and list our results in Tables ??, ??, ?? for Fe V, Co VI and Ni VII, respectively. The only data available in the literature for comparison are by Biémont et al. [34] for the 3d$^4$ 5D$_3$ level, which are 374.3, 140.2 and 58.9 s, for Fe V, Co VI and Ni VII, respectively, which compare favourably with our corresponding values of 379, 138 and 58 s.

5. Conclusions

In this work we have reported energy levels, Landé $g$-factors and the total radiative lifetimes $\tau$ for the lowest 182 levels of the three Ti-like ions Fe V, Co VI and Ni VII. These levels belong to the 3d$^4$, 3d$^3$4s and 3d$^3$4p configurations, and do not have intermixing with those from others, such as 3d$^3$4d and 3d$^3$4f. Experimental energies are available for most levels of Fe V and Co VI, but for only a few of Ni VII.

A large portion of the theoretical level energies differ from the experimental data by only a few hundreds of cm$^{-1}$ or even less. These discrepancies decrease as the ionisation degree increases. As a consequence, the averaged discrepancies for the ground configuration levels are 0.83% for Fe V and 0.75% for Co VI. For the excited configurations where the level energies are larger, these disagreements are noticeably smaller and decrease to 0.12% for both Fe V and Co VI. There is a lack of experimental level energies for Ni VII, but agreement with our results for levels in common is very good. The largest relative discrepancy for the 3d$^3$4p configuration is just 0.13%, and is less than 0.1% for most other levels. This leads to the conclusion that our calculated level energies and the transition wavelengths for Ni VII are highly accurate, and hence suitable for line identifications in future experiments.

For all three ions the radiative lifetimes $\tau$ and the Landé $g$-factors are consistently determined for the first time. There are no available theoretical or experimental $\tau$ data for comparison purposes, but there are no appreciable disagreements with previous theoretical results of $g$, available for only a few levels.

Radiative rates for the three ions have also been reported for all E1, E2 and M1 emission transitions. Earlier data for the E1 transitions are available for Fe V by [18, 19]. However, in comparison to our calculations and those of others [10, 20], their $A$-values appear to be less accurate, and so are their energy levels which differ from the measurements and our work by some 10% for many levels. Unfortunately, no such data are available for transitions in Co VI and Ni VII. Among other types, $A$-values for the M1 and E2 transitions are also available [19, 32], but only among the levels of the 3d$^4$ and 3d$^3$4s configuration of Fe V. The M1 transitions are comparatively stronger than E2, and there are no discrepancies between the present and the earlier results for any type of radiative transition. However, the present data cover the full range of all types of transitions among the lowest 182 levels. We believe our present data will be useful not only for the modelling of plasmas but also for further accuracy assessments.

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Table A

Comparison of energy levels (in cm\(^{-1}\)) of the 3d\(^4\) configuration of Fe V.

| Index | Level | NIST | QR | FAC |
|-------|-------|------|----|-----|
| 1     | \(\frac{3}{2}D_0\) | 0    | 0  | 0   |
| 2     | \(\frac{3}{2}D_1\) | 142  | 144| 134 |
| 3     | \(\frac{3}{2}D_2\) | 418  | 418| 391 |
| 4     | \(\frac{3}{2}D_3\) | 803  | 803| 753 |
| 5     | \(\frac{3}{2}D_4\) | 1283 | 1280| 1204|
| 6     | \(\frac{3}{2}P_0\) | 24056| 24315| 24276|
| 7     | \(\frac{3}{2}H_4\) | 24932| 25134| 28506|
| 8     | \(\frac{3}{2}P_1\) | 24973| 25238| 25141|
| 9     | \(\frac{3}{2}H_5\) | 25226| 25420| 28890|
| 10    | \(\frac{3}{2}H_6\) | 25528| 25715| 29180|
| 11    | \(\frac{3}{2}P_2\) | 26468| 26748| 26560|
| 12    | \(\frac{3}{2}F_2\) | 26761| 27036| 28446|
| 13    | \(\frac{3}{2}F_3\) | 26842| 27110| 28577|
| 14    | \(\frac{3}{2}F_4\) | 26974| 27234| 28831|
| 15    | \(\frac{3}{2}G_3\) | 29817| 30095| 33120|
| 16    | \(\frac{3}{2}G_4\) | 30147| 30419| 33432|
| 17    | \(\frac{3}{2}G_5\) | 30430| 30686| 33740|
| 18    | \(\frac{3}{2}D_3\) | 36630| 36985| 39556|
| 19    | \(\frac{3}{2}G_4\) | 36586| 37041| 39133|
| 20    | \(\frac{3}{2}D_2\) | 36758| 37123| 39666|
| 21    | \(\frac{3}{2}D_1\) | 36925| 37296| 39826|
| 22    | \(\frac{3}{2}H_6\) | 37512| 37822| 43006|
| 23    | \(\frac{3}{2}S_0\) | 39633| 40221| 40264|
| 24    | \(\frac{3}{2}D_2\) | 46291| 46651| 48886|
| 25    | \(\frac{3}{2}F_3\) | 52733| 53173| 57311|
| 26    | \(\frac{3}{2}P_2\) | 61854| 62275| 65971|
| 27    | \(\frac{3}{2}F_4\) | 62238| 62642| 66758|
| 28    | \(\frac{3}{2}F_2\) | 62321| 62798| 66859|
| 29    | \(\frac{3}{2}F_3\) | 62364| 62812| 66885|
| 30    | \(\frac{3}{2}P_1\) | 62914| 63366| 66975|
| 31    | \(\frac{3}{2}P_0\) | 63420| 63890| 67451|
| 32    | \(\frac{1}{2}G_4\) | 71280| 71773| 77163|
| 33    | \(\frac{1}{2}D_2\) | 93833| 94559| 100790|
| 34    | \(\frac{1}{2}S_0\) | 121130| 121948| 127476|

NIST: http://www.nist.gov/pml/data/asd.cfm

QR: Present results in the QR approximation

FAC: Present results with the FAC code with 100 915 level calculations
### Table B

Number of configurations and CSF adopted in the QR calculations.

| Parameter | Fe V | Co VI | Ni VII |
|-----------|------|-------|--------|
| $M_{AC}$  | 4536 | 4536  | 4536   |
| $M_{AC}$  | 3412 | 3412  | 3412   |
| $M_{CSF}$ | 26 770 069 | 26 770 069 | 26 770 069 |
| $M_{CSF}$ | 41 878 914 | 41 878 914 | 41 878 914 |
| $S^c$     | 1103 | 1076  | 1007   |
| $S^o$     | 672  | 656   | 617    |
| $C^c$     | 6 628 071 | 6 411 971 | 5 802 821 |
| $C^o$     | 9 739 792 | 9 468 640 | 8 648 190 |
| $R^c$     | 663 037 | 643 672 | 602 899 |
| $R^o$     | 876 445 | 902 259 | 903 614 |
| $T^c$     | 86 177 | 83 861 | 78 629 |
| $T^o$     | 89 331 | 91 810 | 91 595 |

### Table C

Comparison of Landé $g$-factors (dimensionless) for the 3d$^3$3p ($J = 1$) levels of Fe V.

See Table 1 for definition of all levels.

| Index | Configuration | Level | Present | RCI [20] |
|-------|---------------|-------|---------|----------|
| 80    | 3d$^3$(F)4p  | 5P$^1$ | 0.549   | 0.457    |
| 82    | 3d$^3$(F)4p  | 5D$^1$ | 1.220   | 1.227    |
| 89    | 3d$^3$(F)4p  | 5F$^1$ | 0.231   | 0.317    |
| 97    | 3d$^3$(P)4p  | 5P$^1$ | 2.477   | 2.474    |
| 101   | 3d$^3$(P)4p  | 5D$^1$ | 1.500   | 1.494    |
| 104   | 3d$^3$(P)4p  | 5D$^1$ | 1.521   | 1.513    |
| 122   | 3d$^3$(P)4p  | 3P$^1$ | 1.485   | 1.453    |
| 126   | 3d$^3$(P)4p  | 3D$^1$ | 0.533   | 0.547    |
| 132   | 3d$^3$(D)4p  | 1P$^1$ | 1.159   | 0.949    |
| 133   | 3d$^3$(P)4p  | 3S$^1$ | 1.746   | 1.742    |
| 138   | 3d$^3$(P)4p  | 3D$^1$ | 0.565   | 0.820    |
| 144   | 3d$^3$(D)4p  | 3D$^1$ | 0.566   | 0.536    |
| 150   | 3d$^3$(D)4p  | 3P$^1$ | 1.448   | 1.485    |
| 156   | 3d$^3$(P)4p  | 3S$^1$ | 1.998   | 1.915    |
| 157   | 3d$^3$(P)4p  | 1P$^1$ | 1.003   | 1.063    |
| 168   | 3d$^3$(F)4p  | 3D$^1$ | 0.500   | 0.500    |
| 171   | 3d$^3$(D)4p  | 3D$^1$ | 0.506   | 0.509    |
| 179   | 3d$^3$(D)4p  | 3P$^1$ | 1.494   | 1.490    |
| 182   | 3d$^3$(D)4p  | 1P$^1$ | 1.000   | 0.999    |
Table D

Comparison of oscillator strengths \((f\)-values) for some E1 transitions of Fe V.

| \(i\) | \(j\) | SE    | RCI\(_L\) | RCI\(_V\) | BPRM | QR   |
|------|------|-------|----------|----------|------|------|
| 1    | 80   | 0.163 | 0.110    | 0.116    | 0.2154 | 0.1366 |
| 1    | 82   | 0.041 | 0.060    | 0.064    | 0.0055 | 0.0702 |
| 1    | 89   | 0.059 | 0.061    | 0.065    | 0.0574 | 0.0321 |
| 1    | 97   | 0.076 | 0.072    | 0.073    | 0.0842 | 0.0755 |
| 6    | 80   | 0.039 | 0.036    | 0.041    | 0.0231 | 0.0271 |
| 6    | 89   | 0.061 | 0.046    | 0.051    | 0.0670 | 0.0410 |
| 6    | 122  | 0.153 | 0.141    | 0.148    | 0.0938 | 0.1360 |
| 6    | 133  | 0.028 | 0.011    | 0.012    | 0.0022 | 0.0277 |
| 6    | 144  | 0.024 | 0.020    | 0.020    | 0.0071 | 0.0385 |
| 23   | 122  | 0.010 | 0.010    | 0.011    | 0.0070 |       |
| 23   | 132  | 0.216 | 0.108    | 0.118    | 0.0080 | 0.1560 |
| 23   | 133  | 0.010 | 0.042    | 0.045    | 0.0002 | 0.0277 |
| 23   | 138  | 0.029 | 0.054    | 0.059    | 0.0020 | 0.0257 |
| 23   | 150  | 0.011 | 0.012    | 0.013    | 0.0115 |       |
| 23   | 157  | 0.073 | 0.059    | 0.060    | 0.0786 | 0.0729 |
| 31   | 104  | 0.013 | 0.010    | 0.011    | 0.0101 | 0.0076 |
| 31   | 150  | 0.021 | 0.016    | 0.017    | 0.0520 |       |
| 31   | 156  | 0.088 | 0.074    | 0.082    | 0.0482 | 0.0665 |
| 31   | 168  | 0.168 | 0.136    | 0.145    | 0.1648 | 0.1390 |
| 31   | 179  | 0.046 | 0.045    | 0.042    | 0.0487 | 0.0429 |
| 34   | 182  | 0.379 | 0.289    | 0.295    | 0.3468 | 0.2850 |

SE: Calculations of Fawcett [10] with the semi-empirical relativistic atomic structure code
RCI\(_L\): Calculations of O’Malley et al. [20] in the length form with the RCI code
RCI\(_V\): Calculations of O’Malley et al. [20] in the velocity form with the RCI code
BPRM: Calculations of Nahar and Pradhan [18] with the BPRM code
QR: Present calculations with the QR code
Table E.

Comparison of radiative rates ($\Lambda$-values, s$^{-1}$) for some M1 transitions among the levels of the 3d$^4$ configuration of Fe V.

$\alpha \pm b \equiv \alpha \times 10^{\pm b}$.

| $i$ | $j$ | Garstang [32] Present | $i$ | $j$ | Garstang [32] Present |
|-----|-----|------------------------|-----|-----|------------------------|
| 1   | 2   | 1.6$\cdot$4            | 7   | 9   | 6.5$\cdot$4             |
| 1   | 8   | 1.3$\cdot$1 1.38$\cdot$1 | 7   | 15  | 3.6$\cdot$2             |
| 1   | 21  | 2.2$\cdot$1 2.62$\cdot$1 | 7   | 16  | 3.3$\cdot$2             |
| 2   | 3   | 1.2$\cdot$3 1.16$\cdot$3 | 7   | 19  | 1.8$\cdot$1             |
| 2   | 6   | 1.3$\cdot$0 1.62$\cdot$0 | 8   | 21  | 1.2$\cdot$1             |
| 2   | 12  | 1.0$\cdot$1 1.18$\cdot$1 | 8   | 24  | 6.2$\cdot$2             |
| 2   | 20  | 2.0$\cdot$1 2.18$\cdot$1 | 9   | 10  | 5.8$\cdot$4             |
| 2   | 21  | 1.9$\cdot$1 2.32$\cdot$1 | 9   | 17  | 4.1$\cdot$2             |
| 3   | 4   | 2.6$\cdot$3 2.64$\cdot$3 | 9   | 19  | 2.5$\cdot$1             |
| 3   | 8   | 1.1$\cdot$0 1.23$\cdot$0 | 9   | 22  | 1.1$\cdot$1             |
| 3   | 12  | 2.0$\cdot$1 2.31$\cdot$1 | 10  | 17  | 4.1$\cdot$2             |
| 3   | 13  | 1.6$\cdot$1 2.02$\cdot$1 | 10  | 22  | 1.4$\cdot$1             |
| 3   | 15  | 7.0$\cdot$3 8.10$\cdot$3 | 11  | 18  | 5.6$\cdot$2             |
| 3   | 18  | 9.7$\cdot$2 1.08$\cdot$1 | 11  | 20  | 5.2$\cdot$2             |
| 3   | 20  | 1.8$\cdot$1 1.76$\cdot$1 | 11  | 21  | 3.6$\cdot$2             |
| 4   | 5   | 3.0$\cdot$3 2.91$\cdot$3 | 11  | 24  | 1.8$\cdot$1             |
| 4   | 7   | 4.0$\cdot$4 1.18$\cdot$3 | 12  | 15  | 3.0$\cdot$2             |
| 4   | 11  | 7.1$\cdot$1 7.93$\cdot$1 | 12  | 24  | 2.1$\cdot$1             |
| 4   | 12  | 4.7$\cdot$2 6.39$\cdot$2 | 13  | 15  | 3.7$\cdot$2             |
| 4   | 13  | 4.0$\cdot$1 5.30$\cdot$1 | 13  | 19  | 1.5$\cdot$1             |
| 4   | 14  | 1.6$\cdot$1 1.87$\cdot$1 | 13  | 24  | 4.2$\cdot$1             |
| 4   | 15  | 1.7$\cdot$2 1.94$\cdot$2 | 14  | 16  | 2.7$\cdot$2             |
| 4   | 16  | 7.8$\cdot$2 8.59$\cdot$3 | 14  | 17  | 3.7$\cdot$2             |
| 4   | 18  | 8.9$\cdot$2 1.01$\cdot$1 | 14  | 19  | 3.2$\cdot$1             |
| 4   | 20  | 1.1$\cdot$1 1.20$\cdot$1 | 15  | 19  | 4.2$\cdot$2             |
| 5   | 7   | 1.1$\cdot$3 6.24$\cdot$3 | 15  | 25  | 1.2$\cdot$1             |
| 5   | 13  | 6.6$\cdot$2 7.21$\cdot$2 | 16  | 25  | 1.7$\cdot$1             |
| 5   | 14  | 7.4$\cdot$1 8.98$\cdot$1 | 18  | 24  | 9.0$\cdot$2             |
| 5   | 16  | 3.2$\cdot$2 3.02$\cdot$2 | 18  | 25  | 1.5$\cdot$1             |
| 5   | 18  | 3.7$\cdot$1 4.20$\cdot$1 | 20  | 25  | 7.0$\cdot$2             |
| 6   | 21  | 4.9$\cdot$2 5.91$\cdot$2 | 21  | 24  | 8.0$\cdot$2             |
Table F

Comparison of radiative rates ($A$-values, s$^{-1}$) for some E2 transitions of Fe V. $a \pm b \equiv a \times 10^{\pm b}$.

| $i$ | $j$ | BPRM [19] | Present |
|-----|-----|-----------|---------|
| 1   | 36  | 7.79+3    | 4.19+3  |
| 2   | 35  | 1.54+4    | 8.27+3  |
| 2   | 37  | 1.01+4    | 5.42+3  |
| 3   | 35  | 1.09+4    | 5.87+3  |
| 3   | 36  | 1.26+4    | 6.74+3  |
| 3   | 38  | 1.01+4    | 5.40+3  |
| 4   | 36  | 6.83+3    | 3.66+3  |
| 4   | 37  | 1.35+4    | 7.23+3  |
| 4   | 38  | 6.97+3    | 3.74+3  |
| 4   | 39  | 7.09+3    | 3.81+3  |
| 5   | 37  | 2.94+3    | 1.57+3  |
| 5   | 38  | 1.09+4    | 5.81+3  |
| 5   | 39  | 2.10+4    | 1.13+4  |