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Accurate transition and hyperfine data in Ag I from the multiconfiguration Dirac–Hartree–Fock and relativistic coupled-cluster methods

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ABSTRACT

Context. Silver is a key tracer of the weak r-process in late-type stars. However, when the assumption of local thermodynamic equilibrium is relaxed, accurate abundance determinations become even more sensitive to complete sets of reliable transition data.
Aims. The aim of this work is to provide accurate and extensive results of excitation energies, radiative transitions, and hyperfine data for Ag I.
Methods. The multiconfiguration Dirac–Hartree–Fock (MCDHF) and relativistic coupled-cluster (RCC) methods were used in the present work. The quantitative and qualitative evaluation approach was applied to the MCDHF transition rates to estimate uncertainties using the terminology of the National Institute of Science and Technology Atomic Spectroscopic Database (NIST ASD).
Results. Excitation energies, transition data, and hyperfine structure constants were calculated for 18 states up to $4d^{10}8s$. Fifty-seven electric dipole (E1) transition rates and weighted oscillator strengths were computed, and their uncertainties were estimated to belong to the following NIST ASD classes: four in AA , 12 in A+, five in A, 13 in B+, six in B, and four in C+ with AA ≤ 1%, A+ ≤ 2%, A ≤ 3%, B+ ≤ 7%, B ≤ 10%, C+ ≤ 18%. The remaining transitions, mainly weak transitions involving the $4d^9 5s^2$ states, were estimated to be in the E class >50%. The computed lifetimes from both the MCDHF and RCC methods are in good mutual agreement and mostly fall within the error bars of available experimental values from laser-induced fluorescence measurements. The $4d^9 5s^2\ ^2D_{5/2}$ metastable state, important for establishing the ionization balance, decay through an E2 transition to the ground state. The calculated lifetime is 163 ms. The computed hyperfine interaction constants from the MCDHF and RCC methods are in good agreement and compare well with the scattered experimental constants.

Key words. atomic data – atomic processes – nuclear reactions, nucleosynthesis, abundances

1. Introduction

The origins of elements heavier than iron ($Z = 26$) – specifically, the relative yields from different astrophysical sites of the rapid neutron capture process (r-process) – remain an open question (e.g., Cowan et al. 2021). There is evidence for several different patterns of r-process yields, including a weak r-process that may produce elements up to the second r-process peak ($N = 82$; e.g., Arcones & Thielemann 2023; Thielemann 2023). In this context, silver ($Z = 47$) is of great interest: it is predicted to form mostly from the r-process (e.g., Prantzos et al. 2020), and its lines can be detected in stellar spectra. Consequently, silver abundances in late-type stars are key diagnostics for understanding the weak r-process (e.g., Hansen et al. 2012; Wu et al. 2015; Huang et al. 2025).

However, the accuracy of stellar abundance determinations is closely coupled to the input atomic data (e.g., Mashonkina 2009; Sonnen & Aufdenberg 2025). The transition rate or oscillator strength has a one-to-one relationship with the abundance inferred from a given spectral line, and hyperfine splitting may also significantly impact analyses based on saturated lines (e.g., Thorsbro et al. 2018). Furthermore, when the assumption of local thermodynamic equilibrium (LTE) is relaxed, radiative transition data are required not only for the diagnostic lines used in abundance determinations, but also for all lines that couple levels in the model atom. This is because radiative rates enter the coupled statistical-equilibrium equations for all levels and can therefore affect inferred abundances indirectly through their influence on non-LTE level populations. Therefore, a comprehensive and accurate set of transition rates is essential for non-LTE diagnostics (e.g., Lind & Amarsi 2024).

In the case of silver (e.g., Hansen 2023), abundances are usually inferred from the Ag I 328 nm and 338 nm resonance lines ($5s^2S_{1/2} \rightarrow 5p^2P^o_{3/2,1/2}$). Although the NIST database transition rates (Kramida et al. 2024), given with 10% accuracy, and measured hyperfine structure data (Hansen et al. 2012) for these two lines are well constrained, a detailed 3D radiation-hydrodynamics analysis of the solar spectrum (Grevesse et al. 2015) suggests that these lines are prone to large non-LTE effects – at least in the Sun (Asplund et al. 2021) – and thus may be indirectly affected by the full set of transition data. To test this and ultimately derive accurate silver abundances in late-type stars, a model atom for Ag I is under construction (Caliskan et al., in prep.), which in turn requires a reliable and as complete as possible set of transition data for Ag I.

Being a nominal one-electron system, Ag I has been extensively studied with respect to its hyperfine structures, transition rates, and lifetimes using a variety of experimental and

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theoretical methods. The lifetimes of the first two excited states, $5p_{1/2,3/2}$, were measured with high precision by Carlsson et al. (1990) using a picosecond delayed-coincidence technique. The reported uncertainties are as low as 0.5%, making these lifetimes among the most accurately known in atomic physics and highly valuable for benchmarking purposes; see also Carlsson (1989) for an in-depth discussion about the error sources. Hyperfine interaction constants were also determined through quantum beat spectroscopy. Lifetimes of states in the s and d sequences up to $10s_{1/2}$ and $9d_{3/2}$ were measured using laser-induced fluorescence (LIF) combined with two-step excitations (Jiang et al. 1990). These results showed good agreement with multiconfiguration Hartree–Fock (MCHF) calculations based on a model potential, as reported in the same study. Similarly, the lifetimes of the $6p_{1/2,3/2}$ and $7p_{1/2,3/2}$ states were measured using LIF techniques (Bengtsson et al. 1990, 1991), and these studies also provide hyperfine interaction constants. The hyperfine interaction constant of the $4d^9 5s^2\ ^2D_{5/2}$ state was measured with exceptional accuracy by Blachman et al. (1966) using the atomic-beam magnetic-resonance method.

Numerous theoretical studies are reflected in the NIST database (Kramida et al. 2024). Here, we highlight those most relevant to our work. The pseudo-relativistic Hartree–Fock (HFR) method was employed by Nasr et al. (2023) to compute atomic structures and radiative parameters for highly excited states in the s, p, d, and f sequences, including configurations with holes in the $4d$-subshell. The weakest-bound electron potential model (WBEPM) was used by Zheng et al. (2000) to study transition probabilities, while Civiš et al. (2010) applied the Fues model potential to calculate transition dipole matrix elements. The latter work is particularly comprehensive, providing extensive tables comparing oscillator strengths from both experimental and theoretical sources. Third-order relativistic many-body theory was utilized by Safronova et al. (2003) to compute excitation energies and lifetimes of the lowest states with s, p, d, f, and g symmetries. More recently, Chaudhuri & Chattopadhyay (2022) applied the Fock-space multi-reference coupled cluster (FSMRCC) theory to determine excitation energies, hyperfine constants, and transition parameters for the $5s_{1/2}$ and $5p_{1/2,3/2}$ states. Additionally, hyperfine constants for these states were calculated using the multiconfiguration Dirac–Hartree–Fock (MCDHF) method by Song et al. (2007).

In this work, we employ the advanced FSMRCC theory together with the combined multiconfiguration Dirac–Hartree–Fock and relativistic configuration interaction (MCDHF/RCI) methods to compute excitation energies, hyperfine interaction constants, transition data, and lifetimes for the even $5s_{1/2}$, $6s_{1/2}$, $7s_{1/2}$, $8s_{1/2}$, $5d_{3/2,5/2}$, $6d_{3/2,5/2}$, $4d^9 5s^2\ ^2D_{3/2,5/2}$ states and the odd $5p_{1/2,3/2}$, $6p_{1/2,3/2}$, $7p_{1/2,3/2}$, $4f_{5/2,7/2}$ states in Ag I.

2. Theory and procedure

Detailed descriptions of the MCDHF/RCI methods can be found in Grant (2006); Jönsson et al. (2023) and in the recent comparative study by Sahoo et al. (2025) who use the FSMRCC method. Thus, only the computational procedures are outlined here. The FSMRCC method employed here is similar to that applied by Chaudhuri & Chattopadhyay (2022); however, it incorporates triple excitations and Breit interactions in the calculations.

2.1. MCDHF and RCI

All MCDHF and RCI calculations in this work were performed using the GRASPG package (Si et al. 2025), an extension of GRASP (Froese Fischer et al. 2019) based on configuration state function generators (CSFGs), which enables significantly faster computations with reduced resource requirements (Li et al. 2023b). An initial MCDHF calculation was carried out for states belonging to the reference configurations $4d^{10}\{5s, 6s, 7s, 8s, 5p, 6p, 7p, 5d, 6d, 4f\}$ with additional states from $4d^{10}\{9s, 10s, 8p, 9p, 7d\}$ to introduce spatially extended orbitals into the basis. This is essential for achieving agreement between transition parameters in the length and velocity gauges and reducing uncertainties (Rhodin et al. 2017; Papoulia et al. 2019). Subsequent MCDHF calculations used configuration state function (CSF) expansions generated by allowing single and double (SD) excitations to progressively larger orbital sets from subshells of reference configurations down to $4s^2 4p^6 4d^{10}$, with at most one excitation from this layer. The closed core $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10}$ remained inactive. Following the terminology of Froese Fischer et al. (2019), these calculations account for radial and core-valence (CV) correlation. Orbital sets were increased layer by layer as summarized in Table 1. Finally, RCI calculations were performed using the same CSF expansions, but including Breit and quantum electrodynamic (QED) effects.

Table 1. Layers of correlation orbitals, in nonrelativistic notation, used in the MCDHF/RCI calculations.

Layers	Orbitals
Layer 1	$\{10s\ 9p\ \ 7d\ \ 5f\ \ 5g\}$
Layer 2	$\{11s\ 10p\ \ 8d\ \ 6f\ \ 6g\}$
Layer 3	$\{12s\ 11p\ \ 9d\ \ 7f\ \ 7g\}$
Layer 4	$\{13s\ 12p\ \ 10d\ \ 8f\ \ 8g\}$
Layer 5	$\{14s\ 13p\ \ 11d\ \ 9f\ \ 9g\}$
Layer 6	$\{15s\ 14p\ \ 12d\ \ 10f\ \ 10g\}$

2.2. FSMRCC

Computational details of our FSMRCC method are discussed in a series of previous studies (Sahoo et al. 2004; Dixit et al. 2007; Nandy & Sahoo 2014). We considered Gaussian type orbitals (GTOs) to construct single particle orbitals using the Dirac–Hartree–Fock (DHF) method (Chaudhuri et al. 1999). We generated orbitals up to i-symmetry considering 40 GTOs for each angular momentum symmetry. The Breit interaction terms were included self-consistently in the DHF and FSMRCC methods. Convergence of the results was verified by first considering single and double excitations in the calculations, and then by including triple excitations in the FSMRCC method (Sahoo et al. 2021; Sahoo & Ohayon 2021). In the estimations of the magnetic dipole structure constants ($A_{\rm hfs}$), we also considered corrections due to the Bohr-Weisskopf (BW) effect. The detailed procedure for estimating the BW effect is discussed in Sahoo et al. (2021) and Sahoo (2025). Results obtained with single and double approximation in the FSMRCC method are given under the RCCSD method, while those including the single, double, and triple approximation in the FSMRCC method are listed under the RCCSDT method.

3. Results and discussion

3.1. Excitation energies

The excitation energies from the MCDHF/RCI calculations are presented in Table 2 as functions of the increasing layers of

Table 2. Calculated excitation energies (in cm^{-1}) at different layers using the MCDHF/RCI method compared with experimental values from the NIST ASD database (Kramida et al. 2024).

State	Layer 1	Layer 2	Layer 3	Layer 4	Layer 5	Layer 6	FT	Experiment
$4d^{10}5s\ ^2S_{1/2}$					0	0		0
$4d^{10}5p\ ^2P_{1/2}$	29 666.09	30 354.06	30 471.03	30 566.38	30 582.32	30 603.42	30 603.42	29 552.057
$4d^{10}5p\ ^2P_{3/2}$	30 566.34	31 311.67	31 443.87	31 544.60	31 563.46	31 584.35	31 584.35	30 472.665
$4d^{9}5s^2\ ^2D_{5/2}$	37 669.11	38 789.07	39 066.71	39 222.35	39 260.77	39 305.78	31 323.21	30 242.298
$4d^{9}5s^2\ ^2D_{3/2}$	42 425.88	43 546.51	43 822.39	43 978.36	44 016.75	44 061.73	35 874.87	34 714.226
$4d^{10}6s\ ^2S_{1/2}$	42 626.16	43 743.93	43 959.01	44 094.63	44 105.87	44 127.67	44 127.67	42 556.147
$4d^{10}6p\ ^2P_{1/2}$	48 319.60	49 518.92	49 757.99	49 909.21	49 941.78	49 969.91	49 969.91	48 297.406
$4d^{10}6p\ ^2P_{3/2}$	48 519.77	49 726.64	49 969.27	50 121.69	50 153.99	50 182.13	50 182.13	48 500.810
$4d^{10}5d\ ^2D_{3/2}$	48 769.42	49 978.98	50 236.71	50 400.94	50 425.84	50 453.33	50 453.33	48 743.969
$4d^{10}5d\ ^2D_{5/2}$	48 800.14	49 997.10	50 253.26	50 417.21	50 442.01	50 471.14	50 471.14	48 764.219
$4d^{10}7s\ ^2S_{1/2}$	55 498.52	56 793.66	53 384.75	53 548.46	53 580.45	53 604.78	53 604.78	51 886.965
$4d^{10}7p\ ^2P_{1/2}$	54 025.44	55 316.33	55 582.43	55 740.77	55 773.98	55 802.99	55 802.99	54 041.037
$4d^{10}7p\ ^2P_{3/2}$	54 104.65	55 397.83	55 665.92	55 825.00	55 856.35	55 885.40	55 885.40	54 121.108
$4d^{10}6d\ ^2D_{3/2}$	54 163.05	55 455.75	55 734.23	55 903.50	55 929.97	55 960.34	55 960.34	54 203.119
$4d^{10}4f\ ^2F_{5/2}$	54 105.56	55 456.44	55 759.78	55 938.03	55 938.98	56 002.28	56 002.28	54 204.729
$4d^{10}4f\ ^2F_{7/2}$	54 105.49	55 456.37	55 759.71	55 937.96	55 968.58	56 002.35	56 002.35	54 204.745
$4d^{10}6d\ ^2D_{5/2}$	54 178.48	55 465.47	55 743.41	55 912.57	55 968.65	55 969.55	55 969.55	54 213.564
$4d^{10}8s\ ^2S_{1/2}$	57 347.35	58 674.23	57 144.94	57 309.58	57 317.80	57 342.71	57 342.71	55 581.246
NCSF	13 867	23 803	36 501	51 961	70 183	91 167	91 167	

Notes. The column "FT" reports the energies for which the diagonal elements of the Hamiltonian matrix were fine-tuned to give accurate transition energies to the ^2P and ^2F states. NCSFs is the total number of CSFs in the wave function expansion.

correlation orbitals. The state $4d^{10}7s\ ^2S_{1/2}$ initially appears too high but approaches experimental values after two correlation layers. In contrast, the excitation energies of the $4d^95s^2\ ^2D$ states remain significantly overestimated in the CV model by about 9000 cm^{-1}. To ensure accurate transition parameters, these energies were fine-tuned (FT) by manually adjusting the dominant Hamiltonian matrix element (Li et al. 2023a), chosen to reproduce correct transition energies to the ^2P and ^2F states. On average, excitation energies in the CV correlation model are overestimated by 900 cm^{-1} for lower states and up to 1800 cm^{-1} for higher states. Including core-core (CC) correlations through double substitutions from the core, as well as higher-order effects from triple and quadruple (TQ) substitutions, improves agreement with experiment at the cost of substantially larger CSF expansions.

The second ionization potential of the ground state and the excitation energies of the other states obtained from the FSMRCC method are presented in Table 3. As shown, the excitation energies progressively increase from DHF to RCCSD to RCCSDT, indicating that electron correlation contributes more significantly to the ground state than to the excited states. Breit corrections are relatively small, and the final values are taken as RCCSDT results with added Breit contributions. Comparison with experimental data (Kramida et al. 2024) shows good agreement, except for the $4d^95s^2\ ^2D$ states, which remain overestimated by about 4800 cm^{-1}. For a general discussion about the computational difficulties for core-excited states such as $4d^95s^2\ ^2D$, see for example (Caliskan et al. 2024).

By comparing the MCDHF/RCI results with those obtained from the RCCSD and RCCSDT calculations, we find that the FSMRCC values are generally in better agreement to experiment. Furthermore, unlike the MCDHF/RCI method, the FSMRCC calculations correctly reproduce the ordering of the closely spaced $4d^{10}6d$ and $4d^{10}4f$ configurations.

3.2. Hyperfine interaction constants

Silver has two stable isotopes, ^{107}Ag and ^{109}Ag, with natural abundances of 51.839% and 48.161%, respectively. The dominant isotope, ^{107}Ag, has a nuclear spin $I = 1/2$ and a magnetic dipole moment $\mu = -0.113570\,\mu_N$, while ^{109}Ag has $I = 1/2$ and $\mu = -0.1306905\,\mu_N$. Due to the interaction between the electrons and the magnetic dipole moment, the recorded spectral lines are split into hyperfine components, with the splittings governed by the magnetic dipole interaction constants $A_{\rm hfs}$ of the upper and lower states (Froese Fischer et al. 2019).

The hyperfine interaction constants $A_{\rm hfs}$ obtained from the MCDHF/RCI method are presented in Table 4 as functions of the correlation layers. The convergence pattern shows that the absolute values of the constants in the s and p sequences tend to increase as more CV correlation is included, with particularly large changes for the $7s$ and $8s$ states. This behavior is consistent with general trends observed for nominal one-electron systems (Schiffmann et al. 2020). Calculations accounting for CV correlation tend to overshoot the absolute values for the lowest states. This behavior agrees with observations for similar systems, where the inclusion of CSFs from double (D) substitutions – also accounting for CC correlation – reduces the values and improves agreement with experiment (Schiffmann et al. 2020). Owing to the resulting large expansion sizes, such computations were not attempted.

The FSMRCC values for the hyperfine interaction constants $A_{\rm hfs}$ at different levels of approximation are given in Table 5. The BW corrections are also included (Roberts et al. 2022) in the estimation of these quantities using the RCCSD method. The table shows that the Breit and BW corrections are generally small, except for the ground state where they are more significant.

For convenience, the hyperfine interaction constants obtained from both the MCDHF/RCI and FSMRCC methods

Table 3. Calculated second ionization potential and excitation energies (in cm^{-1}) at different levels of approximation in the FSMRCC theory compared with experimental values from the NIST ASD database (Kramida et al. 2024).

State	DHF	RCCSD	RCCSDT	Breit	Final	Experiment
			Second ionization potential			
$4d^{10}5s\ ^2S_{1/2}$	50 376.11	60 419.22	61 455.66	−58.71	61 396.95	61 106.45
			Excitation energies			
$4d^{10}5p\ ^2P_{1/2}$	23 645.86	29 405.57	29 817.80	−23.15	29 794.65	29 552.057
$4d^{10}5p\ ^2P_{3/2}$	24 227.72	30 324.82	30 774.22	−35.20	30 739.02	30 472.665
$4d^{9}5s^2\ ^2D_{5/2}$	61 491.97	34 897.95	–	198.10	35 096.05	30 242.298
$4d^{9}5s^2\ ^2D_{3/2}$	66 890.45	39 449.04	–	46.05	39 495.09	34 714.226
$4d^{10}6s\ ^2S_{1/2}$	33 261.14	41 963.06	42 897.62	−50.64	42 846.98	42 556.147
$4d^{10}6p\ ^2P_{1/2}$	38 590.28	47 737.47	48 666.10	−50.83	48 615.27	48 297.406
$4d^{10}6p\ ^2P_{3/2}$	38 758.13	47 950.68	48 879.08	−53.48	48 825.60	48 500.810
$4d^{10}5d\ ^2D_{3/2}$	38 393.71	48 101.67	49 088.29	−58.05	49 030.24	48 743.969
$4d^{10}5d\ ^2D_{5/2}$	38 409.24	48 122.18	49 113.99	−58.67	49 055.32	48 764.219
$4d^{10}7s\ ^2S_{1/2}$	41 637.14	51 231.60	52 235.83	−55.99	52 179.84	51 886.965
$4d^{10}7p\ ^2P_{1/2}$	43 717.54	53 410.22	54 405.47	−55.56	54 349.91	54 041.037
$4d^{10}7p\ ^2P_{3/2}$	43 788.97	53 496.26	54 490.84	−56.61	54 434.23	54 121.108
$4d^{10}6d\ ^2D_{3/2}$	43 633.55	53 535.84	54 555.13	−58.40	54 496.73	54 203.119
$4d^{10}4f\ ^2F_{5/2}$	43 518.71	53 525.56	54 558.28	−58.67	54 499.61	54 204.729
$4d^{10}4f\ ^2F_{7/2}$	43 518.64	53 525.48	54 558.04	−58.67	54 499.37	54 204.745
$4d^{10}6d\ ^2D_{5/2}$	43 641.70	53 545.90	54 563.71	−58.70	54 505.01	54 213.564
$4d^{10}8s\ ^2S_{1/2}$	45 071.25	54 908.80	55 931.10	−57.46	55 873.64	55 581.246

Table 4. Calculated hyperfine interaction constants A_{hfs} (in MHz) for ^{107}Ag at different layers using the MCDHF/RCI method compared with experimental values.

State	Layer 1	Layer 2	Layer 3	Layer 4	Layer 5	Layer 6	Experiment
$4d^{10}5s\ ^2S_{1/2}$	−1676	−1736	−1765	−1847	−1847	−1845	−1712.512111(18)[a]
$4d^{10}5p\ ^2P_{1/2}$	−164	−175	−186	−192	−192	−193	−175.4(17)[b]
$4d^{10}5p\ ^2P_{3/2}$	−27.2	−31.1	−33.7	−34.8	−34.4	−34.3	−31.7(5)[b]
$4d^{9}5s^2\ ^2D_{5/2}$	−145	−148	−148	−147	−146	−145	−126.2818(1)[c]
$4d^{9}5s^2\ ^2D_{3/2}$	−267	−266	−265	−266	−266	−268	
$4d^{10}6s\ ^2S_{1/2}$	−199	−204	−219	−239	−241	−241	
$4d^{10}6p\ ^2P_{1/2}$	−32.9	−34.0	−39.4	−39.9	−40.6	−40.3	−38.7(10)[d]
$4d^{10}6p\ ^2P_{3/2}$	−6.7	−7.2	−8.5	−8.5	−8.6	−8.5	−9.05(25)[d]
$4d^{10}5d\ ^2D_{3/2}$	−1.4	−1.4	−1.7	−1.8	−1.8	−1.7	
$4d^{10}5d\ ^2D_{5/2}$	−0.8	−0.8	−0.9	−0.9	−0.9	−0.9	
$4d^{10}7s\ ^2S_{1/2}$	−36.5	−40.4	−79.3	−81.4	−81.5	−81.6	
$4d^{10}7p\ ^2P_{1/2}$	−11.5	−11.8	−15.0	−15.0	−15.7	−15.4	
$4d^{10}7p\ ^2P_{3/2}$	−2.6	−2.8	−3.7	−3.6	−3.8	−3.7	−4.5(2)[e]
$4d^{10}6d\ ^2D_{3/2}$	−0.6	−0.6	−0.8	−0.8	−0.8	−0.8	
$4d^{10}4f\ ^2F_{5/2}$	−0.01	−0.01	−0.01	−0.01	−0.01	−0.01	
$4d^{10}4f\ ^2F_{7/2}$	−0.009	−0.009	−0.009	−0.009	−0.009	−0.009	
$4d^{10}6d\ ^2D_{5/2}$	−0.4	−0.4	−0.4	−0.4	−0.4	−0.4	
$4d^{10}8s\ ^2S_{1/2}$	−15.4	−16.2	−26.1	−30.9	−36.5	−37.0	

Notes. [a]Dahmen & Penselin (1967); [b]Carlsson et al. (1990); [c]Blachman et al. (1966); [d]Bengtsson et al. (1990); [e]Bengtsson et al. (1991).

are summarized in Table 6, along with other theoretical results and experimental data. Comparing the results, we find that the FSMRCC values agree better with experiment for the lower states than the MCDHF/RCI results, although the overall agreement is good. For the $4d^{9}5s^2\ ^2D_{5/2}$ state, where the experimental value is known with high precision, the MCDHF/RCI calculation provides a better estimate. The MCDHF calculations by Song et al. (2007) for the ground and first excited states remain the most accurate to date.

3.3. Transition rates and oscillator strengths

The fundamental quantity from which all parameters for electric dipole (E1) transitions can be derived is the reduced matrix

Table 5. Calculated hyperfine interaction constants $A_{\rm hfs}$ (in MHz) for ^{107}Ag at different levels of approximation in the FSMRCC theory compared with experimental values.

State	DHF	RCCSD	RCCSDT	BW	Breit	Final	Experiment
$4d^{10}5s\ ^2S_{1/2}$	−1198.13	−1761.06	−1799.57	8.78	−0.01	−1790.80	−1712.512111(18)[a]
$4d^{10}5p\ ^2P_{1/2}$	−104.46	−173.89	−181.96	0.06	0.52	−181.38	−175.4(17)[b]
$4d^{10}5p\ ^2P_{3/2}$	−16.06	−29.31	−32.07	0.01	0.01	−32.05	−31.7(5)[b]
$4d^{9}5s^2\ ^2D_{5/2}$	−116.78	−194.35	–	−0.02	−0.96	−195.33	−126.2818(1)[c]
$4d^{9}5s^2\ ^2D_{3/2}$	−287.87	−479.59	–	0.02	−1.87	−481.44	
$4d^{10}6s\ ^2S_{1/2}$	−195.20	−239.90	−238.96	1.20	−0.06	−237.82	
$4d^{10}6p\ ^2P_{1/2}$	−29.02	−39.27	−39.67	0.02	0.05	−39.60	−38.7(10)[d]
$4d^{10}6p\ ^2P_{3/2}$	−0.23	−7.00	−7.78	∼0.0	∼0.0	−7.78	−9.05(25)[d]
$4d^{10}5d\ ^2D_{3/2}$	−0.73	−1.59	−1.79	∼0.0	−0.01	−1.80	
$4d^{10}5d\ ^2D_{5/2}$	−0.32	−0.64	−65	∼0.0	∼0.0	−0.65	
$4d^{10}7s\ ^2S_{1/2}$	−69.50	−82.04	−81.43	0.41	−0.10	−81.12	
$4d^{10}7p\ ^2P_{1/2}$	−12.21	−15.77	−15.80	0.01	−0.04	−15.83	
$4d^{10}7p\ ^2P_{3/2}$	−1.94	−2.87	−3.27	∼0.0	∼0.0	−3.27	−4.5(2)[e]
$4d^{10}6d\ ^2D_{3/2}$	−0.38	−0.82	−0.85	∼0.0	∼0.0	−0.85	
$4d^{10}6d\ ^2D_{5/2}$	−0.17	−0.31	−0.33	∼0.0	∼0.0	−0.33	
$4d^{10}4f\ ^2F_{5/2}$	−0.011	−0.012	−0.014	∼0.0	∼0.0	−0.014	
$4d^{10}4f\ ^2F_{7/2}$	−0.006	−0.007	−0.008	∼0.0	∼0.0	−0.008	
$4d^{10}8s\ ^2S_{1/2}$	−32.66	−37.88	−37.51	0.19	−0.01	−37.33	

Notes. [a]Dahmen & Penselin (1967); [b]Carlsson et al. (1990); [c]Blachman et al. (1966); [d]Bengtsson et al. (1990); [e]Bengtsson et al. (1991).

Table 6. Hyperfine interaction constants $A_{\rm hfs}$ (in MHz) for ^{107}Ag from MCDHF/RCI and FSMRCC calculations compared with experimental values and other theories.

State	MCDHF/RCI	FSMRCC	MCDHF[a]	FSMRCC[b]	Experiment
$4d^{10}5s\ ^2S_{1/2}$	−1845	−1790.80	−1724	−1726	−1712.512111(18)[c]
$4d^{10}5p\ ^2P_{1/2}$	−193	−181.38	−180	−167	−175.4(17)[d]
$4d^{10}5p\ ^2P_{3/2}$	−34.3	−32.05	−30	−28	−31.7(5)[d]
$4d^{9}5s^2\ ^2D_{5/2}$	−145	−195.33			−126.2818(1)[e]
$4d^{9}5s^2\ ^2D_{3/2}$	−268	−481.44			
$4d^{10}6s\ ^2S_{1/2}$	−241	−237.82			
$4d^{10}6p\ ^2P_{1/2}$	−40.3	−39.60			−38.7(10)[f]
$4d^{10}6p\ ^2P_{3/2}$	−8.5	−7.78			−9.05(25)[f]
$4d^{10}5d\ ^2D_{3/2}$	−1.7	−1.80			
$4d^{10}5d\ ^2D_{5/2}$	−0.9	−0.65			
$4d^{10}7s\ ^2S_{1/2}$	−81.6	−81.12			
$4d^{10}7p\ ^2P_{1/2}$	−15.4	−15.83			
$4d^{10}7p\ ^2P_{3/2}$	−3.7	−3.27			−4.5(2)[g]
$4d^{10}6d\ ^2D_{3/2}$	−0.8	−0.85			
$4d^{10}4f\ ^2F_{5/2}$	−0.01	−0.014			
$4d^{10}4f\ ^2F_{7/2}$	−0.009	−0.008			
$4d^{10}6d\ ^2D_{5/2}$	−0.4	−0.33			
$4d^{10}8s\ ^2S_{1/2}$	−37.0	−37.33			

Notes. [a]Song et al. (2007); [b]Chaudhuri & Chattopadhyay (2022); [c]Dahmen & Penselin (1967); [d]Carlsson et al. (1990); [e]Blachman et al. (1966); [f]Bengtsson et al. (1990); [g]Bengtsson et al. (1991).

element (Sahoo et al. 2025). Table A.1 compares the reduced matrix elements obtained at different levels of approximation in the FSMRCC method (using the length gauge) with those obtained from the MCDHF/RCI calculations. The median relative difference between the two methods is 1.7%. While most transitions show very small differences, notable exceptions occur for the $6p_{1/2,3/2} \rightarrow 5s_{1/2}$ and $7p_{1/2,3/2} \rightarrow 5s_{1/2}$ transitions. As discussed in Papoulia et al. (2019), the length-gauge matrix elements in the MCDHF/RCI model for transitions from highly excited states to low-lying states are sensitive to the completeness of the radial orbital basis, which affects the outer part of the wave function. In contrast, the velocity-gauge matrix elements are less sensitive to basis incompleteness and provide more accurate values. Indeed, the velocity-gauge results for these transitions (0.162 and 0.310 for $6p_{1/2,3/2} \rightarrow 5s_{1/2}$, and 0.0411 and 0.104 for $7p_{1/2,3/2} \rightarrow 5s_{1/2}$) are in better agreement with the

FSMRCC values, which do not suffer from this limitation. These transitions also exhibit the largest changes when going from the DHF approximation to RCCSD and further to RCCSDT.

The transition rates A from the MCDHF/RCI and FSMRCC calculations are presented in Table A.2. Due to limitations of the FSMRCC approach, transition rates involving the core-excited $4d^9 5s^2\ ^2D_{3/2,5/2}$ states could not be computed; these transitions are, however, provided by the MCDHF/RCI calculations. For MCDHF/RCI, the quantitative and qualitative evaluation (QQE) approach of Gaigalas and co-workers (Gaigalas et al. 2022; Kitovienė et al. 2024) was used to estimate uncertainties, following the NIST ASD (Kramida et al. 2023) classification: AA ($\leq 1\%$), A+ ($\leq 2\%$), A ($\leq 3\%$), B+ ($\leq 7\%$), B ($\leq 10\%$), C+ ($\leq 18\%$), C ($\leq 25\%$), D+ ($\leq 40\%$), D ($\leq 50\%$), and E ($> 50\%$). Overall, there is good agreement between FSMRCC and MCDHF/RCI transition rates, except for the $6p_{1/2,3/2} \rightarrow 5s_{1/2}$ and $7p_{1/2,3/2} \rightarrow 5s_{1/2}$ transitions, as discussed above. For most transitions between Rydberg states, uncertainties are within 10% according to the QQE approach. Transitions connecting the $4d^9 5s^2\ ^2D_{3/2,5/2}$ core-excited states and the ordinary $4d^{10}nl$ Rydberg states are so-called two-electron one-photon (TEOP) transitions. These transitions vanish in the Dirac–Fock approximation and appear only through electron correlation effects, making them both weak and computationally challenging. Consequently, they fall into the E class (uncertainty > 50%). To the best of our knowledge, these transition rates have not been reported in any previous calculations. The transition rates for the $6p_{1/2,3/2} \rightarrow 5s_{1/2}$ transitions were recently measured using optical emission spectroscopy (OES) by Alhijry et al. (2020) yielding values of $A = (5.53 \pm 1.72) \times 10^5$ s^{-1} and $A = (3.0 \pm 0.91) \times 10^5$ s^{-1}, which are in stark contrast to the present values as well as to the values from the Kurucz database. Furthermore, the OES values contradict the measured lifetimes of the $6p_{1/2,3/2}$ states (Jiang et al. 1990).

The weighted oscillator strengths, gf, obtained from the MCDHF/RCI and FSMRCC calculations are presented in Table A.3. For MCDHF/RCI, the uncertainty estimates from Table A.2 are included. The table also lists the values reported by Civiš et al. (2010) based on the Fues model potential for comparison. Except for the $6p_{1/2,3/2} \rightarrow 5s_{1/2}$ and $7p_{1/2,3/2} \rightarrow 5s_{1/2}$ transitions, there is excellent agreement between MCDHF/RCI and FSMRCC, with a mean relative difference of 3.5%. The Fues model potential values, despite the simplicity of the method, show relatively good agreement with the results from full many-body theories. However, the differences are especially large for the $6p_{1/2,3/2} \rightarrow 5s_{1/2}$ and $7p_{1/2,3/2} \rightarrow 5s_{1/2}$ transitions. Indeed, Table III of Civiš et al. (2010), which compiles gf values from numerous theories, reveals a scatter spanning orders of magnitude for these transitions.

3.4. Lifetimes

Silver is relatively easily accessible for laser excitation, and lifetimes have been measured for states in the s, p, and d sequences using LIF. In Table A.4, the lifetimes obtained using the MCDHF/RCI and FSMRCC methods are compared with results from other theories as well as with experiment. Both MCDHF/RCI and FSMRCC slightly underestimate the lifetime for the resonance transition, which is accurately known (Carlsson et al. 1990). A similar trend, though more distant from experiment, is observed for the FSMRCC and configuration interaction – many-body perturbation theory (CI-MBPT) calculations (Chaudhuri & Chattopadhyay 2022; Dzuba et al. 2021). For the excited states in the p sequence, the MCDHF/RCI method predicts somewhat longer lifetimes than FSMRCC, in agreement with experiment within the error bars. For the states in the d and f sequences, the two methods give lifetimes in very close agreement, which also match experimental values within uncertainties. For the s sequence, the opposite trend is observed: FSMRCC predicts slightly longer lifetimes than MCDHF/RCI, again in good agreement with experiment. Overall, the agreement between theory and experiment is very good. The $4d^9 5s^2\ ^2D_{3/2,5/2}$ states are metastable and decay only via higher-order magnetic and electric transitions. The lifetime for $4d^9 5s^2\ ^2D_{5/2}$ from MCDHF/RCI is 163 ms, in reasonable agreement with the recent CI-MBPT calculation by Dzuba et al. (2021), which gives 192 ms. For $4d^9 5s^2\ ^2D_{3/2}$, the lifetimes from the MCDHF/RCI and CI-MBPT calculations differ by a factor of three. Improved computational methodologies are urgently needed to handle transitions of this type. As a comment, in contrast to the regular states in the s, p, and d sequences, no experimental technique is currently available for determining the lifetime of $4d^9 5s^2\ ^2D_{5/2}$; its value is established entirely through theoretical calculations.

4. Summary: Recommended data

We applied the FSMRCC theory and the MCDHF/RCI method, two well-known many-body approaches, to compute hyperfine interaction constants, transition data, and lifetimes for the even $5s_{1/2}$, $6s_{1/2}$, $7s_{1/2}$, $8s_{1/2}$, $5d_{3/2,5/2}$, $6d_{3/2,5/2}$, and $4d^9 5s^2\ ^2D_{3/2,5/2}$ states and the odd $5p_{1/2,3/2}$, $6p_{1/2,3/2}$, $7p_{1/2,3/2}$, $4f_{5/2,7/2}$ states. The results from the two methods were compared with each other, as well as with existing experimental hyperfine and transition data and results from other calculations. We begin with the hyperfine interaction constants. While the FSMRCC and MCDHF/RCI results show excellent agreement for the excited states, the FSMRCC values are in better agreement with experiment for the ground and first excited states than are those from MCDHF/RCI. For this reason we recommend the FSMRCC hyperfine interaction constants. The agreement with the experimental constants is good, with a mean difference of 3% for the accurately determined $5s_{1/2}, 5p_{1/2,3/2}$ states. For the $4d^9 5s^2\ ^2D_{3/2,5/2}$ core-excited metastable states, contributions from triple excitations cannot be included within the current FSMRCC implementation, and the MCDHF/RCI values for these states are in closer agreement with experiment. Turning to the weighted oscillator strengths, gf, the quantity most frequently used for abundance and atmospheric analysis (Wahlgren 2010), the FSMRCC and MCDHF/RCI values for transitions between the ordinary states of the s, p, d, and f sequences agree very well, with a median relative differences of 2.4%. Using the QQE approach (Gaigalas et al. 2022; Kitovienė et al. 2024) and examining the relative changes from the DHF approximation through RCCSD to RCCSDT, we identified the weak $6p_{1/2,3/2} \rightarrow 5s_{1/2}$ and $7p_{1/2,3/2} \rightarrow 5s_{1/2}$ transitions as comparatively uncertain. The transition data, in terms of lifetimes, were compared with values from LIF measurements. The computed lifetimes for the higher states mainly fall within the experimental error bars. For the accurately known resonance transitions $5p_{1/2,3/2} \rightarrow 5s_{1/2}$, the relative differences between the calculated lifetimes and the experimental lifetimes are 2.8% and 3.8%, respectively. Based on the comparison with the lifetimes, it is not possible to single out either the FSMRCC or MCDHF/RCI method as providing the most accurate transition data. For this reason, the recommended transition parameters are those obtained as the mean of the FSMRCC and MCDHF/RCI values. The uncertainties can be estimated in two ways: by using

the relative differences between the FSMRCC and MCDHF/RCI values to assign transitions to the NIST ASD accuracy classes, or alternatively by using the gauge dependence of the MCDHF/RCI transition parameters within the QQE approach for the same purpose. We used both approaches, taking as the final conservative uncertainty estimate the most stringent of the two classes. As the FSMRCC theory does not provide transition data involving the $4d^9 5s^2\ ^2D$ states, the uncertainty estimates for the corresponding TOEP transitions are based entirely on the QQE approach. The recommended weighted oscillator strengths are displayed in Table A.5 along with the estimated uncertainties. Whereas most transitions fall into the higher accuracy classes, we see that the TOEP transitions mainly fall into class E. Incidentally, we note that our recommended gf values for the resonance transitions are in perfect agreement with the experimental ones from the accurate picosecond delayed-coincidence technique measurements by Carlsson et al. (1990), giving $gf = 0.464$ and $gf = 0.952$ for $5p_{1/2} \rightarrow 5s_{1/2}$ and $5p_{3/2} \rightarrow 5s_{1/2}$, respectively.

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Appendix A: Tables

Table A.1. The calculated E1 matrix elements (in a.u.) at different levels of approximation in the FSMRCC method using the length-gauge expression.

Transition	DHF	RCCSD	RCCSDT	Breit	Final	MCDHF/RCI
$6s_{1/2} \rightarrow 5p_{1/2}$	3.403	2.876	2.786	0.005	2.791(50)	2.736
$6s_{1/2} \rightarrow 5p_{3/2}$	5.073	4.343	4.212	0.004	4.216(75)	4.132
$7s_{1/2} \rightarrow 5p_{1/2}$	0.704	0.684	0.688	~ 0.0	0.688(5)	0.679
$7s_{1/2} \rightarrow 5p_{3/2}$	0.988	0.967	0.967	~ 0.0	0.967(5)	0.962
$7s_{1/2} \rightarrow 6p_{1/2}$	8.215	7.468	7.329	0.008	7.337(76)	7.260
$7s_{1/2} \rightarrow 6p_{3/2}$	12.121	11.100	10.892	0.006	10.90(10)	10.77
$8s_{1/2} \rightarrow 5p_{1/2}$	0.366	0.366	0.370	~ 0.0	0.370(4)	0.363
$8s_{1/2} \rightarrow 5p_{3/2}$	0.509	0.512	0.519	~ 0.0	0.519(5)	0.509
$8s_{1/2} \rightarrow 6p_{1/2}$	1.475	1.445	1.450	~ 0.0	1.450(6)	1.477
$8s_{1/2} \rightarrow 6p_{3/2}$	2.029	1.997	2.011	0.001	2.012(10)	2.037
$8s_{1/2} \rightarrow 7p_{1/2}$	14.864	13.833	13.615	0.013	13.63(12)	13.68
$8s_{1/2} \rightarrow 7p_{3/2}$	21.836	20.453	20.133	0.006	20.139(25)	20.130
$5p_{1/2} \rightarrow 5s_{1/2}$	3.059	2.403	2.318	0.003	2.321(50)	2.188
$5p_{3/2} \rightarrow 5s_{1/2}$	4.302	3.395	3.271	0.004	3.275(80)	3.098
$6p_{1/2} \rightarrow 5s_{1/2}$	0.400	0.183	0.135	0.001	0.133(25)	0.0816*
$6p_{3/2} \rightarrow 5s_{1/2}$	0.643	0.342	0.282	0.001	0.283(23)	0.195*
$6p_{1/2} \rightarrow 6s_{1/2}$	7.673	7.227	7.202	0.001	7.203(20)	7.127
$6p_{3/2} \rightarrow 6s_{1/2}$	10.691	10.067	10.040	0.004	10.044(52)	9.945
$7p_{1/2} \rightarrow 5s_{1/2}$	0.174	0.056	0.031	0.001	0.032(10)	0.0102*
$7p_{3/2} \rightarrow 5s_{1/2}$	0.293	0.128	0.086	0.001	0.087(17)	0.0305*
$7p_{1/2} \rightarrow 6s_{1/2}$	1.036	0.865	0.825	0.003	0.828(30)	0.779
$7p_{3/2} \rightarrow 6s_{1/2}$	1.616	1.395	1.341	0.001	1.342(21)	1.269
$7p_{1/2} \rightarrow 7s_{1/2}$	13.980	13.522	13.523	~ 0.0	13.52(12)	13.42
$7p_{3/2} \rightarrow 7s_{1/2}$	19.405	18.747	18.762	0.003	18.76(15)	18.65
$5d_{3/2} \rightarrow 5p_{1/2}$	5.700	4.540	4.399	0.009	4.408(43)	4.261
$5d_{3/2} \rightarrow 5p_{3/2}$	2.654	2.145	2.075	0.002	2.077(53)	2.016
$5d_{3/2} \rightarrow 6p_{1/2}$	11.980	11.773	11.722	−0.001	11.72(10)	11.62
$5d_{3/2} \rightarrow 6p_{3/2}$	5.318	5.240	5.219	~ 0.0	5.219(86)	5.176
$5d_{3/2} \rightarrow 7p_{1/2}$	1.214	1.799	1.861	−0.008	1.853(25)	1.870
$5d_{3/2} \rightarrow 7p_{3/2}$	0.447	0.689	0.719	−0.002	0.717(12)	0.730
$5d_{5/2} \rightarrow 5p_{3/2}$	7.945	6.416	6.219	0.009	6.228(16)	6.030
$5d_{5/2} \rightarrow 6p_{3/2}$	16.000	15.769	15.728	−0.002	15.73(12)	15.57
$5d_{5/2} \rightarrow 7p_{3/2}$	1.370	2.108	2.220	0.008	2.228(20)	2.226
$6d_{3/2} \rightarrow 5p_{1/2}$	2.051	1.805	1.791	0.002	1.793(51)	1.700
$6d_{3/2} \rightarrow 5p_{3/2}$	0.923	0.824	0.808	~ 0.0	0.808(28)	0.778
$6d_{3/2} \rightarrow 6p_{1/2}$	9.332	7.657	7.418	0.018	7.436(69)	7.310
$6d_{3/2} \rightarrow 6p_{3/2}$	4.406	3.671	3.554	0.005	3.559(47)	3.502
$6d_{3/2} \rightarrow 7p_{1/2}$	24.483	24.176	24.135	−0.001	24.135(67)	24.122
$6d_{3/2} \rightarrow 7p_{3/2}$	10.886	10.777	10.766	~ 0.0	10.766(41)	11.75
$6d_{5/2} \rightarrow 5p_{3/2}$	2.773	2.474	2.406	~ 0.0	2.406(22)	2.333
$6d_{5/2} \rightarrow 6p_{3/2}$	13.156	10.936	10.616	0.018	10.63(11)	10.44
$6d_{5/2} \rightarrow 7p_{3/2}$	32.723	32.407	32.340	0.003	32.343(22)	32.322
$4f_{5/2} \rightarrow 5d_{3/2}$	16.563	15.704	15.556	0.002	15.558(30)	15.321
$4f_{5/2} \rightarrow 6d_{3/2}$	23.873	24.109	24.130	−0.001	24.129(38)	24.510
$4f_{5/2} \rightarrow 5d_{5/2}$	4.440	4.213	4.283	~ 0.0	4.283(46)	4.109
$4f_{7/2} \rightarrow 5d_{5/2}$	19.855	18.842	18.706	~ 0.0	18.706(45)	18.375
$4f_{5/2} \rightarrow 6d_{5/2}$	6.372	6.434	6.444	~ 0.0	6.444(55)	6.544
$4f_{7/2} \rightarrow 6d_{5/2}$	28.495	28.772	28.808	0.001	28.809(86)	29.263

Notes. The final results from the FSMRCC method are listed along with the estimated uncertainties and they are compared with the MCDHF/RCI calculations. The transitions with the largest relative difference for the matrix elements are marked with asterisks $*$, see text.

Table A.2. E1 transition rates A (in length gauge) in s^{-1} from FSMRCC and MCDHF/RCI calculations.

Transition	FSMRCC	MCDHF/RCI	unc.
$6s_{1/2} \rightarrow 5p_{1/2}$	1.735+07	1.877+07	A+
$6s_{1/2} \rightarrow 5p_{3/2}$	3.177+07	3.414+07	A+
$7s_{1/2} \rightarrow 5p_{1/2}$	5.343+06	5.685+06	AA
$7s_{1/2} \rightarrow 5p_{3/2}$	9.303+06	1.002+07	AA
$7s_{1/2} \rightarrow 6p_{1/2}$	2.522+06	2.565+06	A+
$7s_{1/2} \rightarrow 6p_{3/2}$	4.671+06	4.712+06	AA
$8s_{1/2} \rightarrow 5p_{1/2}$	2.446+06	2.555+06	A+
$8s_{1/2} \rightarrow 5p_{3/2}$	4.320+06	4.492+06	A
$8s_{1/2} \rightarrow 6p_{1/2}$	8.231+05	8.859+05	B
$8s_{1/2} \rightarrow 6p_{3/2}$	1.456+06	1.544+06	B+
$8s_{1/2} \rightarrow 7p_{1/2}$	6.853+05	6.922+05	B+
$8s_{1/2} \rightarrow 7p_{3/2}$	1.279+06	1.270+06	B+
$5p_{1/2} \rightarrow 5s_{1/2}$	1.409+08	1.390+08	C+
$5p_{3/2} \rightarrow 5s_{1/2}$	1.537+08	1.531+08	C+
$5p_{3/2} \rightarrow 4d^{-1}_{5/2}$	–	3.57+00	E
$6p_{1/2} \rightarrow 5s_{1/2}$	2.019+06	8.426+05	E*
$6p_{1/2} \rightarrow 4d^{-1}_{3/2}$	–	4.137+04	E
$6p_{1/2} \rightarrow 6s_{1/2}$	9.947+06	1.026+07	A+
$6p_{3/2} \rightarrow 5s_{1/2}$	4.628+06	2.446+06	E*
$6p_{3/2} \rightarrow 4d^{-1}_{5/2}$	–	1.668+05	E
$6p_{3/2} \rightarrow 4d^{-1}_{3/2}$	–	5.026+03	E
$6p_{3/2} \rightarrow 6s_{1/2}$	1.074+07	1.112+07	A+
$7p_{1/2} \rightarrow 5s_{1/2}$	1.637+05	1.834+04	E*
$7p_{1/2} \rightarrow 4d^{-1}_{3/2}$	–	7.304+04	E
$7p_{1/2} \rightarrow 6s_{1/2}$	1.052+06	9.800+05	B+
$7p_{1/2} \rightarrow 5d_{3/2}$	5.170+05	5.426+05	A
$7p_{1/2} \rightarrow 7s_{1/2}$	1.852+06	1.938+06	AA
$7p_{3/2} \rightarrow 5s_{1/2}$	6.078+05	8.22+04	E*
$7p_{3/2} \rightarrow 4d^{-1}_{5/2}$	–	1.971+05	E
$7p_{3/2} \rightarrow 4d^{-1}_{3/2}$	–	8.511+03	E
$7p_{3/2} \rightarrow 6s_{1/2}$	1.411+06	1.325+06	B+
$7p_{3/2} \rightarrow 5d_{3/2}$	4.049+04	4.330+04	A
$7p_{3/2} \rightarrow 5d_{5/2}$	3.865+05	3.982+05	B+
$7p_{3/2} \rightarrow 7s_{1/2}$	1.989+06	2.089+06	AA
$4d^{-1}_{3/2} \rightarrow 5p_{1/2}$	–	1.637+04	E
$4d^{-1}_{3/2} \rightarrow 5p_{3/2}$	–	1.729+03	E
$5d_{3/2} \rightarrow 5p_{1/2}$	6.957+07	7.194+07	B+
$5d_{3/2} \rightarrow 5p_{3/2}$	1.333+07	1.383+07	B+
$5d_{3/2} \rightarrow 6p_{1/2}$	6.197+03	7.732+03	B+
$5d_{3/2} \rightarrow 6p_{3/2}$	1.983+02	2.707+02	B
$5d_{5/2} \rightarrow 5p_{3/2}$	8.016+07	8.273+07	B+
$5d_{5/2} \rightarrow 6p_{3/2}$	1.526+03	1.977+03	B
$6d_{3/2} \rightarrow 5p_{1/2}$	2.439+07	2.386+07	B+
$6d_{3/2} \rightarrow 5p_{3/2}$	4.419+06	4.438+06	B+
$6d_{3/2} \rightarrow 6p_{1/2}$	5.769+06	5.818+06	AA
$6d_{3/2} \rightarrow 6p_{3/2}$	1.190+06	1.199+06	AA
$6d_{3/2} \rightarrow 7p_{1/2}$	1.256+03	1.148+03	B+
$6d_{3/2} \rightarrow 7p_{3/2}$	3.238+01	2.465+01	C+
$6d_{5/2} \rightarrow 5p_{3/2}$	2.616+07	2.665+07	B+
$6d_{5/2} \rightarrow 6p_{3/2}$	7.119+06	7.137+06	AA
$6d_{5/2} \rightarrow 7p_{3/2}$	2.792+02	2.103+02	C+
$4f_{5/2} \rightarrow 4d^{-1}_{3/2}$	–	1.533+04	A+
$4f_{5/2} \rightarrow 4d^{-1}_{5/2}$	–	1.146+03	B+
$4f_{5/2} \rightarrow 5d_{3/2}$	1.331+07	1.354+07	AA
$4f_{5/2} \rightarrow 5d_{5/2}$	9.975+05	9.646+05	AA
$4f_{7/2} \rightarrow 4d^{-1}_{5/2}$	–	1.688+04	A
$4f_{7/2} \rightarrow 5d_{5/2}$	1.427+07	1.447+07	AA

Notes. Uncertainty estimates for MCDHF/RCI based on the QQE approach. Here, $4d^{-1}$ denotes the core-excited configuration $4d^9 5s^2$.

Table A.3. Weighted oscillator strengths gf in length gauge from FSMRCC and MCDHF/RCI calculations.

Transition	FSMRCC	MCDHF/RCI	unc.	FMP
$6s_{1/2} \rightarrow 5p_{1/2}$	0.308	0.308	A+	0.332
$6s_{1/2} \rightarrow 5p_{3/2}$	0.652	0.651	A+	0.684
$7s_{1/2} \rightarrow 5p_{1/2}$	0.0321	0.0322	AA	0.0298
$7s_{1/2} \rightarrow 5p_{3/2}$	0.0608	0.0619	AA	0.0552
$7s_{1/2} \rightarrow 6p_{1/2}$	0.587	0.582	A+	0.644
$7s_{1/2} \rightarrow 6p_{3/2}$	1.222	1.206	AA	1.308
$8s_{1/2} \rightarrow 5p_{1/2}$	0.0108	0.0107	A+	0.00960
$8s_{1/2} \rightarrow 5p_{3/2}$	0.0205	0.0203	A	0.0176
$8s_{1/2} \rightarrow 6p_{1/2}$	0.0465	0.0489	B	0.0466
$8s_{1/2} \rightarrow 6p_{3/2}$	0.08706	0.0903	B+	0.0848
$8s_{1/2} \rightarrow 7p_{1/2}$	0.869	0.876	B+	0.934
$8s_{1/2} \rightarrow 7p_{3/2}$	1.799	1.794	B+	1.896
$5p_{1/2} \rightarrow 5s_{1/2}$	0.484	0.445	C+	0.558
$5p_{3/2} \rightarrow 5s_{1/2}$	0.993	0.921	C+	1.14
$5p_{3/2} \rightarrow 4d^{-1}_{5/2}$	–	0.000314	E	–
$6p_{1/2} \rightarrow 5s_{1/2}$	0.00259	0.00101	E*	0.0222
$6p_{1/2} \rightarrow 4d^{-1}_{3/2}$	–	0.000624	E	–
$6p_{1/2} \rightarrow 6s_{1/2}$	0.905	0.902	A+	0.786
$6p_{3/2} \rightarrow 5s_{1/2}$	0.0118	0.0582	E*	0.0530
$6p_{3/2} \rightarrow 4d^{-1}_{5/2}$	–	0.00281	E	–
$6p_{3/2} \rightarrow 4d^{-1}_{3/2}$	–	0.000147	E	–
$6p_{3/2} \rightarrow 6s_{1/2}$	1.822	1.819	A+	1.584
$7p_{1/2} \rightarrow 5s_{1/2}$	0.000168	0.0000177	E*	0.00568
$7p_{1/2} \rightarrow 4d^{-1}_{3/2}$	–	0.000551	E	–
$7p_{1/2} \rightarrow 6s_{1/2}$	0.0239	0.0215	B+	0.0308
$7p_{1/2} \rightarrow 5d_{3/2}$	0.0552	0.0568	A	–
$7p_{1/2} \rightarrow 7s_{1/2}$	1.1966	1.202	AA	1.086
$7p_{3/2} \rightarrow 5s_{1/2}$	0.00124	0.00158	E*	0.0140
$7p_{3/2} \rightarrow 4d^{-1}_{5/2}$	–	0.00196	E	–
$7p_{3/2} \rightarrow 4d^{-1}_{3/2}$	–	0.000127	E	–
$7p_{3/2} \rightarrow 6s_{1/2}$	0.0633	0.0575	B+	0.0734
$7p_{3/2} \rightarrow 5d_{3/2}$	0.00840	0.00880	A	–
$7p_{3/2} \rightarrow 5d_{5/2}$	0.0808	0.0814	B+	–
$7p_{3/2} \rightarrow 7s_{1/2}$	2.3906	2.409	AA	2.180
$4d^{-1}_{3/2} \rightarrow 5p_{1/2}$	–	0.00353	E	–
$4d^{-1}_{3/2} \rightarrow 5p_{3/2}$	–	0.000563	E	–
$5d_{3/2} \rightarrow 5p_{1/2}$	1.133	1.095	B+	1.194
$5d_{3/2} \rightarrow 5p_{3/2}$	0.239	0.233	B+	0.248
$5d_{3/2} \rightarrow 6p_{1/2}$	0.186	0.198	B+	0.182
$5d_{3/2} \rightarrow 6p_{3/2}$	0.0201	0.0201	B	0.0197
$5d_{5/2} \rightarrow 5p_{3/2}$	2.155	2.086	B+	2.232
$5d_{5/2} \rightarrow 6p_{3/2}$	0.198	0.213	B	–
$6d_{3/2} \rightarrow 5p_{1/2}$	0.241	0.223	B+	0.264
$6d_{3/2} \rightarrow 5p_{3/2}$	0.0471	0.0448	B+	0.0524
$6d_{3/2} \rightarrow 6p_{1/2}$	0.992	0.972	AA	1.016
$6d_{3/2} \rightarrow 6p_{3/2}$	0.219	0.215	AA	0.220
$6d_{3/2} \rightarrow 7p_{1/2}$	0.287	0.278	B+	0.284
$6d_{3/2} \rightarrow 7p_{3/2}$	0.0289	0.0263	C+	0.0286
$6d_{5/2} \rightarrow 5p_{3/2}$	0.417	0.403	B+	0.472
$6d_{5/2} \rightarrow 6p_{3/2}$	1.962	1.917	AA	–
$6d_{5/2} \rightarrow 7p_{3/2}$	0.294	0.267	C+	–
$4f_{5/2} \rightarrow 4d^{-1}_{3/2}$	–	0.000341	A+	–
$4f_{5/2} \rightarrow 4d^{-1}_{5/2}$	–	0.0000169	B+	–
$4f_{5/2} \rightarrow 5d_{3/2}$	4.015	3.956	AA	4.038
$4f_{5/2} \rightarrow 5d_{5/2}$	0.303	0.284	AA	0.289
$4f_{7/2} \rightarrow 4d^{-1}_{5/2}$	–	0.000332	A	–
$4f_{7/2} \rightarrow 5d_{5/2}$	5.782	5.672	AA	5.797

Notes. Uncertainty estimates for MCDHF/RCI based on the QQE approach. Here, $4d^{-1}$ denotes the core-excited configuration $4d^9 5s^2$. FMP refers to values reported by Civiš et al. (2010) based on the Fues model potential.

Table A.4. Lifetimes from MCDHF/RCI and FSMRCC calculations compared with experimental values and other theories.

State	MCDHF/RCI	FSMRCC	FSMRCC[(a)]	MBPT[(b)]	CI-MBPT[(c)]	Experiment
$4d^{10}5p\ ^2P_{1/2}$	7.20 ns	7.10(30) ns	6.718 ns	7.62 ns	6.6 ns	7.41(0.04) ns[(d)]
$4d^{10}5p\ ^2P_{3/2}$	6.53 ns	6.51(30) ns	6.193 ns	6.97 ns	6.1 ns	6.79(0.03) ns[(d)]
$4d^{9}5s^2\ ^2D_{5/2}$	163 ms				192 ms	
$4d^{9}5s^2\ ^2D_{3/2}$	55.2 μs				174 μs	
$4d^{10}6s\ ^2S_{1/2}$	18.9 ns	20.36(71) ns				22(3) ns[(e)]
$4d^{10}6p\ ^2P_{1/2}$	89.7 ns	99(15) ns				95(6) ns[(f)]
$4d^{10}6p\ ^2P_{3/2}$	72.8 ns	65(5) ns				78(5) ns[(f)]
$4d^{10}5d\ ^2D_{3/2}$	11.7 ns	12.06(29) ns				11(3) ns[(e)]
$4d^{10}5d\ ^2D_{5/2}$	12.1 ns	12.48(30) ns				
$4d^{10}7s\ ^2S_{1/2}$	43.5 ns	45.79(65) ns				53(5) ns[(e)]
$4d^{10}7p\ ^2P_{1/2}$	282 ns	279(18) ns				285(25) ns[(g)]
$4d^{10}7p\ ^2P_{3/2}$	241 ns	225(16) ns				255(20) ns[(g)]
$4d^{10}6d\ ^2D_{3/2}$	28.3 ns	28(1) ns				26(4) ns[(e)]
$4d^{10}4f\ ^2F_{5/2}$	68.9 ns	69.89(36) ns				
$4d^{10}4f\ ^2F_{7/2}$	69.0 ns	70.07(34) ns				
$4d^{10}6d\ ^2D_{5/2}$	29.6 ns	30.05(56) ns				
$4d^{10}8s\ ^2S_{1/2}$	87.4 ns	91(2) ns				98(10) ns[(e)]

Notes. Error bars to the FSMRCC values are estimated using the uncertainties of the calculated E1 matrix elements.
[(a)]Chaudhuri & Chattopadhyay (2022); [(b)]Safronova et al. (2003); [(c)]Dzuba et al. (2021); [(d)]Carlsson et al. (1990); [(e)]Jiang et al. (1990); [(f)]Bengtsson et al. (1990); [(g)]Bengtsson et al. (1991)

Table A.5. Recommended weighted oscillator strengths, gf, taken as the mean of the FSMRCC and MCDHF/RCI values, along with estimated uncertainties.

Transition	mean	unc. rel. diff.	unc. QQE	unc. final
$6s_{1/2} \rightarrow 5p_{1/2}$	0.308	AA	A+	A+
$6s_{1/2} \rightarrow 5p_{3/2}$	0.651	AA	A+	A+
$7s_{1/2} \rightarrow 5p_{1/2}$	0.0321	AA	AA	AA
$7s_{1/2} \rightarrow 5p_{3/2}$	0.0613	A+	AA	A+
$7s_{1/2} \rightarrow 6p_{1/2}$	0.584	AA	A+	A+
$7s_{1/2} \rightarrow 6p_{3/2}$	1.214	A+	AA	A+
$8s_{1/2} \rightarrow 5p_{1/2}$	0.0107	AA	A+	A+
$8s_{1/2} \rightarrow 5p_{3/2}$	0.0204	AA	A	A
$8s_{1/2} \rightarrow 6p_{1/2}$	0.0477	B+	B	B
$8s_{1/2} \rightarrow 6p_{3/2}$	0.0887	B+	B+	B+
$8s_{1/2} \rightarrow 7p_{1/2}$	0.872	AA	B+	B+
$8s_{1/2} \rightarrow 7p_{3/2}$	1.796	AA	B+	B+
$5p_{1/2} \rightarrow 5s_{1/2}$	0.464	B	C+	C+
$5p_{3/2} \rightarrow 5s_{1/2}$	0.957	B	C+	C+
$5p_{3/2} \rightarrow 4d^{-1}_{5/2}$	0.000314	–	E	E
$6p_{1/2} \rightarrow 5s_{1/2}$	0.00180	E	E	E
$6p_{1/2} \rightarrow 4d^{-1}_{3/2}$	0.000624	–	E	E
$6p_{1/2} \rightarrow 6s_{1/2}$	0.903	AA	A+	A+
$6p_{3/2} \rightarrow 5s_{1/2}$	0.0350	E	E	E
$6p_{3/2} \rightarrow 4d^{-1}_{5/2}$	0.00281	–	E	E
$6p_{3/2} \rightarrow 4d^{-1}_{3/2}$	0.000147	–	E	E
$6p_{3/2} \rightarrow 6s_{1/2}$	1.820	AA	A+	A+
$7p_{1/2} \rightarrow 5s_{1/2}$	0.0000928	E	E	E
$7p_{1/2} \rightarrow 4d^{-1}_{3/2}$	0.000551	–	E	E
$7p_{1/2} \rightarrow 6s_{1/2}$	0.0227	B	B+	B
$7p_{1/2} \rightarrow 5d_{3/2}$	0.0560	A	A	A
$7p_{1/2} \rightarrow 7s_{1/2}$	1.199	AA	AA	AA
$7p_{3/2} \rightarrow 5s_{1/2}$	0.00141	C	E	E
$7p_{3/2} \rightarrow 4d^{-1}_{5/2}$	0.00196	–	E	E
$7p_{3/2} \rightarrow 4d^{-1}_{3/2}$	0.000127	–	E	E
$7p_{3/2} \rightarrow 6s_{1/2}$	0.0604	B	B+	B
$7p_{3/2} \rightarrow 5d_{3/2}$	0.00860	B+	A	B+
$7p_{3/2} \rightarrow 5d_{5/2}$	0.0811	AA	AA	AA
$7p_{3/2} \rightarrow 7s_{1/2}$	2.400	AA	AA	AA
$4d^{-1}_{3/2} \rightarrow 5p_{1/2}$	0.00353	–	E	E
$4d^{-1}_{3/2} \rightarrow 5p_{3/2}$	0.000563	–	E	E
$5d_{3/2} \rightarrow 5p_{1/2}$	1.114	B+	B+	B+
$5d_{3/2} \rightarrow 5p_{3/2}$	0.236	A	B+	B+
$5d_{3/2} \rightarrow 6p_{1/2}$	0.192	B+	B+	B+
$5d_{3/2} \rightarrow 6p_{3/2}$	0.0201	AA	B	B
$5d_{5/2} \rightarrow 5p_{3/2}$	2.120	B+	B+	B+
$5d_{5/2} \rightarrow 6p_{3/2}$	0.205	B+	B	B
$6d_{3/2} \rightarrow 5p_{1/2}$	0.232	B	B+	B
$6d_{3/2} \rightarrow 5p_{3/2}$	0.0459	B+	B+	B+
$6d_{3/2} \rightarrow 6p_{1/2}$	0.982	A	AA	A
$6d_{3/2} \rightarrow 6p_{3/2}$	0.217	A+	AA	A+
$6d_{3/2} \rightarrow 7p_{1/2}$	0.282	B+	B+	B+
$6d_{3/2} \rightarrow 7p_{3/2}$	0.0276	B	C+	C+
$6d_{5/2} \rightarrow 5p_{3/2}$	0.410	B+	B+	B+
$6d_{5/2} \rightarrow 6p_{3/2}$	1.939	A	AA	A
$6d_{5/2} \rightarrow 7p_{3/2}$	0.280	B	C+	C+
$4f_{5/2} \rightarrow 4d^{-1}_{3/2}$	0.000341	–	A+	A+
$4f_{5/2} \rightarrow 4d^{-1}_{5/2}$	0.0000169	–	B+	B+
$4f_{5/2} \rightarrow 5d_{3/2}$	3.985	A+	AA	A+
$4f_{5/2} \rightarrow 5d_{5/2}$	0.293	B+	AA	B+
$4f_{7/2} \rightarrow 4d^{-1}_{5/2}$	0.000332	–	A	A
$4f_{7/2} \rightarrow 5d_{5/2}$	5.727	A+	AA	A+

Notes. For transitions involving $4d^9 5s^2$, here abbreviated as $4d^{-1}$, the values are from MCDHF/RCI. The uncertainties in column three in terms of the NIST ASD accuracy classes are based the relative differences between the FSMRCC and MCDHF/RCI values and the uncertainties in column four are based on the QQE approach. The final uncertainties, column five, are the worst of column 3 and 4. For transitions involving $4d^9 5s^2$ the QQE approach is used for the uncertainty estimation.