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Calculations for energies, transition rates, and lifetimes in Al-like Kr XXIV

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ABSTRACT

Using the second-order many-body perturbation theory (MBPT) method, a complete and accurate data set of excitation energies, lifetimes, wavelengths, and electric dipole (E1), magnetic dipole (M1), electric quadrupole (E2), and magnetic quadrupole (M2) line strengths, transition rates, and oscillator strengths for the lowest 880 levels arising from the $3l^3$ ($0 \le l \le 2$), $3l^2 4l'$ ($0 \le l \le 2$, $0 \le l' \le 3$), $3s^2 5l$ ($0 \le l \le 4$), $3p^2 5l$ ($0 \le l \le 1$), and $3s3p5l$ ($0 \le l \le 4$) configurations in Al-like Kr XXIV is provided. Comparisons are made with available experimental and theoretical results. Our calculated energies are expected to be accurate enough to facilitate identifications of observed lines involving the $n = 4, 5$ levels. The complete data set is also useful for modeling and diagnosing fusion plasma.

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Contents

1. Introduction

Accurate and complete atomic data have practical applications in astrophysics and fusion science [1,2]. As a rare gas, krypton is widely used as an injected impurity for diagnosing tokamak fusion plasma [3–7] and as a diagnostic element for the X-ray imaging spectrometer system of the ITER project [8,9]. High-precision atomic parameters including energies, transition rates, and lifetimes are required for analyzing observations of Kr ions with different ionization degrees. However, there has been a lack of atomic data. In view of this, we have recently provided complete and accurate excitation energies and transition parameters for Kr XXV [10], Kr XXVII [11], Kr XXIX [12], Kr XXX [13], and Kr XXXI [14]. This work represents our contribution for Al-like Kr XXIV.

Using experimental wavelengths from different sources [15,16], excitation energies of the lowest 12 levels for Kr XXIV have been compiled in the Atomic Spectra Database (ASD) of the National Institute of Standards and Technology (NIST) [17]. The experimental constraints provide limitations on Kr XXIV data sets. Therefore, the bulk of the data must be calculated. Using the multiconfigurational Dirac–Hartree–Fock (MCDHF) method, excitation energies, radiative transition parameters for the lowest 84 levels of Kr XXIV have been calculated by Wang et al. [18]. Using the second-order many-body perturbation theory (MBPT), energy levels and lifetimes for the lowest 40 levels have been provided by Safronova et al. [19,20]. Wang et al. calculated transition rates for electric-dipole (E1) and magnetic quadrupole (M2) transitions while Safronova et al. provided transition rates for E1 transitions alone, whereas the corresponding results for magnetic dipole (M1) and electric quadrupole (E2) transitions may also be required in plasma modeling. For example, the transition between the first excited state $3s^23p\ ^2P_{3/2}$ and the ground state $3s^23p\ ^2P_{1/2}$ is a mixed M1 and E2 transition. The lack of M1 and E2 radiative rates for this transition in plasma modeling can dramatically change the population of the first excited state, and lead to the wrong modeling conclusions. Moreover, energies and transition data from previous calculations are limited to the low-lying $n = 3$ levels. Atomic data involving the $n = 4, 5$ levels of Al-like ions are also important because of their wide applications in plasma modeling. For example, the recent studies [21,22] of Al-like Fe XIV show that the ratio of two lines, i.e., the $3s^25f_{7/2} \rightarrow 3s^24d_{5/2}$ and $3s^25f_{5/2} \rightarrow 3s^24d_{3/2}$ transitions, is sensitive to electron densities in the range of 10^9–10^{11} cm^{-3}, which provides a means for assessing the density of high temperature plasma. Consequently, it may also be required to provide extensive and accurate atomic data involving the $n = 4, 5$ levels of Kr XXIV for modeling and diagnosing fusion plasma of high temperature.

In the present work, energy levels, lifetimes, wavelengths, and E1, E2, M1, and M2 line strengths, transition rates, and oscillator strengths for the lowest 880 levels arising from the $3l^3$ ($0 \le l \le 2$), $3l^24l'$ ($0 \le l \le 2$, $0 \le l' \le 3$), $3s^25l$ ($0 \le l \le 4$), $3p^25l$ ($0 \le l \le 1$), and 3s3p5l ($0 \le l \le 4$) configurations of Kr XXIV are presented. Calculations are performed using the MBPT method implemented in the FAC package [23]. To assess the accuracy of the present results, comparisons are made with experiments and other theoretical calculations. The present excitation energies are in excellent agreement with the NIST compiled values for the $n = 3$ energy levels, i.e., the difference is within ± 250 cm^{-1} on average. The objective of this work is to report a highly accurate atomic data set involving high-lying levels for Al-like Kr. This is a continuation of our recent work for Al-like Zn [24] in which a large amount of atomic data involving the high-lying $n = 4, 5$ levels of Al-like Zn are calculated by employing both MCDHF and MBPT methods. The uncertainty of excitation energies and lifetimes provided in [24] is evaluated to be within 0.1% and 2% for most levels, respectively. Since using the same method, adequate configuration interaction effects are included in the present calculations, results for high-lying levels of Kr XXIV are also expected to be sufficiently accurate for identifications of fusion plasma, and could be of great help for modeling and diagnosing the high temperature plasma.

2. Calculations, results and evaluations

2.1. Calculations and results

In the MBPT method [25–27] implemented in the FAC code [23,28–30], the Hilbert space of the system is divided into two subspaces, including a model space M and an orthogonal space N. By the means of solving the eigenvalue problem of a non-Hermitian effective Hamiltonian in the space M, we can find the true eigenvalues of the Dirac–Coulomb–Breit Hamiltonian. The configuration interaction effects in the M space are exactly considered, and the interaction of the spaces M and N is accounted for with the many-body perturbation theory up to the second order. The $3l^3$, $3l^24l'$, $3s^25l$, $3p^25l$, and 3s3p5l configurations are contained in the model space M, and all possible configurations generated by single and double excitations of the M space are contained in the space N. The maximum principal quantum number n values are 125 and 65 for single and double excitations, respectively, while the maximum orbital quantum number l value is 20. Leading quantum electron dynamics effects (self-energy and vacuum polarization) are included in our calculations.

In relativistic calculations, wavefunctions for states are given as expansions over jj-coupling configuration state functions (CSFs). To give a good consistency with the labeling system used by experimentalists, wavefunctions are transformed from a jj-coupling CSF basis into a LSJ-coupling CSF basis using the method developed by Gaigalas et al. [31]. In Table 1, the computed excitation energies for the lowest 880 energy levels arising from the $3l^3$ ($0 \le l \le 2$), $3l^24l'$ ($0 \le l \le 2$, $0 \le l' \le 3$), $3s^25l$ ($0 \le l \le 4$), $3p^25l$ ($0 \le l \le 1$),

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