

Calculation of bound states and oscillator strengths for Fe VII

ABSTRACT

Data for radiative transitions between all bound and free states of elements with significant stellar abundances are required for opacity calculations that are discussed by Seaton in these proceedings. In the iron ions, valence electron states are interspersed with those of excited configurations. The large spread in energy of these core-excited configurations makes theoretical and experimental analysis very difficult. Recent developments of computer codes and exploitation of modern computer power have made this first attempt at a comprehensive study for Fe VII possible. Our results are not definitive, discrepancies with experimental data are still large, but we hope that they will form a sound basis for future work. A full account of this work is in preparation for submission to Journal of Physics B.

THE CALCULATION

The Fe⁷⁺ target states

Of the seven configurations 3s²3p⁶3d, 4s, 4p, 4d, 4f, and 3p⁵3d², 3s3p⁶3d² all 31 terms are retained to serve as target states. In addition, the 3p⁴3d³(²D) states provide correlation with the ground state 3p⁶3d. The ionic orbitals 1s to 4f are optimised in a statistical model potential (Nussbaumer and Storey, 1978, 1988).

The Fe⁶⁺ bound and free states

In the close coupling expansion the wave function for Fe⁶⁺ is given by

$$\phi^{SL\pi} = A \sum_i \phi_i F_i + \sum_j c_j \phi_j \quad (1)$$

where A is an antisymmetrisation operator, ϕ and F are vector-coupled functions for target and added electrons, and ϕ_j are wave functions for additional configurations of Fe⁶⁺ formed

from target orbitals only. Free variation of the radial part of F and the configuration mixing coefficients c leads to a set of coupled integro differential equations for each SL π . For the solution we use the opacity version of the RMATRIX code described by Berntson et al., 1987.

Restrictions

SL-coupling is used throughout. The angular momenta of the added electron are restricted to $l=0$ to 4. The equations are solved for S=0, 1, and 2 and L=0 to 8. All bound states with energies such that the principal quantum number of the lowest channel is less than 11 are obtained and stored; 515 such states are below the first ionisation limit. We calculate oscillator strengths for all dipole allowed transitions between these terms and photoionisation cross sections from 0 to 10 Rydberg from all these bound states.

SPECIAL FEATURES OF Fe VII

Configuration mixing in bound states

Experimental energies are known for only 8 terms of Fe⁷⁺, (Corliss and Sugar, 1985) out of the 31 terms included here. For these, our target term energies differ by .20 to .46 Ryd (increasing with energy). In a similar way they differ from results by Fawcett, 1989 who has calculated energies for levels J=1/2 to 3 1/2 of configuration 3p⁵3d² using configuration interaction and Slater parameters to fit to the experimental data. Core-excited configurations 3p^x3d^y cover wide bands of the energy, as illustrated in fig. 1. The valence electron states 3dn l couple strongly with core-excited states and this affects their quantum defects, (Ekberg, 1981). Our close coupling expansion takes account of these effects, but, as a consequence of the shortcomings of our target energies our calculation for Fe⁶⁺ does not reproduce the perturbations between the principal series and the excited configurations quite accurately. In particular, terms with open core parent configurations are shifted to higher energies. Table 1 shows the difference between calculated and experimental energies for seven configurations. A table of term energies is available.

Oscillator strengths

Calculated oscillator strengths are very sensitive to the composition of the wave functions. The earlier data as compiled by Fuhr et al., 1988 did not include configuration mixing between core-excited states and valence electron states that we include. But they do include spin-orbit coupling effects that we neglect. Fuhr et al. assign accuracy D⁻ to

