

Multiconfiguration Dirac-Hartree-Fock energy levels, wavefunction compositions, and transition probabilities for W XXXVIII

Charlotte Froese Fischer* and Gediminas Gaigalas†

*National Institute of Standards and Technology, MD 20899-8420, Gaithersburg, USA

†Vilnius University, Institute of Theoretical Physics and Astronomy,
A. Goštauto 12, LT-01108 Vilnius, Lithuania

Abstract.

Energies, lifetimes, and wave function compositions have been computed for all levels of $4p^64d$, $4p^64f$, and $4p^54d^2$ configurations. Single- and double excitations were used to generate expansions for the multiconfiguration Dirac-Hartree-Fock (MCDHF) approximation from an active set of orbitals with maximum nl quantum numbers of $4f$, $5g$, $6h$, respectively. For the even states, the excitations were from $4s^24p^64d$ with an inactive Ni-like core, but for odd levels the excitations were from both $4s^24p^64f$ and $4s^24p^54d^2$. Orbitals were optimized in groups of levels specified by J and parity.

A newly extended version [1] of the general relativistic atomic structure package, GRASP2K [2], was used to deal with configuration state functions with as many as six open shell and with configurations containing as many as three f -electrons in a subshell. Also included in this package is a new JJ2LSJ program that rapidly transforms a specified portion of the wavefunction from jj -coupling to intermediate LSJ-coupling. The present calculations were a test-case for this code for complex, relativistic atomic systems.

Calculations were performed systematically so that the convergence of the levels could be monitored as a function of the increasing size of the orbital sets used in the expansion. Configuration interaction calculations were performed to include Breit and QED corrections.

The E1, E2, M1 transition probabilities between all these levels and their computed and lifetimes will be presented. Results will be compared with other theory [3] and with experiment [4], when available. The present wavelengths are in good agreement with experiment although there is a discrepancy in the composition for the upper level with the highest transition to the ground state.

Keywords: multiconfiguration Hartree-Fock, multiconfiguration Dirac-Hartree-Fock, transition rates, energy structure

PACS: 31.15.am; 31.15.vj; 31.15.xr; 32.70.Cs

REFERENCES

1. P. Jönsson, G. Gaigalas, J. Bieroń, C. Froese Fischer, and I. P. Grant, *Comput. Phys. Commun.* to be submitted (2012).
2. P. Jönsson, X. He, C. Froese Fischer, and I. P. Grant, *Comput. Phys. Commun.* **177**, 597–622 (2007).
3. P. Bogdonovich, O. Rancovai, and A. Stikonas, *Phys. Scr.* **83**, 065302 (2011).
4. A. E. Kramida and T. Shirai, *AT. Data Nucl. Data Tables*, **95**, 305 (2009).