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M. J. Wilkas, Y. Ishikawa, E. Träbert

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Prominent soft x-ray lines of Sr-like Au⁴¹⁺ in low-energy EBIT spectrum

Marius Jonas Vilkas¹ and Yasuyuki Ishikawa

Department of Chemistry, University of Puerto Rico, P.O. Box 23346 San Juan, Puerto Rico 00931-3346 USA

Elmar Träbert

Experimentalphysik III, Ruhr-Universität Bochum, D-44780 Bochum, Germany,
and High Temperature and Astrophysics Division, LLNL, P.O. Box 808, Livermore, CA 94550, U.S.A.

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 (≈ 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.

¹ To whom correspondence should be addressed (marius@hpcf.upr.edu)

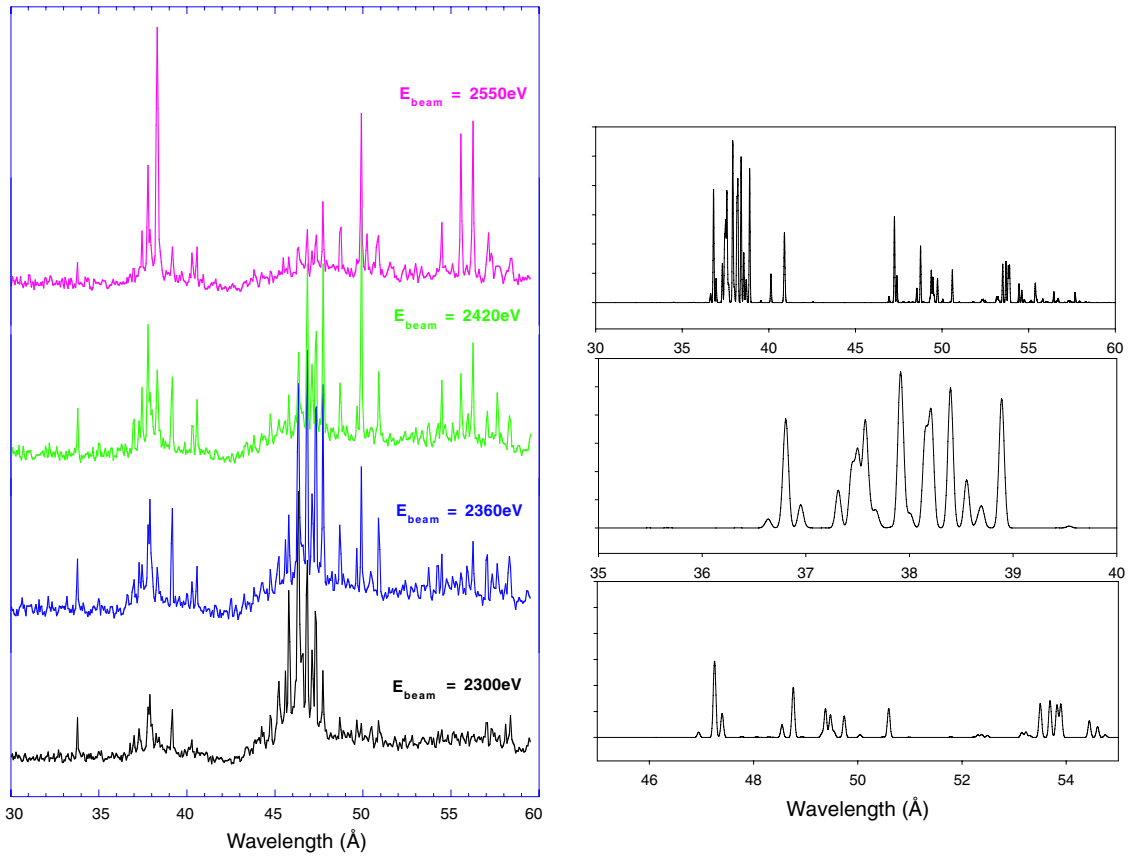


Figure 1. EBIT (left panel) and synthetic theoretical spectra (right panel) of gold ions in the wavelength range 30 to 60 Å. The two lower synthetic spectra are expanded sections of the upper one.

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 correlation 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 $4s^{n_1}4p_{1/2}^{n_2}4p_{3/2}^{n_3}4d_{3/2}^{n_4}4d_{5/2}^{n_5}4f_{5/2}^{n_6}4f_{7/2}^{n_7}$ 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
2242000	2(1)	0	2231200	1(6)*	1861503	2230300	3(17)*	2218387
2242000	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(9)*	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	2240101	2(19)*	2337105
2233000	0(1)*	1449330	2231200	2(10)*	1969579	2240101	3(20)*	2341707
2233000	3(1)*	1461887	2231200	4(10)*	1973026	2240101	1(15)*	2416594
2232100	3(2)*	1586356	2241010	2(11)*	1976524	2143000	2(20)*	2571374
2232100	2(2)*	1603692	2231200	1(8)*	1993166	2142100	3(21)*	2697281
2232100	4(1)*	1612828	2240110	3(11)*	1996206	2142100	2(21)*	2698800
2232100	2(3)*	1625232	2240110	2(12)*	1998282	2142100	1(16)*	2702968
2232100	1(2)*	1632158	2241001	4(11)*	2012670	2142100	0(7)*	2715509
2232100	3(3)*	1643699	2240110	1(9)*	2020271	2143000	1(17)*	2716789
2232100	0(2)*	1644150	2231200	3(12)*	2020621	2142100	4(17)*	2721642
2232100	4(2)*	1645218	2231200	2(13)*	2030829	2142100	2(22)*	2840495
2232100	4(3)*	1676686	2231200	0(4)*	2031184	2141200	3(22)*	2859169
2232100	2(4)*	1681235	2231200	2(14)*	2041432	2141200	4(18)*	2871057
2232100	1(3)*	1681833	2231200	1(10)*	2059988	2141200	2(23)*	2875402
2232100	3(4)*	1684730	2241001	4(12)*	2067437	2142100	3(23)*	2885081
2241010	3(5)*	1733525	2241001	3(13)*	2067441	2141200	1(18)*	2897648
2232100	4(4)*	1734945	2230300	3(14)*	2080723	2141200	0(8)*	2897794
2232100	2(5)*	1745994	2230300	0(5)*	2082786	2141200	2(24)*	2906140
2232100	2(6)*	1771320	2231200	3(15)*	2109897	2142100	4(20)*	2907321
2232100	3(6)*	1785742	2230300	2(15)*	2116220	2142100	1(19)*	2915616
2232100	1(4)*	1805112	2241010	3(16)*	2116380	2141200	3(24)*	2921575
2231200	4(5)*	1812558	2241010	1(11)*	2130188	2142100	2(25)*	2923354
2231200	2(7)*	1817031	2241001	2(16)*	2135655	2142100	3(25)*	2933943
2232100	1(5)*	1831439	2240101	4(13)*	2138085	2141200	4(19)*	2940595
2231200	3(7)*	1854547	2230300	2(17)*	2166047	2141200	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 Au⁴¹⁺. The occupation of the seven relativistic shells $4s^{n_1}4p_{1/2}^{n_2}4p_{3/2}^{n_3}4d_{3/2}^{n_4}4d_{5/2}^{n_5}4f_{5/2}^{n_6}4f_{7/2}^{n_7}$ 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.

λ_{expt} Å	λ_{theor} Å	Upper		Lower		A
		Conf	Key	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)*	224200	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)*	2242000	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 0.05Å) 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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