Isotope shift parameters in Al I for the $3p - 4s$ and $3p - 3d$ lines

L. Filippin[1], J. Ekman[2], S. Fritzsche[3], M. Godefroid[1], and P. Jönsson[2]

[1]*Chimie Quantique et Photophysique, Université Libre de Bruxelles, Brussels, Belgium*
[2]*Materials Science and Applied Mathematics, Malmö University, Malmö, Sweden*
[3]*Helmholtz-Institut Jena, and Theoretisch-Physikalisches Institut, Friedrich-Schiller-Universität Jena, Jena, Germany*

Presenting Author: Livio.Filippin@ulb.ac.be

When the effects of the finite mass and the spatial charge distribution of the nucleus are taken into account in a Hamiltonian describing an atomic system, the isotopes of an element have different electronic energy levels [1]. The isotope shift (IS), which consists of the field shift and the mass shift, plays a key role in extracting nuclear properties of an isotope such as its nuclear mean-square charge radius $\langle r^2 \rangle$ [2]. For a given atomic transition k with frequency ν_k, it is assumed that the *electronic response* of the atom to variations of the nuclear mass and charge distribution can be described by only two parameters : the mass-shift parameter M_k and the field-shift parameter F_k, respectively [2].

Five transitions are of interest for laser spectroscopy experiments of neutral aluminium (Al I) radioactive isotopes in order to determine their nuclear properties : $3s^2 3p\ ^2P^o_{3/2} \to 3s^2 4s\ ^2S_{1/2}$ (396.26 nm), $3s^2 3p\ ^2P^o_{1/2} \to 3s^2 4s\ ^2S_{1/2}$ (394.51 nm), $3s^2 3p\ ^2P^o_{1/2} \to 3s^2 3d\ ^2D_{3/2}$ (308.30 nm), $3s^2 3p\ ^2P^o_{3/2} \to 3s^2 3d\ ^2D_{3/2}$ (309.37 nm) and $3s^2 3p\ ^2P^o_{3/2} \to 3s^2 3d\ ^2D_{5/2}$ (309.36 nm).

We perform *ab initio* calculations of IS parameters using the multi-configuration Dirac-Hartree-Fock (MCDHF) method implemented in the Ris3/Grasp2K [1,3] and Ratip packages [4]. Two strategies are adopted. A first one consists in extracting the relevant parameters from the calculated line shifts for given triads of isotopes. A second one is based on the estimation of the expectation values of the one- and two-body recoil Hamiltonian for a given isotope, including the Shabaev relativistic corrections [5], combined with the calculation of the theoretical total electron densities at the origin. The results of the two approaches are compared. In both of them, different correlation models are explored in a systematic way to determine a reliable computational strategy and estimate theoretical error bars.

References

[1] C. Nazé *et al.*, Comput. Phys. Commun. **184**, 2187 (2013)
[2] B. Cheal, T. E. Cocolios and S. Fritzsche, Phys. Rev. A **86**, 042501 (2012)
[3] P. Jönsson *et al.*, Comput. Phys. Commun. **184**, 2197 (2013)
[4] S. Fritzsche, Comput. Phys. Commun. **183**, 1525 (2012)
[5] V. M. Shabaev, Theor. Math. Phys. **63**, 588 (1985); Sov. J. Nucl. Phys. **47**, 69 (1988)