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Prominent soft x-ray lines of Sr-like Au$^{41+}$ in low-energy EBIT spectrum

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Abstract. Relativistic multireference Møller-Plesset perturbation theory has been employed to calculate with high accuracy the energy levels and transition probabilities of Cu- to Sr-like gold ions. The many-body calculations were carried out to identify the unassigned blended lines in the 35–40 Å region of the low-energy EBIT spectrum of the gold ions [Träbert et al 2001 Can. J. Phys. 79 153]. Most of the prominent lines in the 35–40 Å region were identified as the emission lines in Sr-like gold.

1. Introduction

In the last two decades, the electron-beam ion trap (EBIT) [1] has been successfully employed to produce well-resolved spectra of highly-ionized atomic ions. Using the Livermore EBIT-2, Träbert et al [2] obtained soft-x-ray spectra of Au with well-defined maximum charge states ranging from Br- to Co-like ions. The prominent lines in the spectra of Cu-, Zn-, Ga-, and Ge-like Au ions are well separated and they have been measured to very high accuracy – typically 0.01–0.005 Å. The line classifications for the strongest transitions in Cu-like to Rb-like Au were guided by theoretical calculations with the fully relativistic parametric potential code RELAC [3]. Typically the accuracy achievable with the large-scale RELAC calculations is of the order of 0.5–1.0 Å. Such an accuracy suffices to identify well-separated prominent lines. However, the complex EBIT spectra of Au ions produced at lower-energy electron beam contain numerous lines, many of which are blended. The uncertainties ($\approx 0.5–1.0$ Å) in the extant theoretical predictions are too large to make unique line identifications of the line-rich spectra.

We have recently developed and implemented a relativistic multireference Møller-Plesset (MR-MP) perturbation theory for high-accuracy calculations of spectroscopic quality for the term energies and decay probabilities of multi-valence-electron ions. The method was successfully applied to calculate with high accuracy the spectra of Mg-, Al-, Si-, P-, Zn-, and Ga-like highly-ionized ions [4, 5, 6]. The theoretical predictions were within experimental uncertainties where available, with the estimated theoretical uncertainty of the order of 0.01 Å for the soft-x-ray lines.

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In the present study, our relativistic MR-MP perturbation theory calculations are employed to calculate with high wavelength accuracy the soft-x-ray spectra of Cu-like to Sr-like Au ions. The highly accurate theoretical predictions allow us to make immediate identifications of the individual lines in the line-rich EBIT spectra produced with a lower-energy electron beam.

2. Computational details

The state-averaged matrix multiconfiguration Dirac-Fock-Breit (MCDFB) self-consistent-field (SCF) calculations [7] were performed including 25 relativistic configuration state functions (CSFs) arising from the configurations, \(4s^24p^64d^2\) and \(4s^24p^54d4f\). The state-averaged MCDFB SCF yield a single set of spinors for the ground and excited levels. Subsequently, each of the ground and excited states was subjected to state-specific second-order MR-MP refinement to account for the residual dynamic correlation. The reference space in the MR-MP refinement includes all the CSFs arising from the configurations \(4s^{n1}4p^{n2}4d^{n3}4f^{n4}\) with \(n3 + n4 \leq 3\) and \(n4 \leq 1\). Frequency-independent Breit correction corrections were included in the second-order MR-MP. Frequency-dependent Breit correction, normal and specific mass shifts were evaluated at the first-order of perturbation theory. Lamb shift was estimated using the procedure proposed by Y.-K. Kim [8]. The even-tempered basis set of 26s24p22d20f18g18h Gaussian spinors for up to angular momentum \(L = 5\) and 15 Gaussian spinors for \(L = 6–11\) were employed.
Table 1. Energy levels (cm\(^{-1}\)) in strontiumlike Au\(^{41+}\). In each level the occupation number of the seven relativistic shells \(4s^{2}4p^{6}3\) \(4p^{6}3\) \(4d^{9}4f^{8}\) \(5d^{5}4f^{7}\), of the dominant CSF is given in the columns denoted “Conf”. The “Key” columns contain the \(J\)-value of the level and level number in parentheses. The odd-parity states are labeled by a star.

| Conf  | Key  | E   | Conf  | Key  | E   | Conf  | Key  | E   |
|-------|------|-----|-------|------|-----|-------|------|-----|
| 224200 | 2(1) | 0   | 2231200 | 1(6)* | 1861503 | 2230300 | 3(17)* | 2218387 |
| 224200 | 0(1) | 79342 | 2231200 | 3(8)* | 1870500 | 2230300 | 1(12)* | 2257805 |
| 2241100 | 3(1) | 204681 | 2231200 | 4(6)* | 1871604 | 2240110 | 3(18)* | 2264618 |
| 2241100 | 4(1) | 253344 | 2231200 | 4(7)* | 1881427 | 2240110 | 4(15)* | 2268037 |
| 2241100 | 2(2) | 254103 | 2241010 | 4(8)* | 1896611 | 2240110 | 2(18)* | 2275361 |
| 2241100 | 1(1) | 256919 | 2231200 | 3(9)* | 1899714 | 2240110 | 1(13)* | 2282086 |
| 2240200 | 4(2) | 455122 | 2231200 | 1(7)* | 1914565 | 2240110 | 0(6)* | 2293318 |
| 2240200 | 2(3) | 479178 | 2231200 | 4(10)* | 1915625 | 2230300 | 3(19)* | 2297888 |
| 2240200 | 0(2) | 547523 | 2231200 | 0(3)* | 1918328 | 2230300 | 4(16)* | 2307717 |
| 2233000 | 2(1)* | 1415793 | 2231200 | 2(9)* | 1931078 | 2230300 | 1(14)* | 2334544 |
| 2233000 | 1(1)* | 1432570 | 2231200 | 3(10)* | 1950097 | 2240110 | 2(19)* | 2337105 |
| 2233000 | 0(1)* | 1449330 | 2231200 | 2(10)* | 1969579 | 2240110 | 3(20)* | 2341707 |
| 2232100 | 3(2)* | 1586356 | 2241010 | 2(11)* | 1976524 | 2143000 | 2(20)* | 2571374 |
| 2232100 | 2(2)* | 1603692 | 2231200 | 1(8)* | 1993166 | 2143000 | 3(21)* | 2697281 |
| 2232100 | 4(1)* | 1612828 | 2231200 | 3(11)* | 1996206 | 2143000 | 2(21)* | 2698800 |
| 2232100 | 2(3)* | 1625232 | 2231200 | 1(9)* | 2020271 | 2143000 | 4(17)* | 2816594 |
| 2232100 | 1(2)* | 1632158 | 2231200 | 3(12)* | 2080723 | 2143000 | 0(7)* | 2817699 |
| 2232100 | 3(3)* | 1643699 | 2231200 | 2(13)* | 2092786 | 2143000 | 3(22)* | 2859019 |
| 2232100 | 0(2)* | 1644150 | 2231200 | 2(14)* | 2109897 | 2143000 | 4(18)* | 2871057 |
| 2232100 | 4(2)* | 1733525 | 2241010 | 2(15)* | 2135655 | 2143000 | 3(23)* | 2885081 |
| 2232100 | 3(5)* | 1735325 | 2241010 | 4(16)* | 2138085 | 2143000 | 1(18)* | 2897648 |
| 2232100 | 4(4)* | 1739135 | 2230300 | 3(17)* | 2158623 | 2143000 | 0(8)* | 2897794 |
| 2232100 | 2(5)* | 1745994 | 2230300 | 0(9)* | 2160829 | 2143000 | 2(22)* | 2906149 |
| 2232100 | 2(6)* | 1771320 | 2231200 | 3(15)* | 2199997 | 2142100 | 4(20)* | 2907421 |
| 2232100 | 3(6)* | 1785742 | 2231200 | 4(10)* | 2190987 | 2142100 | 4(20)* | 2907421 |
| 2232100 | 1(3)* | 1805112 | 2241010 | 3(16)* | 2196300 | 2142100 | 3(24)* | 2921575 |
| 2232100 | 3(4)* | 1831439 | 2241010 | 4(13)* | 2138085 | 2142100 | 4(19)* | 2940950 |
| 2231200 | 3(7)* | 1854547 | 2230300 | 2(17)* | 2166047 | 2142100 | 2(26)* | 3008219 |
| 2231200 | 2(8)* | 1855055 | 2230300 | 4(14)* | 2174699 | 2140300 | 4(21)* | 3065255 |

3. Results and discussions
In Figure 1 the EBIT spectra of Au ions are compared with the simulated theoretical spectra of Sr-like Au ion. The synthetic spectra were produced by convoluting with gaussian function the line intensities proportional to “branched” transition probabilities, assuming a uniform level population. At the electron beam energies of 2300 eV there are two wavelength regions containing numerous lines within a 4–5 Å range. The first of these, in 37–40 Å region, was characterized in previous study [2] as containing multiple lines of Br-like Au. Our calculations predicted not a single Br-like gold line in that region, ruling out the possibility that those blends are lines of the Br-like ions. However, theoretical spectra in Figure 1 indicate that there are multiple lines of Sr-like gold blended in the 37–39 Å region (this region is shown separately in Figure 1). The many lines in the second wavelength region 45–48 Å are mostly unidentified. Relativistic MR-MP
Table 2. Identified lines in strontium-like Au\(^{41+}\). The occupation of the seven relativistic shells\(4s^{1}4p_{1/2}^{1}4p_{3/2}^{1}4d_{5/2}^{1}4d_{3/2}^{1}4f_{5/2}^{1}4f_{7/2}^{1}\) in the dominant CSF of the upper and lower states is given in the columns denoted “Conf”. The “Key” columns contain the J-value of the level and level number in parentheses. The odd-parity states are labeled by a star.

| \(\lambda_{\text{expt}}\) | \(\lambda_{\text{theor}}\) | Upper | Lower | \(A\) |
|---|---|---|---|---|
| \(\text{A}\) | \(\text{A}\) | Conf | Key | A | Conf | Key | s\(^{-1}\) |
| 37.42 | 37.443 | 2141200 | 1(18)* | 2241100 | 2(2) | 1.46(+12) |
| 37.75 | 37.702 | 2141200 | 1(21)* | 2240200 | 2(3) | 5.32(+11) |
| 38.00 | 37.939 | 2142100 | 3(23)* | 2241100 | 3(1) | 1.21(+12) |
| 37.910 | 2141200 | 1(22)* | 2240200 | 0(2) | 2.60(+12) |
| 37.915 | 2143000 | 1(17)* | 2242000 | 0(1) | 1.61(+12) |
| 38.009 | 2142100 | 3(23)* | 2241100 | 2(2) | 6.13(+11) |
| 38.26 | 38.210 | 2141200 | 2(27)* | 2240200 | 2(3) | 2.47(+12) |
| 38.35 | 38.396 | 2141200 | 1(20)* | 2241100 | 2(2) | 3.10(+12) |
| 38.60 | 38.552 | 2142100 | 2(22)* | 2241100 | 2(2) | 1.08(+12) |
| 38.699 | 2141200 | 1(21)* | 2240200 | 0(2) | 5.91(+11) |
| 47.27 | 47.251 | 2241010 | 1(11)* | 2242000 | 2(1) | 2.00(+12) |
| 48.64 | 48.760 | 2141200 | 1(21)* | 2240200 | 0(1) | 1.61(+12) |

Calculations were performed to examine if the Sr-like gold ion has any strong radiative emission in that region. The synthetic spectrum has just two prominent lines of Sr-like gold at 47.251 Å and 48.760 Å. The remaining lines instead relate to other charge states such as Y-like Au ions. In the ions of partially occupied \(4d\) shell, numerous low-lying excited states have term energies nearly degenerate with the ground state. The branching of the decays of the higher-lying excited states to the ground state and to the low-lying excited levels produce multiple prominent lines in the same wavelength region. Table 1 lists term energies of the lowest 48 levels. It is clear that decays of the same upper state to the ground state and lowest five even-parity states produce E1 lines in the same wavelength region and highly accurate theoretical predictions must be brought to bear (accurate to 0.05 Å) to identify the lines in such a line-rich spectrum. Table 2 displays the Sr-like gold lines identified by the present theoretical work.

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