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Atomic data for VUV lines of astrophysical interest in singly ionized rhodium

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ABSTRACT

The first theoretical transition probabilities and oscillator strengths are reported for Rh II lines of astrophysical interest in the VUV region (100–200 nm). They have been obtained through the use of a pseudo-relativistic Hartree–Fock model including core-polarization effects and the accuracy has been estimated to be about 10–15% through a comparison with new experimental lifetimes measured using the time-resolved laser-induced fluorescence technique.

1. Introduction

In astrophysics, there is a growing need for spectroscopic data concerning neutral and lowly ionized heavy atoms ($Z \geq 37$) arising mostly from investigation of the atmospheres of chemically peculiar (CP) stars. Atomic data, such as wavelengths, line intensities, transition probabilities and oscillator strengths, are important for computing the opacity of the stellar matter and, consequently, for building models of the stars. In addition, they are essential for deriving abundances from the equivalent widths or line profiles of the observed lines. In particular, the understanding of the large overabundances of some elements in CP stars related to diffusion processes and magnetic field effects, requires a large number of fundamental radiative paramaters for neutral, singly and doubly ionized heavy elements [1,2].

In stellar nucleosynthesis, a detailed analysis of the *r*- and *s*-processes is not possible without accurate atomic data not only for the prominent stellar lines but also for a huge number of weak absorption features which are now observable on the high resolution spectra available both from ground and space observatories in the whole range of the electomagnetic spectrum [1].

In this context, the determination and accuracy of the spectroscopic data for a large number of heavy atoms and ions is of key importance. Although many are now available from modern experimental techniques or sophisticated theoretical methods, they are still insufficient to meet all the needs of the astrophysical community. This is particularly true for singly ionized rhodium for which no radiative data have been published so far in the literature despite the fact that Rh II lines have been identified in different astrophysical spectra such as the spectra of the HgMn type star χLupi [3], the super-rich mercury star HD 65949, the HgMn star HD 175640 and the peculiar Przybylski's star HD 101065 [4].

In the present paper, we report on new theoretical transition rates for VUV Rh II lines obtained within the framework of the relativistic Hartree–Fock (HFR) approach [5] including core-polarization effects. The reliability of these results has been assessed through a comparison with experimental radiative lifetimes measured for some selected levels using the time-resolved laser-fluorescence technique at the Lund High Power Laser Facility, Sweden.

This work is part of an extensive program of radiative rate measurements and calculations for heavy atoms and ions belonging to the fifth and the sixth rows of the periodic table.

2. Atomic structure calculations

Calculations of energy levels and radiative transition rates in Rh II have been carried out using the relativistic Hartree–Fock (HFR) approach [5] modified to take core-polarization effects into account (see e.g. Refs. [6,7]). This method (HFR + CPOL) has been combined with a least-squares optimization process of the radial parameters in order to reduce the discrepancies between the Hamiltonian eigenvalues and the available experimental energy levels.

The following configurations were explicitly introduced in the calculations: $4d^8 + 4d^7 5s + 4d^7 6s + 4d^7 5d + 4d^7 6d + 4d^6 5s^2 + 4d^6 5p^2 + 4d^6 5d^2 + 4d^6 5s6s + 4d^6 5s5d + 4d^6 5s6d$ and $4d^7 5p + 4d^7 6p + 4d^7 4f + 4d^7 5f + 4d^6 5s5p + 4d^6 5s6p + 4d^6 5p5d + 4d^6 5p6s$

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for the even and odd parities, respectively. This configuration list extends considerably the one considered in the previous theoretical investigation of Rh II due to Shadmi [8] who limited the calculations to the 4d^{8} + 4d^{7}5s + 4d^{6}5s^{2} configurations. The ionic core considered for the core-polarization model potential and the correction to the transition dipole operator was a 4d^{6} Rh IV Mo-like core. The dipole polarizability, α_d, for such a core is 4.79 a$_0$^{3} according to Fraga et al. [9]. We used the HFR mean value $\langle r \rangle$ of the outermost 4d core orbital, 1.52 a$_0$, for the cut-off radius, r_c.

Table 1
Experimental and calculated lifetimes obtained in the present work for five levels within the 4d^{7}(^{4}F)5p configuration of Rh II.

Level	E^a (cm^{-1})	τ_{exp} (ns)	τ_{calc} (ns)
z ^{5}F$_{4}^{\circ}$	56547.3	3.9 ± 0.5	4.4
z ^{5}D$_{4}^{\circ}$	59161.5	3.3 ± 0.2	3.9
z ^{5}G$_{6}^{\circ}$	59702.4	3.0 ± 0.2	3.1
z ^{3}G$_{5}^{\circ}$	62194.4	3.2 ± 0.2	3.5
z ^{3}F$_{4}^{\circ}$	62326.1	2.4 ± 0.2	2.8

[a] From Ref. [10].

Table 2
Transition probabilities and oscillator strengths calculated in the present work for selected Rh II lines in the VUV region between 100 and 200 nm. Only transitions with log gf > −1.0 are given. $X(Y)$ stands for $X \times 10^{Y}$.

λ[a] (nm)	Int.[a]	Lower level[a]		Upper level[a]		log gf	gA (s^{-1})
		E (cm^{-1})	Desig.	E (cm^{-1})	Desig.		
126.216	40	8164.4	a ^{1}D$_{2}$	87394.0	v ^{3}D$_{3}^{\circ}$	−0.55	1.18(9)
128.465	60	0.0	a ^{3}F$_{4}$	77842.8	x ^{3}F$_{4}^{\circ}$	−0.91	5.04(8)
129.174	40	10515.0	a ^{3}P$_{1}$	87930.1	v ^{3}D$_{2}^{\circ}$	−0.68	8.34(8)
129.761	20	10760.8	a ^{3}P$_{0}$	87827.5	v ^{3}D$_{1}^{\circ}$	−0.99	4.01(8)
131.085*		11643.7	a ^{3}P$_{2}$	87930.1	v ^{3}D$_{2}^{\circ}$	−0.81	6.05(8)
131.523	90	0.0	a ^{3}F$_{4}$	76032.4	w ^{3}D$_{3}^{\circ}$	−0.20	2.46(9)
131.636	50	3580.7	a ^{3}F$_{2}$	79547.6	z ^{1}P$_{1}^{\circ}$	−0.86	5.28(8)
131.747	50	2401.3	a ^{3}F$_{3}$	78303.9	x ^{3}F$_{2}^{\circ}$	−0.65	8.59(8)
132.012	40	11643.7	a ^{3}P$_{2}$	87394.0	v ^{3}D$_{3}^{\circ}$	−0.68	7.90(8)
133.830	50	3580.7	a ^{3}F$_{2}$	78303.9	x ^{3}F$_{2}^{\circ}$	−0.72	7.07(8)
134.213	200	0.0	a ^{3}F$_{4}$	74509.8	y ^{3}G$_{5}^{\circ}$	0.10	4.62(9)
134.947	100	2401.3	a ^{3}F$_{3}$	76504.5	x ^{3}G$_{4}^{\circ}$	−0.02	3.50(9)
135.041	50	3580.7	a ^{3}F$_{2}$	77633.0	x ^{3}D$_{1}^{\circ}$	−0.73	6.76(8)
135.110	60	3580.7	a ^{3}F$_{2}$	77595.0	x ^{3}G$_{3}^{\circ}$	−0.29	1.86(9)
135.811	50	2401.3	a ^{3}F$_{3}$	76032.4	w ^{3}D$_{3}^{\circ}$	−0.90	4.52(8)
135.824	40	8164.4	a ^{1}D$_{2}$	81788.9	y ^{1}F$_{3}^{\circ}$	−0.77	6.18(8)
135.860	50	2401.3	a ^{3}F$_{3}$	76007.3	w ^{3}D$_{2}^{\circ}$	−0.41	1.41(9)
136.444	10	2401.3	a ^{3}F$_{3}$	75691.1	x ^{3}D$_{3}^{\circ}$	−0.84	5.24(8)
137.231	80	0.0	a ^{3}F$_{4}$	72870.6	z ^{1}G$_{4}^{\circ}$	−0.41	1.38(9)
138.307	30	0.0	a ^{3}F$_{4}$	72303.7	y ^{3}F$_{3}^{\circ}$	−0.86	4.82(8)
138.962	10	2401.3	a ^{3}F$_{3}$	74364.4	z ^{1}F$_{3}^{\circ}$	−0.93	4.10(8)
139.326	30	8164.4	a ^{1}D$_{2}$	79938.8	y ^{1}D$_{2}^{\circ}$	−0.62	8.18(8)
139.652	30	11643.7	a ^{3}P$_{2}$	83251.4	x ^{3}P$_{1}^{\circ}$	−0.41	1.32(9)
139.718	50	3580.7	a ^{3}F$_{2}$	75152.4	y ^{3}F$_{2}^{\circ}$	−0.44	1.24(9)
139.757	20	8164.4	a ^{1}D$_{2}$	79717.5	z ^{1}D$_{2}^{\circ}$	−0.90	4.29(8)
140.834	90	0.0	a ^{3}F$_{4}$	71005.7	y ^{5}D$_{4}^{\circ}$	−0.25	1.91(9)
141.274[b]	100	2401.3	a ^{3}F$_{3}$	73185.7	y ^{3}D$_{3}^{\circ}$	−0.40	1.34(9)
		3580.7	a ^{3}F$_{2}$	74364.4	z ^{1}F$_{3}^{\circ}$	−0.58	8.74(8)
142.224	80	11643.7	a ^{3}P$_{2}$	81955.0	x ^{3}P$_{2}^{\circ}$	−0.11	2.59(9)
142.573	20	8164.4	a ^{1}D$_{2}$	78303.9	x ^{3}F$_{2}^{\circ}$	−0.93	3.85(8)
144.041	20	10515.0	a ^{3}P$_{1}$	79938.8	y ^{1}D$_{2}^{\circ}$	−0.87	4.33(8)
147.110	100	14855.4	a ^{1}G$_{4}$	82830.7	y ^{1}H$_{5}^{\circ}$	−0.12	2.34(9)
148.091	20	8164.4	a ^{1}D$_{2}$	75691.1	x ^{3}D$_{3}^{\circ}$	−0.98	3.20(8)
148.118	80	11643.7	a ^{3}P$_{2}$	79159.7	x ^{3}F$_{3}^{\circ}$	−0.41	1.17(9)
149.403	40	14855.4	a ^{1}G$_{4}$	81788.9	y ^{1}F$_{3}^{\circ}$	−0.62	7.14(8)
150.074	100	14855.4	a ^{1}G$_{4}$	81488.5	y ^{1}G$_{4}^{\circ}$	0.16	4.31(9)
150.664	50	8164.4	a ^{1}D$_{2}$	74537.8	y ^{3}P$_{1}^{\circ}$	−0.97	3.12(8)
151.059	50	8164.4	a ^{1}D$_{2}$	74364.4	z ^{1}F$_{3}^{\circ}$	−0.94	3.34(8)
151.398	50	10515.0	a ^{3}P$_{1}$	76566.6	x ^{3}D$_{2}^{\circ}$	−0.89	3.72(8)
152.543	50	8164.4	a ^{1}D$_{2}$	73720.1	y ^{3}P$_{2}^{\circ}$	−0.88	3.81(8)
152.909	60	14855.4	a ^{1}G$_{4}$	80254.0	y ^{3}H$_{4}^{\circ}$	−0.92	3.43(8)
153.091	100	0.0	a ^{3}F$_{4}$	65321.2	z ^{3}G$_{3}^{\circ}$	−0.52	8.55(8)
154.274	100	0.0	a ^{3}F$_{4}$	64819.4	z ^{3}D$_{3}^{\circ}$	−0.72	5.31(8)
154.933	50	14855.4	a ^{1}G$_{4}$	79399.3	y ^{3}H$_{5}^{\circ}$	−0.86	3.82(8)
155.510	90	14855.4	a ^{1}G$_{4}$	79159.7	x ^{3}F$_{3}^{\circ}$	−0.83	4.04(8)
157.041	100	2401.3	a ^{3}F$_{3}$	66078.8	z ^{3}D$_{2}^{\circ}$	−0.49	8.70(8)
158.257	90	3580.7	a ^{3}F$_{2}$	66769.7	z ^{3}D$_{1}^{\circ}$	−0.77	4.58(8)
158.400	90	10515.0	a ^{3}P$_{1}$	73646.3	z ^{1}P$_{1}^{\circ}$	−0.59	6.96(8)
159.435	100	11643.7	a ^{3}P$_{2}$	74364.4	z ^{1}F$_{3}^{\circ}$	−0.73	4.93(8)
160.445	500	0.0	a ^{3}F$_{4}$	62326.1	z ^{3}F$_{4}^{\circ}$	−0.36	1.14(9)
162.894	500	3580.7	a ^{3}F$_{2}$	64970.4	z ^{3}F$_{2}^{\circ}$	−0.60	6.32(8)
163.472	200	0.0	a ^{3}F$_{4}$	61173.1	z ^{5}G$_{4}^{\circ}$	−0.96	2.76(8)
163.788	200	2401.3	a ^{3}F$_{3}$	63454.9	z ^{3}F$_{3}^{\circ}$	−0.57	6.72(8)
166.717	20	14855.4	a ^{1}G$_{4}$	74836.2	z ^{1}H$_{5}^{\circ}$	−0.79	3.94(8)
168.041	90	14855.4	a ^{1}G$_{4}$	74364.4	z ^{1}F$_{3}^{\circ}$	−0.99	2.43(8)
170.680	80	14855.4	a ^{1}G$_{4}$	73444.3	y ^{3}G$_{5}^{\circ}$	−0.93	2.70(8)
176.509	80	8164.4	a ^{1}D$_{2}$	64819.4	z ^{3}D$_{3}^{\circ}$	−0.89	2.74(8)
179.974	80	10515.0	a ^{3}P$_{1}$	66078.8	z ^{3}D$_{2}^{\circ}$	−0.89	2.63(8)

* Wavelength deduced from experimental levels from Ref. [10].
[a] From Ref. [10]. Note that some strong Rh II lines were also reported in Ref. [14].
[b] Blend.

In addition, the calculated eigenvalues of the Hamiltonian were adjusted to the experimental energy levels from Ref. [10]. For the $4d^8$, $4d^7 5s$ and $4d^7 5p$ configurations, the average energies (E_{av}), the electrostatic direct (F^k) and exchange (G^k) integrals, the spin–orbit (ζ_{nl}) and the effective interaction (α) parameters were allowed to vary during the fitting process. Further more, an additional effective operator (β) for the $4d^7 5s$ configuration was included in the adjustment. All other Slater integrals were scaled down by a factor 0.85 following a well-established procedure [5]. The standard deviations of the fits were 50 cm^{-1} for the even parity and 111 cm^{-1} for the odd parity. Note that the even level at 35012.0 cm^{-1} had to be excluded from the fit because its designation as $4d^7(^2P)5s\ b^3P_0$ given in Ref. [10] appeared questionable. Our HFR predicted eigenvalue for this state was found to be more than 1000 cm^{-1} above the experimental value.

3. Radiative lifetime measurements

In order to assess the accuracy of the calculations, comparisons with experimental results have been performed. Radiative lifetimes for some selected Rh II levels have been measured using the time-resolved laser-induced fluorescence technique applied to a laser-produced plasma. The experimental setup used in the present experiment is the same as the one described in many previous papers (e.g. Refs. [11–13]). Consequently, only a brief description will be given here.

Two Q-switched Nd:YAG lasers were used in our experiment. One of them (Continuum Surelite), characterized by a 10 ns duration and a 2–10 mJ pulse energy at 532 nm, was used as an ablation laser focused on a pure rhodium foil rotating in a 10^{-5}–10^{-6} mbar vacuum chamber and to produce a plasma containing Rh^+ ions. The second Nd:YAG laser (Continuum NY-82) is an injection seeded laser and provides 8 ns pulse duration and 400 mJ pulse energy at 532 nm. The laser beam was compressed to about 1–2 ns by a stimulated Brillouin scattering (SBS) compressor. These pulses were used to pump a dye laser (Continuum Nd-60) operating with a DCM dye. We used a KDP crystal and Raman shifting in a H_2 cell to extend the tunable range of the laser radiation. The excitation pulse was sent horizontally into the vacuum chamber to interact with the plume about 10 mm above the foil. The ablation and the excitation pulses were synchronized by external triggering from a digital delay generator. The emitted fluoresence light was collected by a fused-silica lens, filtered by a 1/8 m monochromator and finally detected by a PMT microchannel plate (Hamamatsu R 1564) with a rise time of 160 ps. The excitation laser pulse was detected separately by a fast photodiode. Both signals were then recorded and averaged over 1000 pulses by a transient digitizer and transferred to a computer for the lifetime evaluations. The computer code DECFIT was used to analyze the fluorescence signals. Radiative lifetimes are extracted by a weighted least-squares fit of a single exponential decay convoluted with the shape of the laser pulse to the fluorescence signal. In addition, a polynomial background representation can be added in the fit.

During the experiment, about 10 curves were recorded for each level under different experimental conditions in order to minimize systematic errors and the averaged lifetime value was adopted as the final result.

4. Results and discussion

In Table 1, we present the experimental radiative lifetimes measured in the present work for 5 levels belonging to five different terms within the $4d^7(^4F)5p$ configuration, i.e. z $^5F^\circ$, z $^5D^\circ$, z $^5G^\circ$, z $^3G^\circ$ and z $^3F^\circ$. These values are compared with the theoretical results obtained using the HFR + CPOL model. As shown in this table, the over-all agreement between theory and experiment is very good. However, the HFR + CPOL results seem to be systematically 5–15% longer than the measurements.

Calculated oscillator strengths ($\log gf$) and transition probabilities (gA) for Rh II lines in the VUV spectral region between 100 and 200 nm are reported in Table 2. Due to the large number of computed transitions in the present study, this table is restricted to the transitions with $\log gf \geq -1.0$. The complete table is available upon request to the authors. Based on the comparison between experimental and theoretical lifetimes in Table 1, we expect an accuracy of 10–15% for the new oscillator strengths and transition probabilities at least for the strongest transitions and for the transitions not affected by cancellation effects reported in Table 2.

The present work will be extended to Rh II lines in the near UV and visible in a further paper.

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