Disclaimer for Missing, the user friendly interface for atomic multiplet calculations

The user friendly interface Missing has been written by Riccardo Gusmeroli, in collaboration with Prof. Claudia Dallera and relying on the advisory capacity of Prof. Lucio Braicovich.
The program greatly simplifies the use of the atomic multiplet calculation programs based on the code by Robert D. Cowan with further additions. Our work consisted in writing the Graphical User Interface, and implementing the procedures that allow a rapid processing and viewing of the calculated spectra and the parameters used in the calculations.
We want here to give credit to the researchers who mainly contributed to the development of the codes.

The modules *RCN, RCN2* and *RCG* were written and developed by R.D. Cowan. These modules serve to calculate energy parameters, exchange and spin orbit integrals in spherical symmetry for the requested configurations and compute absorption and photoemission spectra. The most recent, bug free version of the RCG module was used in the current suite of programs.

RACER is the crystal field multiplet program. It was written by B. T. Thole based on the point group program by P. H. Butler.

BANDER is the charge transfer multiplet program. It was written by B. T. Thole with the help of B. Searle and in collaboration with A. Kotani, H. Ogasawara and K. Okada. *BANDER* was used as a basis for the development of the program for calculating x-ray emission spectra based on the Kramers-Heisenberg formula. The first version of the program was called *Fluor* and was written by B. T. Thole. Fluor was later developed and extended into *TotalFluor* by C. M. Bertoni and P. Ferriani.

Information on the development of the programs can be found in the following papers:

G. van der Laan, J. Electron Spectrosc. Relat. Phenomen. 86, 41 (1997), Section 2
A. Kotani, J. Electron Spectrosc. Relat. Phenom. 100, 75-104 (1999), on p.84 (see also the footnote).

The right to use the software free of charge is granted to scientific institutions, provided a proper reference to the code and its author is included in any publication issued with the help of the code. Any commercial use is instead prohibited without explicit authorization by the author.
In porting the original code from the PC-compatible version bugs unavoidably arose. Many of them have been found and removed by the author but some might still be present. The users of Missing should recognize when results are suspicious and undoubtedly contradicting physical expectations. In such cases please contact the author enclosing the indicted results (see below for contact information).

Comments, suggestions and bug reports can be sent to:

Prof. Claudia Dallera
Dipartimento di Fisica
Politecnico di Milano
Piazza L. Da Vinci, 32
20133 Milano (MI)
Email: claudia.dallera@fisi.polimi.it