

W XLV: atomic data for ITER diagnostics

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Abstract. Tungsten is a potential material for the lining of the walls of the divertor region of the International Thermonuclear Experimental Reactor (ITER), because of its low rate of erosion and hence long lifetime. A knowledge of decay rates of various ions of this element, both radiative and by electron collision, are important in analysing the impurities in the plasma.

To this end, we are investigating the properties of highly ionised Tungsten, specifically W XLV. We have used the CIV3 program [1] which incorporates relativistic effects via the Breit-Pauli Hamiltonian, to undertake configuration interaction calculations of the levels associated with configurations $\{1s^2 2s^2 2p^6 3s^2 3p^6\} 3d^{10}[4s^2, 4s4p, 4s4d, 4s4f, 4p^2, 4p4d]; 3d^9[4s^2 4p, 4s^2 4d, 4s^2 4f, 4s4p4d]$. The CI expansions also include the configurations $3d^{10}[4p4f, 4d^2, 4d4f, 4f^2]; 3d^9[4s4p4f$ and $4p4d4f]$ to allow for correlation effects.

The $n=4$ orbitals were optimised by including the one-body mass correction and Darwin terms of the Breit-Pauli Hamiltonian in addition to the usual non-relativistic Hamiltonian, both directly and by means of a model potential, following the procedure of Cowan and Griffin [2]. The optimised orbitals were very similar in these two approaches, but their mean radii were smaller than those of a purely non-relativistic optimisation, thus displaying the relativistic contraction of the outer orbitals.

The states with occupations including $3d^9$ are strongly mixed, so it is important to obtain accurate values for their separations. This is especially true for the $J = 1$ odd parity as these levels have a direct E1 transition to the 1S_0 ground state. Particularly important are the very strong transitions from the $3d^9 4s^2 4f$ levels, for which the dipole matrix element is non-zero. These levels mix strongly with those of $3d^9 4s4p4d$, but only the $3d^9 4s^2 4f$ configurations contribute directly to the dipole matrix, being just one orbital different from that of the ground state. It is therefore crucial that this mixing is determined accurately.

The results of oscillator strengths for these and other transitions will be presented at the conference. It is our intention to use the wavefunctions as target state wavefunctions in an electron-impact calculation, to compute collision cross sections and excitation rates. For this aspect of the work, we will use parallel R-matrix codes.

REFERENCES

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2. R. D. Cowan, and D. C. Griffin, *J. Opt. Soc. Am.* **66**, 1010–1014 (1976).