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Atomic Data and Nuclear Data Tables

journal homepage: www.elsevier.com/locate/adndt

Transition rates and radiative lifetimes of Ca I

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ARTICLE INFO

Article history:
Received 9 February 2017
Received in revised form 20 February 2017
Accepted 28 March 2017
Available online xxxx

Keywords:
Atomic data
Transition probabilities
Lifetime

ABSTRACT

We tabulate spontaneous emission rates for all possible 811 electric-dipole-allowed transitions between the 75 lowest-energy states of Ca I. These involve the 4s*n*s (n = 4–8), 4s*n*p (n = 4–7), 4s*n*d (n = 3–6), 4s*n*f (n = 4–6), $3d^2$, $4p^2$, 3d4p, and 4s5g electronic configurations. We compile the transition rates by carrying out *ab initio* relativistic calculations using the combined method of configuration interaction and many-body perturbation theory. The results are compared to the available literature values. The tabulated rates can be useful in various applications, such as optimizing laser cooling in magneto-optical traps, estimating various systematic effects in optical clocks and evaluating static or dynamic polarizabilities and long-range atom–atom interaction coefficients and related atomic properties.

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http://dx.doi.org/10.1016/j.adt.2017.03.002
0092-640X/

Contents

1. Introduction

Alkaline-earth atoms and divalent-like atoms (such as Yb and Hg) became a subject of interest to the cold atom community in the past decade. These atoms possess two valence electrons outside a tightly bound core and in the LS coupling scheme, the atomic states can be classified by being either singlet or triplet states. The availability of relatively wide spin-allowed and narrow spin-forbidden electric-dipole (E1) transitions enables stacking laser cooling on both types of transitions, with the spin-allowed transitions used for the initial rapid cooling and spin-forbidden transitions—for reaching much lower Doppler-limit temperatures. Moreover, the narrow inter-combination transitions, such as the $4s^2\ ^1S_0 - 4s4p\ ^3P_1$ transition, can be used as an optical frequency Refs. [1,2]. The highly-forbidden $4s^2\ ^1S_0 - 4s4p\ ^3P_0$ transition can be potentially used for an optical lattice clock scheme [3]. However, due to peculiarities of its electronic structure, Ca, unlike other alkaline-earth atoms, has a relatively short lifetime in conventional magneto-optical traps (MOT). To improve the MOT efficiency, several re-pumping schemes were proposed and demonstrated [4]. That work required reliable electric-dipole transition data for many transitions between the 75 lowest energy states of neutral Ca. Here, we compile the results of our computational work that served as a basis of the MOT performance analysis [4]. We anticipate that the tabulated data will be useful in multiple other contexts, such as estimating various systematic effects in optical clocks and computing static or dynamic polarizabilities and long-range inter-atomic interaction coefficients.

There have been a number of atomic-structure calculations for neutral calcium. The earlier work includes multi-configuration Hartree–Fock (MCHF) calculation [5] and semi-empirical model-potential calculations [6–9]. These computations provide oscillator strengths for spin-allowed transitions for levels up to 4s10s, 4s9p and 4s6d. Most of them are non-relativistic with very limited numbers of low-lying levels treated with *ab initio* relativistic methods. In particular, Fisher and Tachiev [10] reported energies and E1 transition rates for levels below $3d4p\ ^1F_3$. Porsev et al. [11] and Savukov and Johnson [12] computed the $4s^2 - 4s4p$, $4s4p - 3d4s$, and $4s4p - 4s5s$ transition rates using a combination of configuration-interaction (CI) and many-body perturbation theory (MBPT) (referred to as the CI+MBPT method). The CI+MBPT method results were in excellent agreement with high-precision experimental values. This fact partially motivated our use of the relativistic CI+MBPT method for the present work.

2. Computational details

The CI+MBPT method employs a systematic formalism that combines advantages of both configuration interaction (CI) method and many-body perturbation theory (MBPT) [13]. This method has been used extensively for evaluation of atomic properties (see, e.g., review [14] for optical lattice clock applications and references therein). Relativistic effects are included exactly as the formalism starts from the Dirac equation and employs relativistic bi-spinor wave functions throughout the entire calculation. In our treatment, the CI model space is limited to excitations of the two valence electrons. Contributions involving virtual excitations of core orbitals are treated within the MBPT. In this approach, we first solve for the valence electron orbitals and energies in the field of core electrons. The one-electron effective potential includes both the frozen-cored Dirac–Hartree– Fock (DHF V^{N-2}) and self-energy (core-polarization) potentials. The self-energy correction is computed using second-order MBPT diagrams involving virtual core excitations. At the next step, the computed one-electron valence orbitals are used to diagonalize the atomic Hamiltonian in the model space of two valence electrons within the CI method. The CI model-space Hamiltonian includes the residual (beyond DHF) Coulomb interaction between the valence electrons and also their core-polarization-mediated interaction. The latter was computed in the second-order MBPT. This step yields two-electron wavefunctions and energies. Finally, with the obtained wave-functions we calculated the required electric-dipole matrix elements. In calculations of transition rates we used experimental energy intervals and the computed CI+MBPT matrix elements.

We used two independent CI+MBPT implementations: (i) by the Reno group (see the description of the earlier version in Ref. [15]) and (ii) the recently published package [16]. The practical goal of the calculations was not reaching the best possible accuracy, but rather the generation of massive amounts of reliable data for the transition array involving 75 lowest-energy levels. The Reno code was run on a large basis set but without including core-polarization-mediated interaction in the CI Hamiltonian due to considerable computational costs. The production runs with package [16] employed a smaller basis set (due to code limitations) but treated the correlation problem more fully.

While using the package [16] we employed the one-electron basis set that included the 1s−17s, 2p−17p, 3d−17d, 4f−17f, and 5g−17g orbitals, where the core and 4s, . . . , 6f orbitals are DHF ones, while the remaining orbitals were represented by a B-spline basis set. The Reno code used the dual-kinetic-balance basis set generated in the DHF V^{N-2} potential using spherical cavity of 75 Bohr radius [17]. The basis included orbitals with orbital angular momentum ℓ up to 6. The total number of positive-energy (in the Dirac sense) orbitals per partial wave was 40 with the 35 lowest-energy orbitals used in the calculations.

For most states, the values of transition rates obtained with package [16] were in close agreement with the NIST recommended

Please cite this article in press as: Y. Yu, A. Derevianko, Transition rates and radiative lifetimes of Ca I, Atomic Data and Nuclear Data Tables (2017), http://dx.doi.org/10.1016/j.adt.2017.03.002.