

Atomic properties of Li, Na, K, Rb, Ga, Cs, Tl, Fr, Mg⁺, Ca⁺, Sr⁺, Cd⁺, Ba⁺, Hg⁺, and Ra⁺

M.S. Safronova,¹ Dansha Jiang,¹ E. Iskrenova-Tchoukova,¹ Bindiya Arora,¹ U. I. Safronova,²
Charles W. Clark,³ W.R. Johnson⁴

¹ *University of Delaware, Newark, Delaware, USA*

² *University of Nevada, Reno, Nevada, USA*

³ *National Institute of Standards and Technology, Gaithersburg, Maryland, USA*

⁴ *University of Notre Dame, Notre Dame, Indiana, USA*

msafrono@udel.edu

Domain : Other

We conducted a systematic high-precision calculation of the atomic properties of systems with one valence electron above closed core using a relativistic all-order method. This method is a linearized coupled-cluster method, where single and double excitations of Dirac-Fock wave functions are included to all orders of perturbation theory. Partial triple excitations are also included in some of the calculations. The energy levels, fine-structure intervals, electric-dipole and electric-quadrupole matrix elements, lifetimes, hyperfine constants, static and dynamic polarizabilities, isotope shifts, as well as other properties are calculated for various systems. Systematic comparison with available experiment is carried out and excellent agreement is found in most cases. This work provides benchmark values for a large number of yet unmeasured properties.

As a result of these calculations, we have created an extensive theoretical database of more than 500 reduced electric-dipole matrix elements of the alkali-metal atoms and other systems with one valence electron above the closed core. The database includes all allowed electric-dipole transitions between four lowest ns states and four lowest $np_{1/2,3/2}$ states, four lowest $np_{1/2}$ states and three lowest $nd_{3/2}$ states, and four lowest $np_{1/2,3/2}$ states and three lowest $nd_{3/2,5/2}$ states for the alkali-metal atoms. A number of transitions for other systems are included as well. The database includes three values for each transition: lowest-order DHF values and two state-of-the-art calculations: all-order calculation with single and double excitations and all-order calculation with single, double, and partial triple excitations. Listing all three values in the database allows to evaluate the accuracy of the results as it allows to calculate the approximate relative size of the correlation correction and estimate the importance of certain classes of the higher-order terms.