Energy levels, oscillator strengths, and effective collision strengths for transitions in Fe XIV

K M Aggarwal¹, T Kato² and F P Keenan¹

¹Astrophysics Research Centre, School of Mathematics and Physics, Queen’s University Belfast, Belfast BT7 1NN, Northern Ireland, UK
²National Institute for Fusion Science, Oroshi-cho, Toki, Gifu, 509-5292 Japan
E-mail: K.Aggarwal@qub.ac.uk

Abstract. In this paper we report atomic data, namely energy levels, radiative rates, lifetimes, collision strengths, and excitation rate coefficients, for transitions among 162 levels of the (1s²2s²2p⁶) 3s²3p, 3s3p², 3s²2d, 3p³, 3s3p3d, 3p²3d, 3s3d², 3p3d², 3d³, 3s3p4s, and 3s²4f configurations of Fe XIV. For the calculations of energy levels and radiative rates both the GRASP and FAC codes have been adopted, whereas for the collision strengths only FAC is employed.

1. Introduction

Emission lines of Fe XIV have been widely observed in a variety of solar and other astrophysical plasmas, and over a wide wavelength region varying from optical to extreme ultra-violet. The strongest observed forbidden transition is from the coronal green line (3s²3p) ²P₂¹/₂ → ²P₂³/₂ with the wavelength 5303 Å. Many of the line pairs are density and/or temperature sensitive, and hence provide useful information about physical conditions of the plasmas. However, to reliably analyse observations, atomic data are required for many parameters, including energy levels, radiative rates (A-values), and excitation rates. Since experimental data are not available, except for some energy levels, theoretical results are required.

Considering the importance of Fe XIV many calculations have been performed in the past, particularly for the A-values, such as by Huang [1], Storey et al. [2], Safronova et al. [3], Gupta and Msezane [4], Froese-Fischer et al. [5], Dong et al. [6], and Wei et al. [7]. However, most of these calculations are confined to transitions among the lowest 40 levels of the n = 3 configurations, although Gupta and Msezane and Wei et al. have also included some levels of the n = 4 configurations. Similarly, in a more recent paper Tayal [8] has reported energy levels, radiative rates, and effective collision strengths for some transitions among the lowest 59 levels of the (1s²2s²2p⁶) 3s²2p, 3s3p², 3s²2d, 3p³, 3s3p3d, and 3p²3d configurations of Fe XIV. Furthermore, most of these workers have reported A-values for the electric dipole (E1) transitions alone, whereas in the modelling and diagnostics of plasmas corresponding results are also required for other types of transitions, namely electric quadrupole (E2), magnetic dipole (M1), and magnetic quadrupole (M2). Similarly, for the modelling of plasmas atomic data for all transitions are preferable. Therefore, the aim of the present work is to extend and improve upon the earlier available calculations, apart from reporting a complete set of results for all transitions, which can be confidently applied in plasma modelling.
2. Calculations
For our calculations we have adopted the GRASP (general-purpose relativistic atomic structure package) code, originally developed by Grant et al. [9] but revised by Dr. P. H. Norrington. It is a fully relativistic code, based on the jj coupling scheme. Further relativistic corrections arising from the Breit interaction and QED effects have also been included. Additionally, we have used the option of extended average level (EAL), in which a weighted (proportional to \(2j+1\)) trace of the Hamiltonian matrix is minimized. This produces a compromise set of orbitals describing closely lying states with moderate accuracy. A series of calculations have been performed with increasing amount of CI (configuration interaction) included with up to \(n = 5\) orbitals, which generate up to 332 levels. However, the presentation of the results is confined to the lowest 162 levels of the 3s\(^2\)3p, 3s3p\(^2\), 3s\(^2\)3d, 3p\(^3\), 3s3p3d, 3p\(^2\)3d, 3s3d\(^2\), 3d\(^3\), 3s3p4s, and 3s\(^2\)3d\(^{\ell}\) configurations alone. Among these the lowest 135 levels were included by Tayal [8], who adopted the multi-configuration Hartree-Fock (MCHF) code of Froese-Fischer [10] for calculating energy levels and \(A\) values, and the \(R\)-matrix code of Berrington et al. [11] for calculating collision strengths (\(\Omega\)) and subsequently the effective collision strengths (\(\Upsilon\)).

Additionally, in order to make a rigorous accuracy assessment of our results, we have also performed calculations from the Flexible Atomic Code (FAC) of Gu [12], available from the website http://kipac-tree.stanford.edu/fac. This is a fully relativistic code and provides a variety of atomic parameters. Furthermore, the code yields results comparable to those obtained from other atomic structure codes such as CIV3 and GRASP - see, for example, Aggarwal et al. [13] and references therein, and scattering codes such as \(R\)-matrix - see, for example, Aggarwal et al. [14] and references therein. Furthermore, FAC is based on the well-known and widely-used distorted-wave (DW) method and yields results for collision strengths (\(\Omega\)) comparable with those from the \(R\)-matrix method, particularly for the allowed transitions, as demonstrated in several of our earlier papers on a variety of ions, including many of iron, i.e. Fe XI - Fe XXVI.

As from GRASP, with FAC also we have performed a series of calculations with increasing amount of CI with up to \(n = 5\) orbitals, generating a maximum of 3146 levels. However, for the calculations of \(\Omega\) and \(\Upsilon\) values, only 162 levels of the 3s\(^2\)3p, 3s3p\(^2\), 3s\(^2\)3d, 3p\(^3\), 3s3p3d, 3p\(^2\)3d, 3s3d\(^2\), 3p3d\(^2\), 3d\(^3\), 3s3p4s, and 3s\(^2\)3d\(^{\ell}\) configurations have been considered. These calculations will provide a direct comparison with the most recent results of Tayal [8].

3. Energy levels, radiative rates, and lifetimes
Our energy levels from GRASP and FAC agree with each other in both magnitude and orderings, and the agreement with the experimental values compiled by NIST (http://physics.nist.gov/PhysRefData) is also highly satisfactory, generally within 1%. Similarly, the agreement with the energy levels of Tayal [8] is generally satisfactory, but our energy for the 3s\(^2\)3p \(^2\)P\(^o\)\(_{3/2}\) level is particularly closer to the experimental result, whereas Tayal’s value is lower by 6%. Similarly, the two sets of \(A\) values from GRASP and FAC agree within 20% for a majority of strong transitions (\(f \geq 0.01\)), although differences are larger for the weaker ones. Tayal has reported \(A\) values for only some of the transitions among the lowest 59 levels alone, and there is no discrepancy with his results for the strong transitions. A complete set of \(A\) values among 162 levels and for all four types of transitions can be obtained on request from KMA (K.Aggarwal@qub.ac.uk). Furthermore, detailed results for transitions among the lowest 332 levels, along with lifetimes, are reported in a separate paper by Aggarwal et al. [15].

4. Collision strengths and effective collision strengths
We have calculated values of \(\Omega\) (which is related to the better known quantity collision cross section \(\sigma\) as \(\Omega = k_i^2 \omega_i \sigma_{ij} (\pi a_0^2)\), where \(k_i^2\) is the electron energy and \(\omega_i\) is the statistical weight of the lower level \(i\)) for all the 13 041 transitions among the above listed 162 levels of Fe XIV over a wide energy range up to \(\sim 160\) Ryd. This energy range is similar to that of Tayal [8], who
calculated values of $\Omega$ up to $E = 150$ Ryd. No comparisons can be made with the calculations of Tayal, because he has not reported values of $\Omega$. However, comparisons can be made for $\Upsilon$ values, which are obtained after integrating the $\Omega$ values over a Maxwellian distribution of electron velocities. A comparison of our values of $\Upsilon$ with those of Tayal in the common temperature range of $3 \times 10^5 \leq T_e \leq 10^7$ K is generally satisfactory for the allowed transitions, as shown in Fig. 1 for three resonance (allowed) transitions, namely 1-8 ($3s^23p^2 P^o_{1/2} - 3s3p^2 S_{1/2}$), 1-9 ($3s^23p^2 P^o_{1/2} - 3s3p^2 P_{1/2}$), and 1-10 ($3s^23p^2 P^o_{1/2} - 3s3p^2 P_{3/2}$). Some anomaly between the two independent calculations, particularly towards the lower end of the temperature range, is perhaps due to the inclusion of resonances by Tayal. Since resonances for allowed transitions are often not prominent, their effect on the calculations of $\Upsilon$ is confined to very low temperatures alone. Similarly the slightly anomalous behaviour of the $\Upsilon$ values of Tayal towards the higher temperatures for these transitions is perhaps due to the limited range of partial waves with angular momentum $J \leq 25$ included by him. This range of partial waves is insufficient for the convergence of $\Omega$ for a majority of the allowed and some forbidden transitions, particularly those among the excited levels. Since he has accounted for the contribution of higher neglected partial waves through a top-up, there is no major discrepancy between the two calculations for a majority of the common allowed transitions, although the $\Upsilon$ values differ by $\sim 10\%$ over the entire temperature range for some of the transitions, such as 1-8. A part of the differences are due to the corresponding differences in the $f$-values. As an example, our $f$-value for the 1-8 transition is 0.199 whereas that of Tayal is 0.191, i.e. lower by 4%.

In Fig. 2 we compare the $\Upsilon$ values for three transitions among the excited levels, namely 2-10 ($3s^23p^2 P^o_{3/2} - 3s3p^2 P_{3/2}$), 2-12 ($3s^23p^2 P^o_{3/2} - 3s^23d^2 D_{5/2}$), and 5-27 ($3s3p^2 P_{5/2} - 3s3p3d D^o_{5/2}$). For these transitions also there is no (major) discrepancy with the corresponding results of Tayal [8], particularly at higher temperatures. However, differences between the two calculations are significant for a majority of the forbidden and some intercombination transitions, because Tayal has resolved resonances in the thresholds region whereas we have not. Resonances often enhance the values of $\Upsilon$, by up to an order of magnitude (or even more), depending upon the transition and/or the temperature. Therefore, for the transitions for which Tayal has reported results ($\sim 5\%$), his values of $\Upsilon$ may be preferable, but only for the forbidden transitions. Since his results for both $\Lambda$ and $\Upsilon$ values are restricted to a subset of the total 13 041 transitions, these are of limited applications. Therefore, under the circumstances, a complete set of our results for all transitions can be confidently applied for the modelling of plasmas. The entire set of data for all transitions for $\Lambda$ and $\Upsilon$ values over a wide range of temperatures are reported in a separate paper [15].
5. Conclusions
In this paper results for energy levels, radiative rates, and effective collision strengths for transitions in Fe XIV have been discussed. For calculating energy levels and A- values, both GRASP and FAC codes have been used whereas for the Y values FAC alone is adopted. Energy levels and A- values agree in general with the already available data in the literature, but the present results cover a wider range of levels and hence the transitions. Similarly, for Y values there is a general agreement for many allowed transitions with the most recent calculations of Tayal [8], but differences are notable for the forbidden transitions, because resonances have not been resolved in the present work. Detailed results in numerical form for all atomic parameters can be obtained on request from KMA (K.Aggarwal@qub.ac.uk). Furthermore, a larger calculation involving 332 lowest levels of Fe XIV has also been recently reported by Aggarwal et al. [15]. This paper contains detailed comparisons as well as a complete set of data for all atomic parameters.

Acknowledgments
This work has been financed by the EPSRC and STFC of UK. FPK is grateful to AWE Aldermaston for the award of a William Penney Fellowship and KMA would like to acknowledge the hospitality of NIFS enjoyed during a visit in November 2007.

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