Electric dipole transitions among low lying levels of Fe IV

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Abstract. We report a large-scale configuration interaction (CI) calculation for the fine-structure levels of Fe IV belonging to the 3d^5, 3d^4s and 3d^4p configurations. In order to generate well-represented CI wave functions, we use the Hartree-Fock functions for 1s, 2s, 2p, 3s, 3p and 3d orbitals of the 3d^5S level, augmented by seven more orbitals (4s, 4p, 4d, 4f, 5s, 5p and 5d), optimised on different energies: 4s and 4p are optimised on spectroscopic levels, while the remaining orbitals are optimised to account for the effect of different 3d^4 cores and correlation effects. Relativistic effects are included through the Breit-Pauli operators. Excitation energies of all the fine-structure levels of the three lowest configurations and oscillator strengths for all E1 transitions among these levels are calculated in the present investigation. A number of these oscillator strengths, for transitions between some low-lying sextet levels, are presented and compared with other available calculations.

1. Introduction

Data for low ionization stages of iron (Fe I to Fe IV) with dominant contributions from Fe IV are important for non-local thermal equilibrium spectral models. In Galactic H II regions one can expect iron to be in three ionization stages: Fe II, Fe III and Fe IV. The Fe II and Fe III abundances can be determined from several optical [Fe II] and [Fe III] lines (although one should be careful about [Fe II] emission, since some optical lines are affected by fluorescence [1,2]). The total iron abundance in the gas then can be obtained by correcting for the contribution of Fe IV. The ionization potential of Fe IV is 54.8 eV which is very close to that of He II at 54.4 eV. Thus, in a photoionized H II region such as the great diffuse nebula in the constellation of Orion, stellar ionizing flux is effectively shielded by helium to prevent extensive ionization of iron beyond Fe IV. It is because of this reason that hot stars of spectral types O and B have a 54 eV “cut-off” which attenuates the ionizing flux.

Fe IV is a challenging open d-shell problem with a large number of strongly interacting levels. The lowest three configurations 3d^5, 3d^4s and 3d^4p give as many as 108 LS states. Some of their levels differ only by seniority of 3d^5 or of the 3d^4 core and they interact very strongly. Accurate knowledge of oscillator strengths for Fe IV is important in probing physical conditions within various astronomical objects. Only a few calculations [3-6] are reported on E1 transitions in Fe IV levels. While some of these calculations lack the direct introduction of relativistic effects [5], with transition data for individual lines being obtained by an algebraic transformation of non-relativistic, LS-coupled oscillator strengths, others take account of relativistic and correlation effects but use a more limited number of configurations.

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2. Method of calculation

In the present calculation we have used the configuration interaction code CIV3 [7], augmented [8] to include relativistic effects via the Breit-Pauli Hamiltonian, to obtain configuration interaction (CI) wave functions which we then use to calculate oscillator strengths of electric-dipole and intercombination transitions. The calculation proceeds in several stages.

The first stage is the determination of the radial functions used in the configuration state functions (CSFs). This stage is undertaken purely in the \(LS\) coupling scheme. The radial functions for \(1s, 2s, 2p, 3s, 3p\) and \(3d\) orbitals are chosen to be the Hartree-Fock functions [9] of the \(3d^5(6S)\) state. Other radial functions of the one-electron orbitals \(4s, 5s, 4p, 5p, 4d\) and \(5d\) were optimised on the energies of various atomic states, as follows. The \(4s\) orbital is optimised on the energy of \(3d^4(5D)4s^6D\) and so is a ‘spectroscopic’ orbital. \(5s\) is optimised on the third lowest \(^4P\) state, (corresponding to \(3d^4(3P_i)4s\)), using the configurations \(3d^5, 3d^4s, 3d^45s\). Hence \(5s\) represents a means of allowing some \(LS\) dependence in the orbital functions, and so we regard it as a ‘correction’ orbital. \(4p\) is optimized on \(3d^44p^6P^o\) and is therefore spectroscopic. \(5p\) is taken as a correction to \(4p\) and is optimized on the lowest eigenvalue of the two configurations \(3d^44p^6D^o\) and \(3d^55p^6D^o\). \(4d\) is optimized on \(3d^4(^2D1)\) – the third lowest \(^2D\) state – using configurations \(3d^5\) and \(3d^44d\), so that \(4d\) acts as a correction to \(3d\) for a different total \(LS\) symmetry (and one which is relatively high-lying in energy) from the state on which the \(3d\) is optimised. \(5d\) is optimised on the \(3d^5\) \(^2P\) state, using the configurations \(3d^5, 3d^44d^2, 3d^44d5d, 3d^55d^2\), so that \(5d\) represents one of the major correlation effects in the states under investigation. \(4f\) is optimised on the \(3d^5(6S)\) state, using the configurations \([3d^5, 3d^44f^2]\), so that \(4f\) represents the other major correlation effect in the states under investigation.

The next stage is the choice of the configurations in the CI expansions of the wave functions used for the determination of energy levels and the oscillator strengths of transitions among them. Firstly, we included up to two orbital replacements from the \(3p\) and \(3d\) subshells of the reference set of \(3p^63d^5, 3p^63d^44s\) and \(3p^63d^44p\) configurations to all the available orbitals, to obtain a set of CSFs for each of the relevant \(LS\) symmetries. Using these CSFs, we determined the \(LS\) energies and CI coefficients of all possible states which are conventionally labelled by the configurations in the reference set. Many of the eigenvector components are very small in all the eigenvectors of interest, and their omission would have little influence on the accuracy of the wave functions, but would result in a considerable saving of computer time in the \(LSJ\) calculation.

Consequently, in the subsequent work, those CSFs with CI coefficients having magnitudes less than 0.001 in all our \(LS\) wave functions were deleted from the list of CSFs. We then allowed a limited opening of the \(3s^2\) subshell by including those CSFs obtained by the replacements \(3s \rightarrow 3d, 3s^2 \rightarrow 3d^2, 3s \rightarrow 4s, 3s^2 \rightarrow 3d4s\) (for even parity) or \(3s \rightarrow 4p, 3s^2 \rightarrow 3d4p\) (for odd parity) in the reference configurations.

All the fine structure levels corresponding to the seven even \(J\) values (0.5 – 6.5) and eight odd \(J\) values (0.5 – 7.5) were then calculated with the above reduced set of configurations, combining all possible \(LS\) contributions for a particular \(J\) value. Our \textit{ab initio} energies were then fine-tuned to fit the energy differences listed by the National Institute of Standards and Technology (NIST) [10]. Most of the levels were brought into agreement to within a few cm\(^{-1}\) though a few of them could not be fixed very well because of strong mixing between the levels of same \(LS\pi\) but with different seniority. As a result of this fine-tuning the \textit{ab initio} mixing coefficients are slightly refined. These wave functions are then used to calculate oscillator strengths and radiative rates for all the E1 transitions among the lowest three configurations of Fe\textsc{iv}.

3. Results and discussions

In Table 1 we compare some of our energy-adjusted \(LSJ\) oscillator strengths with those of Nahar & Pradhan [5] and Nahar [6] for transitions among low-lying sextet levels. For all these oscillator strengths the lower and upper levels belong to \(3d^5\) and \(3d^44p\) configurations,
respectively; the full set of our results will be published elsewhere. For the \(a^6S \rightarrow z^6P^o\) transition the present oscillator strengths and radiative rates are about 10\% lower than those of the other two sets of results. The radiative rates for these three transitions remained almost independent of the \(J\) values of the upper levels in all three calculations, as expected since the states are spectroscopically pure (almost no mixing with other \(LS\) terms with the same \(J\)).

| LL→UL | \(\lambda (\text{Å})\) | \(g_i\) | \(g_f\) | \(f_{if} (\text{Present})\) | \(f_{if} [5]\) | \(A_{fi} (\text{Present})\) | \(A_{fi} [5]\) | \(A_{fi} [6]\) |
|-------|-----------------|-----|-----|-----------------|--------|-----------------|--------|--------|
| \(a^6S \rightarrow z^6P^o\) | 525.69 | 6 | 8 | 1.69(-1) | 1.88(-1) | 3.06(+9) | 3.40(+9) | 3.48(+9) |
| | 526.29 | 6 | 6 | 1.24(-1) | 1.41(-1) | 2.99(+9) | 3.39(+9) | 3.47(+9) |
| | 526.63 | 6 | 4 | 8.20(-2) | 9.39(-2) | 2.96(+9) | 3.38(+9) | 3.47(+9) |
| \(a^6D \rightarrow z^6P^o\) | 1632.41 | 10 | 8 | 1.92(-1) | 1.82(-1) | 6.01(+8) | 5.68(+8) | 6.65(+8) |
| | 1621.14 | 8 | 8 | 5.56(-2) | 6.55(-2) | 1.41(+8) | 1.66(+8) | 1.68(+8) |
| | 1619.99 | 8 | 6 | 1.08(-2) | 1.46(-2) | 2.09(+7) | 2.81(+7) | 2.60(+7) |
| | 1626.89 | 8 | 6 | 1.31(-1) | 1.17(-1) | 4.41(+8) | 3.93(+8) | 4.77(+8) |
| | 1617.68 | 6 | 6 | 9.83(-2) | 1.12(-1) | 2.51(+8) | 2.86(+8) | 2.99(+8) |
| | 1610.85 | 4 | 6 | 4.11(-2) | 5.52(-2) | 7.05(+7) | 9.46(+7) | 9.63(+7) |
| | 1620.90 | 4 | 6 | 6.86(-2) | 5.69(-2) | 2.61(+8) | 2.17(+8) | 2.73(+8) |
| | 1614.05 | 4 | 4 | 1.22(-1) | 1.29(-1) | 3.11(+8) | 3.29(+8) | 3.63(+8) |
| | 1609.81 | 2 | 4 | 1.50(-1) | 1.84(-1) | 1.93(+8) | 2.37(+8) | 2.42(+8) |
| \(a^6D \rightarrow z^6F^o\) | 1631.08 | 10 | 12 | 3.61(-1) | 3.58(-1) | 7.54(+8) | 7.48(+8) | 8.45(+8) |
| | 1651.58 | 10 | 10 | 6.38(-2) | 5.42(-2) | 1.56(+8) | 1.33(+8) | 1.64(+8) |
| | 1668.42 | 10 | 8 | 5.19(-3) | 4.32(-3) | 1.55(+7) | 1.29(+7) | 1.63(+7) |
| | 1640.04 | 8 | 10 | 2.91(-1) | 3.02(-1) | 5.78(+8) | 5.99(+8) | 6.62(+8) |
| | 1656.64 | 8 | 8 | 1.08(-1) | 9.99(-2) | 2.63(+8) | 2.43(+8) | 2.86(+8) |
| | 1669.81 | 8 | 6 | 1.41(-2) | 1.25(-2) | 4.51(+7) | 3.98(+7) | 4.42(+7) |
| | 1647.09 | 6 | 8 | 2.40(-1) | 2.54(-1) | 4.42(+8) | 4.69(+8) | 5.11(+8) |
| | 1660.11 | 6 | 6 | 1.41(-1) | 1.36(-1) | 3.42(+8) | 3.29(+8) | 3.78(+8) |
| | 1669.59 | 6 | 4 | 2.50(-2) | 2.33(-2) | 8.98(+7) | 8.37(+7) | 9.82(+7) |
| | 1652.92 | 4 | 6 | 2.01(-1) | 2.12(-1) | 3.27(+8) | 3.45(+8) | 3.77(+8) |
| | 1662.32 | 4 | 4 | 1.68(-1) | 1.67(-1) | 4.06(+8) | 4.03(+8) | 4.55(+8) |
| | 1668.08 | 4 | 2 | 3.35(-2) | 3.24(-2) | 1.60(+8) | 1.55(+8) | 1.78(+8) |
| | 1657.82 | 2 | 4 | 1.75(-1) | 1.82(-1) | 2.13(+8) | 2.21(+8) | 2.44(+8) |
| | 1663.56 | 2 | 2 | 2.26(-1) | 2.28(-1) | 5.45(+8) | 5.50(+8) | 6.16(+8) |

It is interesting to note that for the transitions between the multiplets \(a^6D\) and \(z^6P^o\) the oscillator strengths and hence the transition probabilities of Nahar & Pradhan [5] are higher than those of ours for \(g_f \geq g_i\) and lower for \(g_f < g_i\). For the transitions at 1611.99 Å and 1610.85 Å they [5] are higher by over 30%. We note here that the E1 transition rates obtained by Nahar & Pradhan [5] were determined with the R-matrix code with a limited set of relativistic operators in the Hamiltonian. Nahar [6], on the other hand, used SUPERSTRUCTURE, including relativistic effects through a more complete set of Breit-Pauli operators. However, in neither case was the refinement of fine-tuning introduced: even though Nahar used experimental transition energies, the CI mixing coefficients were not adjusted from their \(ab\initio\) values. We therefore consider our results to be more accurate.
In Table 2 we present our radiative rates in length and velocity gauges for a few intercombination transitions. For all these transitions the results in the two gauges agree within 10%. This level of agreement for these relatively weak transitions is a pointer to the accuracy of our CI wavefunctions, although we note that the velocity form would really require further relativistic corrections to the agreement to be a stronger indication of accuracy.

### Table 2. Comparison of our radiative rates in length and velocity gauge for some intercombination transitions. $A(N)$ stands for $A \times 10^N$

| LL   | Term         | UL   | Term         | $\lambda$ (Å) | $A_L$         | $A_V$         |
|------|--------------|------|--------------|----------------|---------------|---------------|
| $3d^6$ | $^6S_{5/2}$ | $3d^4(^3P)4p$ | $^2S_{3/2}$ | 388.34 | 0.870(+5) | 0.866(+5) |
| $4P_{3/2}$ | $3d^4(^3P)4p$ | $^2P_{3/2}$ | 446.91 | 0.152(+7) | 0.141(+7) |
| $4P_{3/2}$ | $3d^4(^1G)4p$ | $^2F_{5/2}$ | 434.71 | 0.259(+6) | 0.252(+6) |
| $D_{3/2}$ | $3d^4(^3P)4p$ | $^2P_{1/2}$ | 453.22 | 0.943(+6) | 0.975(+6) |
| $F_0/2$ | $3d^4(^1D)4p$ | $^2F_{7/2}$ | 428.52 | 0.165(+7) | 0.168(+7) |
| $F_{7/2}$ | $3d^4(^1D)4p$ | $^2F_{7/2}$ | 428.65 | 0.489(+6) | 0.457(+6) |
| $G_9/2$ | $3d^4(^3F)4p$ | $^2F_{7/2}$ | 451.20 | 0.356(+7) | 0.380(+7) |
| $G_{9/2}$ | $3d^4(^1G)4p$ | $^2G_{9/2}$ | 431.81 | 0.209(+5) | 0.205(+5) |
| $G_{7/2}$ | $3d^4(^1G)4p$ | $^2G_{7/2}$ | 433.48 | 0.209(+5) | 0.203(+5) |
| $G_{7/2}$ | $3d^4(^1G)4p$ | $^2F_{7/2}$ | 429.59 | 0.374(+5) | 0.361(+5) |

In conclusion, we have carried out an atomic structure calculation for Fe iv. Fine-structure levels belonging to the lowest three configurations ($3d^5$, $3d^44s$ and $3d^44p$) and dipole-allowed and intercombination transitions between these levels are calculated in a large scale CI calculation using the CIV3 program. All major correlation and core-valence effects are carefully accounted for and relativistic effects are included through the Breit-Pauli operator. Our fine-tuning process has been used to improve the accuracy of the CI mixing coefficients prior to the calculation of the oscillator strengths and radiative rates. A number of these dipole-allowed and intercombination transitions are reported and compared here with other recent calculations.

### Acknowledgments

The authors would like to thank PPARC, UK, for support under the Rolling Grant PP/D00103X/1.

### References

[1] Rodriguez M 1999 *A&A* **348** 222
[2] Verner E M et al 2000 *ApJ* **543** 831
[3] Fawcett B C 1989 *Atom Data Nucl Data Tables* **41** 181
[4] Fischer C F and Rubin R 2004 *MNRAS* **355** 461
[5] Nahar S N and Pradhan A 2005 *A&A* **437** 345
[6] Nahar S N 2006 *A&A* **448** 779
[7] Hibbert A 1975 *Comp Phys Comm* **9** 141
[8] Hibbert A, Glass R and Fischer C F 1991 *Comp Phys Comm* **64** 455
[9] Clementi E and Roetti C 1974 *Atom Data Nucl Data Tables* **14** 177
[10] NIST Website: http://physics.nist.gov/cgi-bin/AtData