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Energy levels and strong electric dipole transitions in magnesium-like gold

Gülay Günday Konan, Leyla Özdemir*, Güldem Ürer

Department of Physics, Sakarya University, 54187 Sakarya, Turkey

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ABSTRACT

We have reported the energy levels and strong electric dipole transition parameters such as wavelengths, weighted oscillator strengths and transition rates (or probabilities) in magnesium-like gold (Au^{67+}, $Z=79$) using AUTOSTRUCTURE atomic code. Recently reported data for heavy Au ions and Au plasma diagnostics are important, in particular for modeling of M-shell spectra of Au ions. In calculations, we have considered the correlation, relativistic and quantum electrodynamics effects. The obtained results have been compared with those from other works. All lines obtained from electric dipole transitions have been also presented.

1. Introduction

Highly charged ions (HCIs) mainly exist in hot plasmas such as the solar corona and fusion plasmas [1]. Most of the universe consists of these ions. The scientific studies and applications of highly ionized ions have been limited because these ions are rare on Earth and the data obtained from observing cosmic sources by the relatively high X-ray absorption of Earth's atmosphere are not enough [2]. Therefore the theoretical works for HCIs have crucial importance. In addition, these ions are also interesting for fundamental atomic physics because electrons moving fast near a heavy nucleus provide a suitable system to test the fundamental atomic theory involving relativistic effects and quantum electrodynamics in a strong field [1].

In the spectra of highly charged ions, relativistic and quantum electrodynamics contributions in addition to correlation effects play an essential role [3,4]. An accurate atomic structure and spectral data of highly ionized gold (Au, $Z=79$) ions are needed, in particular, in plasma science, fusion reaction, biomedical applications, high-energy astrophysics and other scientific research fields [4]. Commonly, gold and its ions are used in fusion reactors as a work material and are of great importance for plasma diagnostics for analyzing the radiation emission profile of fusion plasma [5]. Especially, Au nanoparticles have received extensive attention in biomedical research, recently [6]. In addition, Auger electrons in gold ions have been important as a new method for cancer therapy [7,8].

Accurate atomic data for a large range of charge states of gold have been recently presented in the literature. Accurate calculations on some magnesium-like ions were carried out by Safronova et al. [9,10]. Yang et al. calculated the transition data from a Ni-like Au ion to an As-like Au ion using the GRASP code [11]. Mixing of dielectronic and multiply excited states in electron–ion recombination of Au^{24+} was studied by Gribakin et al. [12]. Vilkas et al. [3] made the relativistic multi-reference many-body perturbation theory calculations on Au^{64+}–Au^{69+}. Oscillator strengths, line strengths and radiative decay rates were presented for all 1s–2p transitions in gold ions by Nahar et al. [13]. Ballance et al. [14] demonstrated the first full intermediate-coupling level-resolved DR calculation for Au^{20+}. Hamasha and Alshaiub [4] presented theoretical data for the atomic structure and transition rates for gold

* Corresponding author.
E-mail address: lozdemir@sakarya.edu.tr (L. Özdemir).

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ions from Mg-like Au (Au^{67+}) through Cl-like Au (Au^{62+}) using the relativistic configuration interaction method (RCIM) in the flexible atomic code (FAC). In addition Hamasha [15] reported the multipole transitions (E1, E2, M1, M2). Also there are several works for Au spectra in the literature [16–25].

Relativistic and QED effects are strongly dependent on the nuclear charge Z, which makes highly charged heavy ions suitable for investigations of QED effects. Also, ions including only a few valence electrons outside the last closed shell are useful for testing QED calculations in multielectron systems. Mg-like ions, which have only two valence electrons, have a relatively simple atomic system to treat theoretically. The electronic configuration for Mg-like Au ion is $1s^22s^22p^63s^2$. In this work, we have calculated the excited energy levels in Au^{67+} using atomic structure code (AUTOSTRUCTURE) developed by Badnell [26]. Also we have reported wavelengths, transition probabilities (or rates) and weighted oscillator strengths for strong electric dipole transitions (E1) in Mg-like gold (Au^{67+}). We have here investigated QED (self-energy and vacuum polarization) and Breit interaction (magnetic interaction between the electrons and retardation effects of the electron–electron interaction) contributions. These contributions play an essential role in electronic structure and spectroscopic properties of many electron systems [4]. In addition, the electron correlation effects due to the Coulomb interaction between the electrons are also important, in particular, on fine structure and transitions. In this work, we considered two different configuration sets for calculations according to valence–valence correlation and core–valence correlation by the configuration interaction expansion. For valence–valence correlation, we have taken into account only the configurations including one electron excitation from valence to other high subshells: 3snl, 3pnl and 3dnl (n=3–7 and l=0–6). For core–valence correlation, we have also taken into account the configurations including one electron excitation from 2p subshell to other high subshells: $2p^63snl$ (n=3–6, l=0–4), $2p^63pnl$ (n=3–4, l=0–3), $2p^63p5s$, $2p^63dnl$ (n=3–4, l=0–3), $2p^53s^23p$, $2p^53s3p^2$, $2p^53p^3$, $2p^53s^23d$, $2p^53s^24s$, $2p^53s3p3d$, $2p^53p^23d$, $2p^53d^3$, $2p^53s3d^2$, $2p^53s3p4s$. The core of $1s^22s^22p^6$ is fixed in the valence–valence correlation calculations whereas $1s^22s^2$ is fixed in the core–valence correlation calculations.

2. Calculation method

AUTOSTRUCTURE code [26,27] is a general program for the calculation of atomic and ionic energy levels, radiative and autoionization rates and photoionization cross-sections using non-relativistic or semi-relativistic wavefunctions. It is based on SUPERSTRUCTURE [28]. In this code, the configuration set is chosen optionally and new configuration is added to improve accuracy (a configuration interaction expansion, CI expansion). The CI expansion is related to the choice of radial functions. Each (nl) radial function is calculated in Thomas-Fermi or Slater-Type-Orbital potential model. The Hamiltonian in any coupling model (LS, IC or ICR) is diagonalized to obtain eigenvalues and eigenvectors with which to construct the rates. This code uses non-relativistic or kappa-averaged relativistic wavefunctions and the full Breit interaction in the Pauli approximation. Detailed information on the method of this code can be found in [26,27,29]. We shall here provide information briefly.

For an ion with N electrons, a set of configurations

$$c = \prod_{nl}(nl)^{q_{nl}}, \quad \sum_i q_i = N \tag{1}$$

defines a trial solution $\Psi(\gamma)$ to a suitable Hamiltonian H in the multi-configurational sum form

$$\Psi(\gamma|\mathbf{x}_1,\ldots\mathbf{x}_N) = \sum_k a_k \Phi_k(c_k(\gamma)|\mathbf{x}_1,\ldots\mathbf{x}_N) \tag{2}$$

where γ denotes configuration and coupling scheme. In intermediate coupling (IC) wave functions can be written as

$$\Psi = \Psi(\Gamma SLJM_J|\mathbf{x}_1,\ldots\mathbf{x}_N) \tag{3}$$

which are eigenvectors to the Breit–Pauli matrix $\langle k|H_{BP}|k'\rangle$ with eigenvalues E_k.

Quantum electrodynamics (QED) contributions include vacuum polarization and self-energy contributions to level energies. The finite-nucleus effect is taken into account by assuming an extended Fermi distribution for the nucleus.

Both of Breit and QED contributions are treated as perturbation. Orbitals are fixed, but the mixing coefficients are calculated by diagonalizing the modified Hamiltonian. The correlation effects are taken into account using configuration interaction (CI) method. The correlation contribution should be separated for three parts: correlation of core electrons, correlation between core and valence electrons, and correlation of two valence electrons [10].

For transitions from (2) code computes Einstein coefficients and associated quantities for multipole transitions of low multipolarity (for electric dipole, E1, radiation). Generally, electric multipole transitions exist in both LS coupling and intermediate coupling (or jj-coupling). Electric quadrupole (E2) and magnetic dipole (M1) transitions come into their own only in intermediate coupling. As intermediate coupling wave functions contain admixtures of order α^2, radiative operators must also be expanded up to the Breit contributions order.

In the long wavelength low intensity approximation the probability for spontaneous emission by E1 radiation is as follows:

$$A_{i'\to i} = 2.6774\times 10^9 \frac{(E_i - E_{i'})^3}{g_i} S(i,i') \tag{4}$$

where g_i is statistical weighted of level, E_i and $E_{i'}$ are energies of levels and $S(i,i')$ is line strengths in form

$$S(i,i') = |<i'||R^{[k]}||i>|^2 \tag{5}$$

where $R^{[k]}$ is a transition operator and describes each multipole and k is 1 for electric dipole radiation.

In addition, weighted absorption or emission oscillator strength (gf) value can be written in terms of line strengths as follows:

$$(gf)_{i,i'} = (gf)_{i',i} = \frac{|E_i - E_{i'}|}{3} S(i,i') \tag{6}$$