Abstract Submitted for the MAR12 Meeting of The American Physical Society

Atomic Multiplets in X-ray spectroscopies revisited¹ BERNARD DELLEY, Paul Scherrer Institut, CMT, WHGA123, CH-5232, Villigen PSI, FRANCOIS VERNAY, University of Perpignan, France, ANNE-CHRISTINE ULDRY, Paul Scherrer Institut, CMT, WHGA123, CH-5232, Villigen PSI — Atomic multiplets are known since a long time to produce specific, crystal field dependent, fingerprints of open d- and f- shells in X-ray spectroscopies. Older computer programs originating from gas-phase optical spectroscopy of atoms tend to be difficult to apply to crystal field environments with lower symmetries. In order to study changes of X-ray absorption near edge spectra and resonant inelastic X-ray scattering (RIXS) across symmetry lowering phase transitions, a new multiplet program was developed. Starting from a Dirac-Slater spherical atom calculation we evaluate electron-electron interaction and crystal field in the Hilbert space spanned by the open shells by diagonalization. The crystal field can be simply defined by nominal charges and cartesian atomic positions relative to the core-hole atom. To overcome limitations of the model and for fitting known spectra, spin-orbit splitting, el-el interaction and crystal-field can be scaled independently. The nominal charges may be taken as further crystal field parameters. Various XAS and RIXS examples will be discussed, in particular in view of the polarisation dependence and symmetry of the crystal.

¹Supported by grant SNF 200021-129970.

Bernard Delley Paul Scherrer Institut, CMT, WHGA123, CH-5232, Villigen PSI

Date submitted: 18 Oct 2011

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