Relativistic effects on hyperfine structures in light atoms and negative ions estimated from non-relativistic MCHF orbitals

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Relativistic effects in light atoms have been often neglected as they generally manifest on scales that are difficult to tackle in *ab initio* methods. However, today, correlation models have caught up with relativity so that most often, neglecting those corrections limits the accuracy of the calculations. Furthermore, relativistic effects can sometimes be unexpectedly large, leading to strong disagreement of non-relativistic approaches with experiment. In both cases, it is necessary to include relativistic effects in the model. Approaching these problems with fully relativistic methods, more computationally demanding, does not necessarily solve the problem.

Computing hyperfine structures is challenging as it is highly sensitive to configuration mixing which only weakly affect the energy. Furthermore, it is necessary to consider high order inner shells correlation effects to correctly describe the electronic wave function close to the nucleus. Finally, symmetry plays an important role in the calculation of hyperfine constants so that term mixing can have a drastic effect on the computed values. In order to better understand the physical effects that govern hyperfine structures in light atoms (e.g. orbital contraction, term mixing, interplay of correlation and relativistic effects), it is useful to compare methods which differ in well controlled ways.

Here, we summarise recently obtained theoretical results on hyperfine structures in ground and excited states of negative ions (C^-, Si^-, P^-, S^-, Cl^-) and neutral atoms (C, O, F, Si, P, S, Cl), with emphasis on relativistic corrections. They are obtained using the Multi-Configuration Hartree Fock approach as implemented in the ATSP2K package [1] combined with relativistic methods in which non-relativistic orbitals are used: either based on the Breit-Pauli approximation [2], or on Relativistic Configuration Interaction (RCI) calculations using the GRASP2K package [3] with orbitals converted to Dirac spinors in the Pauli approximation. When possible, these calculations are compared with experiment and fully relativistic results. In general, a satisfactory agreement is obtained.

References:

[1] C. Froese Fischer *et al., Comp. Phys. Comm.* **176**, 559 (2007).
[2] C. Froese Fischer *et al., Computational Atomic Structure: An MCHF Approach,* Taylor & Francis, 1997
[3] P. Jönsson *et al., Comp. Phys. Comm.* **177**, 597 (2007).