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A systematic and detailed investigation of radiative rates for forbidden transitions of astrophysical interest in doubly ionized iron peak elements

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Abstract. We carried out a systematic study of the electronic structure of doubly-ionized Fe-peak species, from Sc III to Ni III. The magnetic dipole (M1) and electric quadrupole (E2) transition probabilities were computed using the pseudo-relativistic Hartree-Fock (HFR) method and the central Thomas-Fermi-Dirac-Amaldi potential approximation implemented in the AUTOSTRUCTURE code. This multi-platform approach allowed for consistency checks and intercomparison and has proven very useful in many previous works for estimating the uncertainties affecting the radiative data.

Keywords. atomic data, atomic processes

Reliable atomic data for lowly-ionized Fe-peak species are of great importance for the analysis of the high resolution astrophysical spectra currently available. The third spectra of several iron group elements have been observed in different galactic sources like Herbig-Haro objects in the Orion Nebula and the Weigelt blob of Eta Carinae. However, forbidden transitions between low-lying metastable levels of these ions have been very little investigated so far and atomic data for such lines remain sparse or non existent.

The first theoretical approach used in this work is the pseudo-relativistic Hartree-Fock (HFR) method. Using the experimental energies compiled at NIST, the HFR method was combined with a least-squares optimization routine minimizing the differences between the experimental and calculated energy levels belonging to $3d^k$ and $3d^{k-1}4s$. The following configurations were explicitly included in the model : $3d^k + 3d^{k-1}4s + 3d^{k-1}5s + 3d^{k-1}4d + 3d^{k-2}4s^2 + 3d^{k-2}4p^2 + 3d^{k-2}4d^2 + 3d^{k-2}4s4d + 3d^{k-2}4s5s + 3s3p^63d^{k+1} + 3s3p^63d^k4s + 3s3p^63d^{k-1}4s^2$. We also used the multiconfiguration Breit-Pauli (MCBP) approach implemented in the AUTOSTRUCTURE code. Single electron orbitals were constructed by diagonalizing the Hamiltonian using a scaled statistical Thomas-Fermi-Amaldi model potential $V(\lambda_{nl})$. The λ_{nl} parameters were optimized by minimizing a weighted sum of the energies for the terms of the $3d^k$ and $3d^{k-1}4s$ configurations. Semi-empirical term energy corrections (TEC) were applied to those terms. The model adopted here was similar to the HFR one in which we added the $3d^{k-1}4p$ and $3d^{k-2}4s4p$ configurations in order to achieve a better representation of the 4p orbital.

We computed radiative data for transitions between all metastable levels belonging to the $3d^k$ and $3d^{k-1}4s$ configurations of 8 doubly-ionized iron-peak ions (Sc III, Ti III, V III, Cr III, Mn III, Fe III, Co III, Ni III). For most of the ions considered, the HFR and the AUTOSTRUCTURE results agree within 20% to 30%, which is the expected uncertainty for theoretical forbidden transitions. The complete set of data will be published in *Astronomy & Astrophysics*.