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Electric-dipole allowed and intercombination transitions among the $3d^5$, $3d^44s$ and $3d^44p$ levels of Fe IV

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ABSTRACT

Oscillator strengths and transition rates for the electric-dipole (E1) allowed and intercombination transitions among $3d^5$, $3d^44s$ and $3d^44p$ levels of Fe IV are calculated using the CIV3 code of Hibbert and coworkers. Using the Hartree–Fock functions up to 3d orbitals we have also optimized 4s, 4p, 4d, 4f, 5s, 5p and 5d orbitals of which 4s and 4p are taken to be spectroscopic and the remaining orbitals represent corrections to the spectroscopic orbitals or the correlation effects. The *J*-dependent levels of 108 *LS* states are included in the calculation and the relativistic effects are accounted for via the Breit–Pauli operator. Configurations are chosen in two steps: (a) two promotions were allowed from the 3p, 3d, 4s and 4p subshells, using all the orbitals; and (b) selective promotions from the 3s subshell are included, but only to the 3s and 4s orbitals. The ab initio fine-structure levels are then fine tuned to reproduce observed energy levels as closely as possible, and the resulting wavefunctions are used to calculate oscillator strengths and transition rates for all possible E1 transitions. For many of these transitions, the present results show good agreement between the length and velocity forms while for some transitions, some large disagreements are found with other available results. The complete list of weighted oscillator strengths, transition rates, and line strengths for transitions among the fine structure levels of the three lowest configurations are presented in ascending order of wavelength.

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1. Introduction

Low ionization stages of iron (Fe I–Fe IV) are of considerable interest to the astrophysical community. Early detections [1,2] of many allowed and forbidden lines in the bright planetary nebula NCG 7027 gave an impetus to further study. Lines of iron peak elements (Fe, Co, Ni and their ions) were also found in η-Carinae [3] and R R Telescopii [4]. Later McKenna et al. [5] reported some more allowed and forbidden lines of iron ions along with lines of other ions. Using the Goddard High-Resolution Spectrograph on the Hubble Space Telescope, Rubin et al. [6] first detected an Fe IV forbidden line in the Orion nebulae at a wavelength, λ, of 2836.56 Å.

Because of the complex nature of the atomic structure calculation of Fe IV, very few calculations have so far been are attempted. Kurucz [7] compiled the most extensive set of data for iron ions, which are widely used for astrophysical modeling. Using the Cowan code [8], Fawcett [9] presented simple calculations for low charge states of iron ions including Fe IV, but with limited treatment of correlation effects. Sawey and Berrington [10] and Bautista and Pradhan [11] presented *LS* coupling calculations of Fe IV although the main purpose of their work was to obtain collision strengths. Nahar and Pradhan [12] included a very large number of bound states (up to $n \leqslant 11$, $l \leqslant 9$) within the *R*-matrix program [13] to carry out *LS* calculations for the radiative data for Fe IV. They then resolve these *LS* data into individual fine-structure lines using an algebraic transformation. This calculation does not include explicitly relativistic effects in the Hamiltonian. The SUPERSTRUCTURE calculation of Nahar [14] includes explicit relativistic effects through the Breit–Pauli approximation.

In a recent calculation Deb and Hibbert [15] have demonstrated large discrepancies among some of the existing atomic data for Fe IV, and they have also presented some possible explanations for these discrepancies. Here we give a more complete list of oscillator strengths and transition rates obtained for optically allowed and intercombination transitions among the fine-structure levels of $3d^5$, $3d^4 4s$ and $3d^4 4p$ configurations of Fe IV. The present calculation uses the CIV3 codes [16,17] of Hibbert and coworkers to calculate ab initio energies of all the fine-structure levels belonging to the above configurations, fine tune only those energies for which NIST recommended values are available, and use the corresponding wavefunctions to calculate the atomic parameters. A brief description of the theoretical method is presented in the next section.

2. Theoretical method

Using Hartree–Fock [18] radial functions for the 1s, 2s, 2p, 3s, 3p and 3d orbitals, we have optimized the 4s and 4p as real spectroscopic orbitals on the energies of $3d^4(^5D)4s\ ^6D$ and $3d^4(^5D)4p\ ^6F^o$. In order to account for the corrections due to various *LS* symmetries, we took 4d as a correction to 3d orbital and optimized on the third lowest of the ^2D levels arising from the $3d^5$ and $3d^4 4d$ configurations, while 4f was optimized on the $3d^5\ ^6S$ state, using the configurations $3d^5$ and $3d^3\ 4f^2$, so that 4f represents a major correlation effect. The 5s function was optimized on the third lowest ^4P state, using $3d^5$, $3d^4 4s$ and $3d^4 5s$ and hence represents a correction orbital allowing some *LS* dependence in the optimal orbital function. Similarly 5p was chosen as a correction orbital and was optimized on the lowest $^6D^o$ eigenvalue arising from the $3d^4 4p$ and $3d^4 5p$ configurations. Finally, 5d was optimized on the $3d^5\ ^2P$ state, using $3d^5$, $3d^3 4d^2$, $3d^3 4d 5d$ and $3d^3 5d^2$, so that it represents another major correlation. The parameters of the optimized orbitals are presented in Table 1.

The optimizations of all radial functions were done in the *LS* coupling scheme using the state wavefunction

$$\Psi(LS) = \sum_{i=1}^{K} a_i \phi_i(\alpha_i LS), \tag{1}$$

where *L* and *S* are the total orbital and spin angular momenta, *K* is the number of terms in the configuration interaction (CI) expansion, a_i are the expansion coefficients and α_i specifies the angular momentum coupling scheme of the *i*th term in Eq. (1). The radial part of the one-electron functions is expressed as the sum of the Slater-type orbitals

$$P_{nl}(r) = \sum_{j=1}^{k} c_{jnl} r^{l_{jnl}} \exp(-\xi_{jnl} r) \times \left[\frac{(2\xi_{jnl})^{2l_{jnl}+1}}{(2l_{jnl})!}\right]^{1/2}, \tag{2}$$

where $k \geqslant n - l$. The coefficients c_{jnl} and the exponents ξ_{jnl} are determined variationally, imposing in addition the condition of orthonormality

$$\int_0^\infty P_{nl}(r) P_{n'l}(r)\, dr = \delta_{nn'}. \tag{3}$$

Once the orbitals were optimized, we proceeded to choose the configurations sets additional to the three main $3d^5$, $3d^4 4s$ and $3d^4 4p$ configurations. This was done in two steps:

1. Two promotions were allowed from the 3p, 3d, 4s and 4p subshells to all the optimized orbitals; this generated 103 even and 87 odd configurations. These configurations were then used to construct configuration state functions (CSFs) of all possible *LS* couplings. We note that there are 40 even and 68 odd *LS* states spanning 14 even (^2S–^2I, ^4P–^4H, ^6S, ^6D) and 18 odd ($^2S^o$–$^2K^o$, $^4S^o$–$^4I^o$, $^6P^o$, $^6D^o$, $^6F^o$) symmetries. A very large number of CSFs was generated for each of these symmetries and *LS* energies were calculated for the states of interest. It was found that many of these CSFs have negligibly small contributions to the eigenenergies of our interest. We therefore deleted those CSFs whose absolute eigenvector components are less than 0.001, in all eigenvectors corresponding to the states being considered in this work.
2. A small number of CSFs were then added to each of the symmetries to incorporate the important $3s \rightarrow 3d$ or $4s$ and $3s^2 \rightarrow 3d^2$ or 3d4s correlations.