Oscillator strengths for transitions among Fe III levels belonging to the three lowest configurations

N C Deb and A Hibbert
School of Mathematics and Physics, Queen's University Belfast, Belfast BT7 1NN, Northern Ireland, UK
E-mail: a.hibbert@qub.ac.uk

Abstract. Accurate oscillator strengths and Einstein $A$-coefficients for some $E1$ and $E2$ transitions among $3d^6$, $3d^54s$ and $3d^54p$ levels of Fe III are presented and compared with other available results. The present results comprise by far the largest configuration interaction calculation for this astrophysically important ion, and include relativistic effects through the Breit-Pauli operator. The core-valence effects from a large number of $3d^6$ and $3d^5$ cores are carefully treated by optimising $4d$, $4f$, $5s$, $5p$, $5d$, $5f$ and $6p$ orbitals either as a correction or as a correlation orbital while $1s$, $2s$, $2p$, $3s$, $3p$ and $3d$ Hartree-Fock functions are used. The $4s$ and $4p$ functions are optimised as spectroscopic orbitals. Fine-tuning of the $ab\ initio$ energies was done through adjusting by a small amount some diagonal elements of the Hamiltonian matrix. It is found that for many of the relatively strong dipole transitions, our calculated oscillator strengths agree with available calculations, while for the weaker transitions our results often disagree with the previously determined results. We also present $gA$ values for five $E2$ transitions for the multiplets $3d^55D_J \rightarrow 3d^5(4S)4s^2S_2$. The present results for these transitions show a 30-40% increase over the results previously published.

1. Introduction
Accurate oscillator strengths and radiative rates associated with spectral lines from low stages of ionisation of iron are very important in order to determine the relative abundance of iron in many astrophysical objects. Fe III lines are detected in supernova remnants [1], in Herbig-Haro objects [2] and in inferred destruction of dust in shocks [3]. Forbidden and fluorescent Fe III lines were also identified [4] by the Hubble Space Telescope in the spectra of η Carinae. In the present paper we present some of these electric dipole and electric quadrupole transitions of Fe III.

In the recent past, several groups of scientists have undertaken a theoretical study of Fe III. Nahar & Pradhan [5] reported $E1$, $E2$ and $M1$ transitions among the fine-structure levels of $3d^6$, $3d^54s$ and $3d^54p$ configurations. While their calculation of $E1$ transitions lacks explicit relativistic effects, (the transition rates for individual lines being obtained by an algebraic transformation of non-relativistic, $LS$-coupled results), $E2$ and $M1$ transitions do include relativistic effects. Raassen & Uylings [6] employed an orthogonal operator method to generate transition data among fine-structure levels of the above configurations. The level energy separations obtained by this method show excellent agreement with those of experimental energy separations. Toner & Hibbert [7] studied a small number of specific allowed and forbidden transitions ($a^7S_3 \rightarrow z^7P_J$, $a^5D_J \rightarrow z^7P_J$, and $a^5D_J \rightarrow a^5S_2$) using the CIV3 program of Hibbert and coworkers [8,9]. Their work has recently been extended by Deb & Hibbert [10].
to account for all major correlation and core-valence effects by including a very large number of configuration state functions (CSFs) in the configuration interaction expansions of the wave functions.

2. Calculation method

In the present analysis we have used the same CIV3 program to calculate the oscillator strengths and transition probabilities among the Fe\textsuperscript{III} fine-structure levels of configurations 3\textit{d}\textsuperscript{6}, 3\textit{d}\textsuperscript{5}4\textit{s} and 3\textit{d}\textsuperscript{5}4\textit{p}. The details of the theoretical method, orbitals and the manner in which they were optimised are presented in our recent work [10]. Here we describe how the different sets of configurations are chosen. These lowest three configurations of Fe\textsuperscript{III} give 136 \(LS\) states belonging to 19 even and 23 odd symmetries. We generate configurations of all these symmetries using the orbitals available from our optimisations: 3\textit{d}, 4\textit{s}, 4\textit{p}, 4\textit{d}, 5\textit{s}, 5\textit{p}, 5\textit{d}, 5\textit{f} and 6\textit{p}. We include all one- and two-electron promotions from 3\textit{d}\textsuperscript{6}, 3\textit{d}\textsuperscript{5}4\textit{s}, 3\textit{d}\textsuperscript{5}4\textit{d} for the even levels and from 3\textit{d}\textsuperscript{5}4\textit{p} for the odd levels, maintaining the parity and keeping up to 3\textit{p} fixed. For each of these symmetries the associated CSFs were then used to calculate \(LS\) energies. It turns out that some of the CSFs have very small configuration interaction (CI) mixing coefficients in all the states of interest. We find that the energy separations are changed very little by removing those CSFs whose eigenvector strengths were smaller in magnitude than 0.001 in all the eigenvectors of a given \(LS\) symmetry. This reduces the configuration sets significantly and, therefore, the computation time.

Additionally, we open up the 3\textit{s}\textsuperscript{2} and 3\textit{p}\textsuperscript{6} subshells, but in a more limited way than for the outer subshells. We found that for the even levels, the 3\textit{s}3\textit{p}\textsuperscript{4}3\textit{d}\textsuperscript{3}, 3\textit{s}3\textit{p}\textsuperscript{4}3\textit{d}\textsuperscript{3}4\textit{s}, 3\textit{s}3\textit{p}\textsuperscript{5}3\textit{d}\textsuperscript{2}, 3\textit{p}\textsuperscript{5}3\textit{d}\textsuperscript{2}, 3\textit{p}\textsuperscript{3}3\textit{d}\textsuperscript{4}4\textit{s}, 3\textit{p}\textsuperscript{4}3\textit{d}\textsuperscript{4} and 3\textit{p}\textsuperscript{4}3\textit{d}\textsuperscript{4}4\textit{s} configurations make significant contributions to the energies and oscillator strengths, while for the odd levels, the 3\textit{s}3\textit{p}\textsuperscript{5}3\textit{d}\textsuperscript{3}, 3\textit{p}\textsuperscript{5}3\textit{d}\textsuperscript{3}, 3\textit{s}3\textit{p}\textsuperscript{5}3\textit{d}\textsuperscript{3}4\textit{s}, 3\textit{p}\textsuperscript{5}3\textit{d}\textsuperscript{3}4\textit{p} and 3\textit{p}\textsuperscript{5}3\textit{d}\textsuperscript{3}4\textit{p} configurations were particularly important. Mostly, these represent correlation within the \(n = 3\) complex. Using these sets of configurations we have calculated the \textit{ab initio} energies of all the fine-structure levels of the three lowest configurations of Fe\textsuperscript{III}. These \textit{ab initio} energies were then fine-tuned to match the level energy differences with those of experiment. As a result of this fine-tuning, the eigenvector components of the major configurations in the CI wavefunction are only slightly changed from their \textit{ab initio} values. These wavefunctions are then used to calculate oscillator strengths and transition probabilities for E1 and E2 transitions in Fe\textsuperscript{III}.

3. Results and discussions

In Table 1 we present our oscillator strengths and radiative transition rates for some allowed (E1) transitions and compare our results for transition rates with other recent calculations, namely those of Nahar & Pradhan [5], Raassen & Uylings [6] and Ekberg [12]. In our earlier work [10] we had given oscillator strengths in both length and velocity form, and showed good agreement between them, indicating that our calculations had included sufficient configurations to give a good description of correlation effects. Hence in Table 1, we present only the length forms of oscillator strengths and transition rates.
Table 1. Comparison of present oscillator strengths and radiative rates (in s⁻¹) with other calculations.

| LL      | UL       | λ (Å) | f (Present) | A(Present) | A([6]) | A([5]) | A([12]) |
|---------|----------|-------|-------------|------------|--------|--------|--------|
| a ⁵S₃   | ⁷P₄      | 1895.46 | 0.39       | 5.69(8)⁸   | 6.74(8) | 5.36(8) | 6.77(8) |
|         | ⁷P₅      | 1914.06 | 0.30       | 5.52(8)⁸   | 6.50(8) | 5.21(8) | 6.59(8) |
|         | ⁷P₆      | 1926.30 | 0.22       | 5.42(8)    | 6.40(8) | 5.11(8) | 4.63(8) |
| a ⁵G₆   | ⁵G₆      | 1987.50 | 0.29       | 4.90(8)    | 5.68(8) | 4.40(8) | 5.85(8) |
|         | ⁵G₇      | 1989.98 | 0.028      | 5.69(7)    | 7.26(7) | 3.70(7) | 2.32(7) |
| a ⁵G₇³  | ⁵G₇³     | 1989.13 | 0.0025     | 3.59(6)    | 1.33(6) | 3.13(7) | 3.13(7) |
|         | ⁵G₇⁴     | 1991.61 | 0.256      | 4.30(8)    | 4.90(8) | 3.78(8) | 5.30(8) |
|         | ⁵G₇⁵     | 1993.26 | 0.044      | 9.06(7)    | 1.14(8) | 6.58(7) | 9.36(7) |
| a ⁵G₄   | ⁵G₄      | 1992.42 | 0.0046     | 6.31(6)    | 5.67(6) | 5.39(7) | 1.98(7) |
|         | ⁵G₅      | 1994.08 | 0.23       | 3.87(8)    | 4.39(8) | 3.36(8) | 4.64(8) |
|         | ⁵G₆      | 1995.27 | 0.051      | 1.09(8)    | 1.31(8) | 8.28(7) | 1.04(8) |
| a ⁵G₃   | ⁵G₃      | 1994.36 | 0.009      | 1.21(7)    | 1.24(7) | 6.45(7) | 2.78(6) |
|         | ⁵G₄      | 1995.56 | 0.22       | 3.62(8)    | 4.13(8) | 3.29(8) | 4.40(8) |
|         | ⁵G₅      | 1996.40 | 0.040      | 9.27(7)    | 1.12(8) | 7.75(7) | 8.24(7) |
| a ⁵G₂   | ⁵G₂      | 1995.58 | 0.014      | 1.63(7)    | 1.72(7) | 5.54(7) |         |
|         | ⁵G₃      | 1996.42 | 0.23       | 3.91(8)    | 4.46(8) | 3.88(8) | 4.58(8) |
| b ⁵D₅   | ⁵F₅      | 1931.51 | 0.33       | 4.83(8)    | 5.84(8) | 4.50(8) | 7.30(8) |
|         | ⁵F₆      | 1940.02 | 0.027      | 4.81(7)    | 7.63(7) | 7.40(7) | 7.12(7) |
|         | ⁵F₇      | 1948.82 | 0.0001     | 2.27(5)    | 2.53(6) | 6.25(6) | 1.01(6) |
| b ⁵D₉   | ⁵F₅      | 1945.34 | 0.30       | 4.11(8)    | 4.85(8) | 3.67(8) | 6.49(8) |
|         | ⁵F₆      | 1954.20 | 0.048      | 8.42(7)    | 1.35(8) | 1.30(8) |         |
|         | ⁵F₇      | 1961.19 | 0.0019     | 4.48(6)    | 1.24(7) | 1.72(7) |         |
| b ⁵D₂   | ⁵F₅      | 1954.23 | 0.286      | 3.57(8)    | 4.03(8) | 2.98(8) | 5.98(8) |
|         | ⁵F₆      | 1961.23 | 0.082      | 1.41(8)    | 1.97(8) | 1.72(8) | 1.96(8) |
|         | ⁵F₇      | 1966.21 | 0.0069     | 1.98(7)    | 2.83(7) | 2.84(7) | 1.67(7) |
| b ⁵D₁   | ⁵F₅      | 1959.33 | 0.271      | 2.82(8)    | 3.21(8) | 2.41(8) | 5.63(8) |
|         | ⁵F₆      | 1964.29 | 0.101      | 1.88(8)    | 2.39(8) | 2.00(8) | 3.64(8) |
| b ⁵D₀   | ⁵F₅      | 1962.72 | 0.363      | 2.10(8)    | 2.56(8) | 2.00(8) | 7.98(8) |
| b ³D₃   | ³F₃      | 2062.42 | 0.331      | 4.04(8)    | 4.11(8) | 6.19(8) |         |
|         | ³F₄      | 2054.18 | 0.017      | 2.69(7)    | 4.64(7) | 2.87(7) |         |
|         | ³F₅      | 2062.71 | 0.00084    | 1.86(6)    | 1.84(6) | 2.47(6) |         |
| b ³D₂   | ³F₃      | 2060.35 | 0.342      | 3.84(8)    | 3.67(8) | 6.24(8) |         |
|         | ³F₄      | 2058.89 | 0.042      | 6.64(7)    | 6.45(7) | 9.00(7) |         |
| b ³D₁   | ³F₃      | 2057.72 | 0.373      | 3.52(8)    | 3.48(8) | 6.70(8) |         |

*: A(B) denotes $A \times 10^B$
†: corrected from the value 3.88(7) given in [5]

The comparisons we make in Table 1 are between the transition rates of various authors – the oscillator strengths can easily be deduced from the transition rates. The calculations have been undertaken using a variety of methods. Nahar & Pradhan [5] use the close-coupling approximation within the context of the R-matrix code ([11]), which is based on LS-coupling. This code requires FeIV wave functions as input, and the difference between the orbitals, particularly 3d in the FeIII and FeIV states, is only partially accounted for by the use of continuum orbitals. Moreover, transition data for individual lines are obtained by an algebraic
transformation from the \textit{LS}-coupled data. However, while this will not allow the mixing of contributions from different \textit{LS} terms in an \textit{LSJ} wave function, we would remark that this mixing is relatively small for the transitions we are considering, compared with mixings encountered in ions such as Fe\textsubscript{II}.

Raassen & Uylings [6] use their orthogonal operators method, which incorporates the effect of higher configurations as well as other effects using additional operators in the Hamiltonian. By this process, the calculated energies match the experimental energies very closely.

Ekberg [12] presents some calculations using the Cowan [13] code to augment his experimental determination of energy levels. These calculations are relatively simple, compared with other more recent work. Each of the three main configurations is treated independently, but without explicit correlation effects, the energy agreement with experiment being achieved by a least-squares process using the various radial integrals involved in the energy expression as variable parameters, though some additional parameters were included to model the effects of energetically higher configurations.

The transition rates shown in Table 1 are, with some exceptions, in qualitative agreement across the different calculations, even though for the larger rates differences of up to 50\% occur between different methods. It is difficult to generalise, but our results seem to be in somewhat closer agreement with those of Raassen & Uylings [6] than with the other calculations. This is perhaps not surprising, since both are extensive calculations and both seek to obtain close agreement with experiment for the energy values of the various levels. A particular exception to this close agreement with the results of [6] is the set of three \textit{<Fe\textsubscript{III}>} fluorescent lines listed at the top of Table 1. For these transitions, we agree much more closely with Nahar & Pradhan [5], whereas Raassen & Uylings agree closely with Ekberg [12]. Nevertheless, except for the results of Ekberg, the transition rates for the three transitions are very similar within each calculation. The difference between them is largely due to the \textit{\lambda}^{-3} dependence of the \textit{A}-value, a consequence of both levels being almost 100\% pure. For the weaker transitions there is a wider distribution of values. Here, cancellation effects due to CI are frequently the cause of the smallness of the transition rates and our fine-tuning process is designed to represent that CI mixing as accurately as possible. A full set of results will be published elsewhere.

We have also calculated \textit{E2} and \textit{M1} rates for transitions between the levels considered here. In Table 2 we compare our \textit{gA} values for the five electric quadrupole transitions \textit{3d}^6\textit{5D}_J \rightarrow \textit{3d}^5\textit{(6S)}\textit{4s}5\textit{S}_2 with those reported by Johansson et al. [4] and in our earlier \textit{CIV3} calculations (Toner & Hibbert [7]). The results of [7] were already about 25\% higher than those of [4], obtained using the Cowan code [13]. Our new \textit{gA}-values are slightly higher again, by about a further 8\%. This further increase is an indication of the effect of convergence in this more extended calculation.

| \textit{J} | \textit{\lambda}_{\text{exp}}(\textit{\AA}) [4] | [4] | [7] | \textit{Present} |
|---|---|---|---|---|
| 4 | 2439.019 | 111 | 134.7 | 147.6 |
| 3 | 2465.222 | 80 | 99.7 | 107.7 |
| 2 | 2483.760 | 55 | 68.8 | 73.7 |
| 1 | 2495.755 | 32 | 40.4 | 43.0 |
| 0 | 2501.683 | 10 | 13.3 | 14.1 |

In conclusion, we have carried out an atomic structure calculation for the computationally difficult open \textit{d}-shell ion Fe\textsubscript{III}. Fine-structure energy levels belonging to the lowest three configurations (\textit{3d}^5, \textit{3d}^4\textit{4s} and \textit{3d}^4\textit{4p}) have been determined in a large scale CI calculation using the \textit{CIV3} program of Hibbert [8,9]. All the major correlation and core-valence effects are carefully incorporated; relativistic effects are included through the Breit-Pauli operators. The diagonal elements of the Hamiltonian matrix are adjusted by small amounts to bring the \textit{ab initio} energies
into agreement with experimental values, and in so doing, improve the accuracy of the mixing coefficients in the CI expansions of the wave functions. Oscillator strengths and radiative rates for all E1 and some E2 transitions were then calculated and compared with the available results.

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