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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 $3d^4$, $3d^3 4s$ and $3d^3 4p$ 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 ($f \geq 0.1$), 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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Contents

1. Introduction

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^{3}4s and 3d^{3}4p 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^{3}4d and 3d^{3}5s 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^{3}4p configurations and none has been measured for 3d^{3}4s—see Table 3 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 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 ~15 000 vectors, and determined energies for 5 ($J = 0$) levels of the 3d^4 and 19 ($J = 1$) of 3d^{3}4p configurations. They achieved a good accuracy within ~3% of the measurements—see their table III. The largest *ab initio* calculation available so far is by Nahar and Pradhan [19], 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^{3}4s, 3d^{3}4p, 3d^{3}4d, and 3d^{2}4s^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

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