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Atomic data for radioactive elements Ra I, Ra II, Ac I and Ac II and application to their detection in HD 101065 and HR 465⋆

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ABSTRACT

Radiative data for transitions of astrophysical interest in radioactive elements Ra I, Ra II, Ac I and Ac II have been computed using a semi-empirical relativistic Hartree-Fock approach including core polarization effects. Most of the oscillator strengths reported in the present paper are new. A possible detection of radium (Ra II) and actinium (Ac II) in the spectrum of the stars HD 101065 and HR 465 is examined and discussed.

Key words. atomic data – stars: chemically peculiar

1. Introduction

In astrophysics, the first detection of short-lived radioactive elements in stellar atmospheres was made by Merrill (1952) who identified Tc I lines in the spectra of S-type stars. A few years later, Przybylski (1961) discovered a star (HD 101065) with properties that placed it far outside of the known limits of the stellar peculiarities. More precisely, Cowley et al. (2000) performed abundance determination of this star for 54 elements and found that lanthanides were overabundant by 4–5 dex. The overabundance of thorium and uranium was also reported in the same paper while Cowley (2003) and Cowley et al. (2004) confirmed with a high degree of confidence the presence of lines of radioactive technetium and promethium. In addition, Gopka et al. (2004) presented the results on new identification of the lines of all radioactive elements with atomic numbers from $Z = 84$ to $Z = 99$, except for $Z = 85$ (At) and $Z = 87$ (Fr). The presence of these heavy short-lived radioactive elements in Przybylski's star is enigmatic. Cowley et al. (2004) proposed that some unrecognized processes, such as flare activities, were taking place in the atmosphere of the star. On the other hand, Gopka et al. (2004) suggested that the presence of elements with $Z < 92$ is due to the natural radioactive decay of thorium and uranium in the upper atmosphere while the existence of elements with $Z > 92$ could be due to neutron capture in the stratified layers of the atmosphere with large overabundance of thorium and uranium. A discussion about possible explanation for the existence of short-lived radioactive elements in stellar atmospheres can also be found in Goriely & Arnould (2001), Gopka et al. (2006) and Yushchenko et al. (2006, 2007). In a recent paper, Goriely (2007) has stressed the importance of spallation nucleosynthesis compared to diffusion processes as a possible explanation of the peculiar abundances spectroscopically determined at the surface of HD 101065. Although it remains difficult to disentangle the effect of both processes theoretically, this conclusion does not necessarily reduce the role of the diffusion processes which have proven to be of first importance to understand the atmosphere of CP stars. As stressed by Goriely (2007), "*the contribution of the nuclear process would be greatly strengthened if spectroscopic observation could confirm the presence of short-lived radioelements at the surface of CP stars and, if confirmed, hopefully in a close future provide abundance determination for these clear tracers of nuclear activity*". Unfortunately, for most of the 72 lines of radioactive elements listed by Gopka et al. (2004) in the spectrum of HD 101065, oscillator strengths are not known. As a first attempt to fill in this gap, we report in the present paper atomic structure calculations for transitions of astrophysical interest in Ra I, Ra II ($Z = 88$), Ac I and Ac II ($Z = 89$).

2. Available atomic data

According to the NIST compilation (Moore 1971), very few energy levels are known in Ra I. In fact, 13 even- and 28 odd-parity levels have been identified by Rasmussen (1934a) with the revisions suggested by Russel (1934) on the basis of the comparison of Ra I with the analogous Be I, Mg I, Ca I, Sr I and Ba I spectra. These levels were established from 69 classified lines from 2955.65 Å to 9932.21 Å and interpreted as belonging to the $7s^2$, 7s7p, 7s6d, 7s8s, 6d7p, 7s8p, $7p^2$, 7s7d, 7s9s, 7s5f, 7s6f, 7s7f and 7s8f configurations. In Ra II, Rasmussen (1933, 1934b) classified 64 lines between 1888.7 Å and 9453.57 Å, from a hollow-cathode source and stressed the similarity of this spectrum with the Ba II one. This gave rise to well-established ns ($n = 7$–11), np ($n = 7$–9), nd ($n = 6$–12), nf ($n = 5$–7) and ng ($n = 5$–11) Rydberg series.

For Ac I and Ac II, the energy levels reported in the NIST compilation (Moore 1971) are based on the observation of the emission spectrum of actinium due to Meggers et al. (1957) who analyzed arc and hollow-cathode spectrograms made at

⋆ Tables 1–4 are only available in electronic form at http://www.aanda.org

the Argonne National Laboratory by Fred et al. (1955). In these spectra, 87 Ac I lines, with wavelengths ranging from 2968.82 Å to 7866.10 Å, were classified as combinations among 6 even and 34 odd energy levels while 226 Ac II lines, with wavelelengths from 2261.75 Å to 7886.82 Å, were classified as combinations of 27 even and 38 odd levels. These levels were interpreted as belonging to the $6d7s^2$, $6d^27s$, $7s^27p$, $6d7s7p$, $6d^27p$ configurations (Ac I) and to the $7s^2$, 7s6d, $6d^2$, 7s7p, 6d7p, 7s5f, 7s8s and 5f7p configurations (Ac II).

In a more recent compilation on actinide elements due to Blaise & Wyart (1992), the spectrum of Ac I was not reanalyzed. For Ac II, however, the energy levels from the early analysis by Meggers et al. (1957) were reinvestigated by the parametric Slater-Condon method which led to a few changes in the theoretical assignments. The studied configurations were $7s^2 + 6d^2 + 6d7s + 5f^2 + 5f7p$ and 5f6d + 5f7s + 6d7p + 7s7p, respectively. This led to reject the two levels 5f7p $^3G_5$ and 6d5f $^3H^\circ_5$ reported in the NIST compilation (Moore 1971) and to find four new even levels between 56 491 and 64 285 cm^{-1} from the 80 lines which remained unclassified after the analysis by Meggers et al. (1957).

Available transition rates and lifetime values in neutral and singly ionized radium and actinium are very sparse.

In the case of Ra I, oscillator strengths were calculated for the $7s^2$–7s7p transitions using the relativistic pseudo-potential approach (Hafner & Schwarz 1978), the multiconfiguration Dirac-Fock method (Bruneau 1984) and the relativistic local spin density functional (Sen & Puri 1989a). More recently, the multiconfiguration Dirac-Hartree-Fock model was employed to compute oscillator strengths for the $7s^2\ ^1S_0$–$7s7p\ ^1P^\circ_1$ electric dipole and the $7s^2\ ^1S_0$–$7s6d\ ^3D_2$ electric quadrupole transitions (Bieron et al. 2004) while relativistic Hartree-Fock method (Dzuba et al. 2000) and many-body perturbation theory (Dzuba & Ginges 2006) were used to compute transition probabilities for lines connecting the low-lying states belonging to the $7s^2$, 7s7p and 7s6d configurations. The lifetime of the $7s7p\ ^3P^\circ_1$ level was experimentally determined by Scielzo et al. (2006) by measuring the exponential decay of fluorescence after illuminating a thermal atomic beam with pulses of laser light.

For Ra II, the only attempts to obtain radiative data are due to Lindgård & Nielsen (1977), who considered a simple Coulomb approximation and to Sen & Puri (1989b), Glushkov (1991) and Glushkov et al. (1996), who used essentially model-potential approaches. In one recent work (Biémont et al. 2004), oscillator strengths were computed for the first ions along the francium isoelectronic sequence, including Ra II, using the pseudo-relativistic Hartree-Fock and the fully relativistic Dirac-Fock methods.

In the case of actinium, the only available results were obtained by Sen & Puri (1989a) who used the relativistic spin density functional approach to compute oscillator strengths for the $7s^2$–7s7p transition array in Ac II. However, to our knowledge, no transition rates were published for Ac I.

3. Energy levels

For heavy neutral and lowly ionized atoms such as those considered in the present work, accurate calculations of atomic structure should allow for both intravalence and core-valence correlation. In addition relativistic effects must normally play an important role. A method which has appeared as a suitable compromise between a gratifying accuracy of the results (tested by comparison with accurate laser lifetime measurements), the moderate complexity of the codes used and the ability to obtain many new results in a limited period of time, is the relativistic Hartree-Fock (HFR) technique as described by Cowan (1981) but modified by us for the inclusion of core-polarization (CPOL) effects. In this approach (HFR+CPOL), most of the intravalence correlation is represented within a configuration interaction scheme while core-valence correlation is described by a core-polarization model potential and a correction to the dipole operator depending upon two parameters, i.e. the dipole polarizability of the ionic core, α_d, and the cut-off radius, r_c (for details see e.g. Quinet et al. 1999). Although based on the Schrödinger equation, this method takes the most important relativistic effects, such as the mass-velocity contribution and the Darwin correction, into account.

3.1. Ra I

We have introduced in the model explicit intravalence interactions between the configurations $7s^2 + 7s8s + 7s9s + 7s6d + 7s7d + 7s8d + 7s9d + 6d8s + 6d9s + 6d7d + 6d8d + 6d9d + 6d^2 + 7p^2 + 7d^2 + 5f^2 + 5f7p + 5f8p + 5f9p + 5f6f + 5f7f + 5f8f + 5f9f$ (for the even parity) and $7s7p + 7s8p + 7s9p + 7s5f + 7s6f + 7s7f + 7s8f + 7s9f + 6d7p + 6d8p + 6d9p + 7p7d + 7p8d + 7p9d + 7p8s + 7p9s + 6d5f + 6d6f + 6d7f + 6d8f + 6d9f + 5f7d + 5f8d + 5f9d + 5f8s + 5f9s$ (for the odd parity). Core-polarization effects were included using the dipole polarizability, α_d, equal to 18.62 a_0^3, as tabulated by Fraga et al. (1976) for the ionic core Ra^{2+} while the cut-off radius, r_c, was chosen to be equal to 2.07 a_0 which corresponds to the expectation value of r for the outermost core orbital ($6p^6$) as calculated with Cowan's codes. The HFR+CPOL method was combined with a least-squares optimization routine minimizing the discrepancies between calculated and experimental energy levels compiled by Moore (1971). More precisely, for the even parity, the average energies, E_{av}, the exchange Slater integrals, G^2(s,d), and the spin-orbit parameters, ζ_d, corresponding to the 7s6d and 7s7d configurations were adjusted while only the average energies of $7s^2$, 7s8s, 7s9s and $6d^2$ were optimized. It should be noted here that the average energy parameter of $6d^2$ was fitted instead of the one corresponding to $7p^2$ because the three energy levels (at 31248.84, 32214.84 and 32941.13 cm^{-1}) identified in the NIST compilation (Moore 1971) as belonging to $7p^2$ were predicted, in our calculations, as mainly belonging to $6d^2$, the $7p^2$ configuration appearing a few thousands of cm^{-1} above (around 37 000 cm^{-1}). This prediction is confirmed when comparing Ra I with the analogous Ba I spectrum in which the $6p^2$ configuration is situated ~10 000 cm^{-1} above $5d^2$. For the odd parity, all the radial parameters (E_{av}, F^k, G^k, ζ_{nl}) corresponding to the 7s7p, 7s8p and 6d7p configurations were adjusted while only average energies were fitted for 7s5f, 7s6f, 7s7f and 7s8f configurations. The standard deviations, as defined by Cowan (1981) were found to be equal to 194 cm^{-1} for the even parity (13 levels and 10 variable parameters) and 260 cm^{-1} for the odd parity (28 levels and 16 adjustable parameters).

3.2. Ra II

The physical HFR+CPOL model used here was exactly the same as the one described in our previous paper related to Fr-like ions Ra II, Ac III, Th IV and U VI (Biémont et al. 2004). In this model, all the ns, np, nd, nf, ng and nh configurations up to $n = 12$ were included while core-polarization corrections were considered with $\alpha_d = 18.62\ a_0^3$ and $r_c = 2.07\ a_0$. The semi-empirical process was then performed using all the experimental

energy levels taken from the NIST compilation (Moore 1971). More precisely, the average energies (E_{av}) and the spin-orbit parameters (ζ_{nl}) were adjusted to reproduce exactly the doublet energy levels belonging to the ns (n = 7–12), np (n = 7–9), nd (n = 6–12), nf (n = 5–7) and ng (n = 5–11) configurations.

3.3. Ac I

For this atom, intravalence correlation was considered by means of the inclusion of the following configurations in the HFR model : $6d7s^2 + 6d^27s + 6d^28s + 6d^3 + 6d^27d + 7s^27d + 7s^28s + 6d7p^2 + 7s7p^2 + 7p^27d + 7p^28s + 5f6d7p + 5f6d8p + 5f7s7p + 5f7s8p + 5f7p7d + 5f7p8s + 6d7s7d + 6d7s8s + 6d7p8p + 6d7d8s + 7s7p8p + 7s7d8s$ (even parity) and $7s^27p + 7s^28p + 7p^3 + 5f6d^2 + 6d^27p + 6d^28p + 5f7s^2 + 5f7p^2 + 7p^28p + 5f6d7s + 5f6d8s + 5f6d7d + 5f7s7d + 5f7s8s + 5f7p8p + 6d7s7p + 6d7s8p + 6d7p7d + 6d7p8s + 6d7d8p + 6d8s8p + 7s7p7d + 7s7p8s + 7s7d8p + 7s8s8p$ (odd parity). Core-polarization effects were considered with the dipole polarizability tabulated by Fraga et al. (1976) for the Ac^{3+} ion, i.e. $\alpha_d = 13.50\ a_0^3$, and the cut-off radius taken from Cowan's code as the expectation value of r for the $6p^6$ orbital in actinium, i.e. $r_c = 1.97\ a_0$. For the even parity, the six experimental energy levels belonging to the $6d7s^2\ ^2D$ and $6d^2(^3F)7s\ ^4F$ multiplets tabulated by Blaise & Wyart (1992) allowed us to adjust the average energies and spin-orbit parameters corresponding to these configurations. Unfortunately, for the odd parity, despite the fact that all but two energy levels of the 6d7s7p configuration are reported in Blaise & Wyart's compilation, we were unable to obtain a reasonable fit by adjusting the corresponding radial parameters. More precisely, when adjusting all the radial parameters (average energy, spin-orbit parameters and electrostatic integrals) corresponding to 6d7s7p, the average deviation between calculated and experimental energy levels was found to be equal to 853 cm^{-1}, this value being only reduced to 826 cm^{-1} when introducing the "illegal-k" effective operators (Cowan 1981). This could be due to the fact that one or several experimental energies are affected by large uncertainties. Another reason could be that the $6d^27p$ configuration, which is expected to interact strongly with some 6d7s7p levels, is unsufficiently known to allow a simultaneous adjustment of all parameters, including configuration interaction integrals, corresponding to both configurations. Other low-lying configurations such as $7s^27p$, $7s^28p$, $5f7s^2$ could also play a role. Although included in our physical model, the fact that these latter configurations are completely unknown experimentally could explain the poor quality of the fitting process. Consequently, in the present work, only average energies were adjusted for 6d7s7p and $6d^27p$ configurations. However, in order to optimize the final results, the theoretical transition energies were replaced by experimental values when computing the oscillator strengths.

3.4. Ac II

The Ac II ion belongs to the radium isoelectronic sequence. Consequently, the same set of interacting configurations as the one used for Ra I was explicitly included in the physical model. For the core-polarization parameters, we used the same values as for Ac I, i.e. $\alpha_d = 13.50\ a_0^3$ and $r_c = 1.97\ a_0$. The semi-empirical procedure was applied to the $7s^2$, 7s8s, 7s6d, $6d^2$ even configurations and to the 7s7p, 7s5f, 6d7p, 6d5f odd configurations for which all the corresponding radial parameters were adjusted using the experimental level energies tabulated by Blaise & Wyart (1992). In addition, in order to reduce as much as possible the discrepancies between calculated and experimental energy levels, an effective interaction parameter α (Trees 1951a,b; Racah 1952) associated to the $6d^2$ configuration was considered in the fitting process while the generalized Slater integrals R^k corresponding to the configuration interactions between 6d7p and 7s5f, on the one hand, and between 6d7p and 7s7p, on the other hand, were also adjusted. It is worth noting that the new spectroscopic designations of some levels proposed by Blaise & Wyart (1992) compared to the previous analysis due to Meggers et al. (1957) were confirmed in the present work. Although some levels belonging to 5f7p are known experimentally, we preferred not to include those levels in the fitting procedure because, according to our calculations, they are situated in a region (from ~55 000 to ~65 000 cm^{-1}) where many levels of unknown configurations such as $7p^2$, 6d8s, 6d7d and 7s7d appear. The standard deviations were found to be equal to 179 cm^{-1} for the even parity (15 levels and 10 variable parameters) and 280 cm^{-1} for the odd parity (38 levels and 22 adjustable parameters).

The computed energies, Landé g-factors and eigenvector compositions as obtained in the present work for low-lying levels in Ra I, Ra II, Ac I and Ac II are reported in Tables 1–4 together with the available experimental data.

Table 5. Oscillator strengths for transitions in Ra I.

λ(Å)[a]	Int[a]	E_l (cm^{-1})	J_l	E_u (cm^{-1})	J_u	log gf
4825.91	1000	0.00 (*e*)	0	20 715.71 (*o*)	1	0.31
5400.23	200	13 993.97 (*e*)	2	32 506.59 (*o*)	2	–0.13
5406.81	200	14 707.35 (*e*)	3	33 197.46 (*o*)	3	0.11
5555.85	200	13 999.38 (*o*)	1	31 993.41 (*e*)	2	0.00
5660.81	500	14 707.35 (*e*)	3	32 367.78 (*o*)	4	0.40
6200.30	300	13 993.97 (*e*)	2	30 117.78 (*o*)	3	0.17
6446.20	200	16 688.54 (*o*)	2	32 197.28 (*e*)	3	0.19
6487.32	200	14 707.35 (*e*)	3	30 117.78 (*o*)	3	–0.36
6980.22	200	13 715.85 (*e*)	1	28 038.05 (*o*)	2	–0.10
7118.50	200	13 993.97 (*e*)	2	28 038.05 (*o*)	2	–0.38
7141.21	500	0.00 (*e*)	0	13 999.38 (*o*)	1	–1.08
7225.16	200	17 081.45 (*e*)	2	30 918.14 (*o*)	2	0.20
7838.12	200	13 999.38 (*o*)	1	26 754.05 (*e*)	1	–0.16

[a] From Sansonetti & Martin (2005) (see also `http://physics.nist.gov/PhysRevData/Handbook/Tables/radiumtable2.htm`).

Table 6. Oscillator strengths for transitions in Ra II.

λ(Å)[a]	Int[a]	E_l (cm^{-1})	J_l	E_u (cm^{-1})	J_u	log gf
2708.96	100	12 084.38 (*e*)	3/2	48 987.98 (*o*)	5/2	0.24
2813.76	150	13 743.11 (*e*)	5/2	49 272.31 (*o*)	7/2	0.38
3649.55	500	21 351.20 (*o*)	1/2	48 744.04 (*e*)	3/2	0.30
3814.42	1000	0.00 (*e*)	1/2	26 208.86 (*o*)	3/2	0.19
4340.64	500	26 208.86 (*o*)	3/2	49 240.48 (*e*)	5/2	0.48
4436.27	100	26 208.86 (*o*)	3/2	48 744.04 (*e*)	3/2	–0.48
4533.11	150	21 351.20 (*o*)	1/2	43 405.01 (*e*)	1/2	–0.23
4682.28	500	0.00 (*e*)	1/2	21 351.20 (*o*)	1/2	–0.20
5813.63	100	26 208.86 (*o*)	3/2	43 405.01 (*e*)	1/2	–0.04
8019.70	250	13 743.11 (*e*)	5/2	26 208.86 (*o*)	3/2	–0.12

[a] From Sansonetti & Martin (2005) (see also `http://physics.nist.gov/PhysRevData/Handbook/Tables/radiumtable2.htm`)

4. Radiative rates and lifetimes

Oscillator strengths obtained in the present work are reported in Tables 5–8 for selected transitions of Ra I, Ra II,

Table 7. Oscillator strengths for transitions in Ac I.

λ(Å)[a]	Int[a]	E_l (cm^{-1})	J_l	E_u (cm^{-1})	J_u	log gf
3885.56	400	0.00 (e)	3/2	25 729.03 (*o*)	1/2	0.15
4034.63	200	2231.43 (e)	5/2	27 009.84 (*o*)	3/2	–0.15
4063.10	200	2231.43 (e)	5/2	26 836.20 (*o*)	5/2	0.51
4179.98	1000	0.00 (e)	3/2	23 916.84 (*o*)	5/2	0.14
4183.12	500	0.00 (e)	3/2	23 898.86 (*o*)	5/2	–0.28
4194.40	400	2231.43 (e)	5/2	26 066.04 (*o*)	3/2	–0.72
4384.53	300	0.00 (e)	3/2	22 801.10 (*o*)	3/2	–1.46
4396.71	400	2231.43 (e)	5/2	24 969.30 (*o*)	7/2	–1.82
4462.73	400	0.00 (e)	3/2	22 401.52 (*o*)	1/2	–2.92
4613.93	300	2231.43 (e)	5/2	23 898.86 (*o*)	5/2	–1.24
4705.78	200	2231.43 (e)	5/2	23 475.94 (*o*)	7/2	–1.56
4716.58	500	0.00 (e)	3/2	21 195.87 (*o*)	5/2	–1.37
5258.24	300	0.00 (e)	3/2	19 012.46 (*o*)	3/2	–0.41
5569.26	200	0.00 (e)	3/2	17 950.71 (*o*)	5/2	–1.29
6359.86	300	2231.43 (e)	5/2	17 950.71 (*o*)	5/2	–0.98
6691.27	200	0.00 (e)	3/2	14 940.72 (*o*)	5/2	–0.93
7290.40	300	0.00 (e)	3/2	13 712.90 (*o*)	3/2	–1.18
7866.10	200	2231.43 (e)	5/2	14 940.72 (*o*)	5/2	–1.24

[a] From Sansonetti & Martin (2005) (see also `http://physics.nist.gov/PhysRevData/Handbook/Tables/actiniumtable2.htm`).

Table 8. Oscillator strengths for transitions in Ac II.

λ (Å)[a]	Int[a]	E_l (cm^{-1})	J_l	E_u (cm^{-1})	J_u	log gf
2847.16	100	9087.54 (*e*)	2	44 199.94 (*o*)	1	–0.07
2994.17	130	0.00 (*e*)	0	33 388.61 (*o*)	1	–0.21
3043.30	300	9087.54 (*e*)	2	41 937.05 (*o*)	3	0.19
3069.36	130	13 236.46 (*e*)	2	45 807.06 (*o*)	3	–0.17
3112.83	130	4739.63 (*e*)	1	36 855.50 (*o*)	1	–0.31
3153.09	300	5267.16 (*e*)	2	36 972.94 (*o*)	3	0.29
3154.41	300	7426.52 (*e*)	3	39 119.02 (*o*)	4	–0.93
3164.81	150	5267.16 (*e*)	2	36 855.50 (*o*)	1	–0.13
3230.59	130	7426.52 (*e*)	3	38 371.64 (*o*)	2	0.10
3260.91	300	4739.63 (*e*)	1	35 397.12 (*o*)	2	0.14
3383.53	130	7426.52 (*e*)	3	36 972.94 (*o*)	3	–1.17
3413.84	130	9087.54 (*e*)	2	38 371.64 (*o*)	2	–0.24
3417.77	200	0.00 (*e*)	0	29 250.40 (*o*)	1	–0.19
3481.16	300	7426.52 (*e*)	3	36 144.35 (*o*)	3	0.30
3489.53	130	4739.63 (*e*)	1	33 388.61 (*o*)	1	–0.21
3554.99	130	5267.16 (*e*)	2	33 388.61 (*o*)	1	–0.91
3565.59	700	5267.16 (*e*)	2	33 304.96 (*o*)	2	–0.19
3756.67	150	5267.16 (*e*)	2	31 878.87 (*o*)	2	–0.23
3799.82	70	9087.54 (*e*)	2	35 397.12 (*o*)	2	–0.76
3863.12	700	7426.52 (*e*)	3	33 304.96 (*o*)	2	–0.08
4061.60	150	5267.16 (*e*)	2	29 881.09 (*o*)	3	–0.47
4088.44	1000	7426.52 (*e*)	3	31 878.87 (*o*)	2	–1.02
4168.40	700	5267.16 (*e*)	2	29 250.40 (*o*)	1	–0.46
4209.69	100	7426.52 (*e*)	3	31 174.60 (*o*)	3	–0.49
4359.13	130	5267.16 (*e*)	2	28 201.11 (*o*)	2	–0.44
4386.41	500	9087.54 (*e*)	2	31 878.87 (*o*)	2	0.08
4507.20	700	0.00 (*e*)	0	22 180.52 (*o*)	1	–1.04
4605.45	300	4739.63 (*e*)	1	26 446.96 (*o*)	2	–1.66
4720.16	300	5267.16 (*e*)	2	26 446.96 (*o*)	2	–1.14
4812.22	200	7426.52 (*e*)	3	28 201.11 (*o*)	2	–3.07*
5732.05	70	4739.63 (*e*)	1	22 180.52 (*o*)	1	–0.93
5758.97	130	9087.54 (*e*)	2	26 446.96 (*o*)	2	–1.37
5910.85	300	5267.16 (*e*)	2	22 180.52 (*o*)	1	–0.60
6164.75	200	4739.63 (*e*)	1	20 956.40 (*o*)	0	–0.85
6167.83	30	16 756.90 (*e*)	4	32 965.55 (*o*)	4	–0.50
6242.83	100	13 236.46 (*e*)	2	29 250.40 (*o*)	1	–0.58

[a] From Sansonetti & Martin (2005) (see also `http://physics.nist.gov/PhysRevData/Handbook/Tables/actiniumtable2.htm`).
* Affected by severe cancellation effects.

Ac I and Ac II, respectively. For most of these transitions, listed as strong lines by Sansonetti & Martin (2005), radiative data are reported for the first time (see also `http://physics.nist.gov/PhysRevData/Handbook/Tables/radiumtable2.htm` and `http://physics.nist.gov/PhysRevData/Handbook/Tables/actiniumtable2.htm`).

For Ra I, a comparison between radiative lifetimes deduced from our calculations and available results is shown in Table 9. With the exception of the 6d7s ^{1}D$_2$ level (E = 17 081.45 cm^{-1}), for which our computed transition probabilities are affected by large cancellation effects, a good agreement (5–20%) is observed between the values calculated in the present work and the recent ones obtained by Dzuba & Ginges (2006) using the many-body perturbation theory. For the 7s7p ^{3}P$^\circ_1$ level, our calculated lifetime (τ = 281 ns) is ∼30% shorter than the experimental measurement due to Scielzo et al. (2006). In order to see whether this difference could be due to an underestimation of core-polarization effects included in our theoretical model, we have performed semi-empirical HFR calculations including explicitly core-valence correlations by means of additional configurations with one hole in the 6s or 6p subshell, instead of considering the core-polarization potential. More precisely, the following configurations were added to the ones considered in the physical model presented in Sect. 3.1.: 6s^{2}6p^{5}7p^3 + 6s^{2}6p^{5}6d^{2}7p + 6s^{2}6p^{5}7s^{2}7p + 6s^{2}6p^{5}6d7s7p + 6s6p^{6}6d^3 + 6s6p^{6}6d^{2}7s + 6s6p^{6}6d7s^2 + 6s6p^{6}6d7p^2 + 6s6p^{6}7s7p^2 (even parity) and 6s^{2}6p^{5}6d^3 + 6s^{2}6p^{5}6d^{2}7s + 6s^{2}6p^{5}6d7s^2 + 6s^{2}6p^{5}6d7p^2 + 6s^{2}6p^{5}7s7p^2 + 6s6p^{6}7p^3 + 6s6p^{6}6d^{2}7p + 6s6p^{6}7s^{2}7p + 6s6p^{6}6d7s7p (odd parity). Using this model, the calculated lifetime for the 7s7p ^{3}P$^\circ_1$ level was found to be equal to 250 ns, i.e. ∼10% shorter than our HFR+CPOL calculation and ∼40% shorter than the measurement due to Scielzo et al. (2006). This indicates that core-polarization corrections were not underestimated in our HFR+CPOL model, having in mind that HFR calculations without core-polarization gave a lifetime value of 215 ns. It was also verified that, for the levels at 13 715.85, 13 999.38, 16 688.54, 17 081.45 and 20 715.71 cm^{-1}, the magnetic dipole (M1) and electric quadrupole (E2) contributions were negligible.

For Ra II, a comparison between our oscillator strengths and previous results was already presented in our recent paper related to Fr-like ions (Biémont et al. 2004). In that paper, we pointed out that our multiplet f-values were 25% lower than the results obtained for the 7s–7p transition by Sen & Puri (1989b) using the quasi-relativistic local spin density functional approach. However, the results obtained in our work were considered to be more reliable than those published by Sen & Puri in view of the excellent agreement observed between the accurate lifetimes measured by Zhao et al. (1997) and Simsarian et al. (1998) for the levels 7p$_{1/2}$ and 7p$_{3/2}$ in the isoelectronic francium atom and our calculations performed using exactly the same model as the one used for Ra II (Biémont et al. 1998). It was also shown in Biémont et al. (2004) that our results were in reasonable agreement with those of Lindgård & Nielsen (1977), Glushkov (1991) and Glushkov et al. (1996), using the Coulomb approximation and a model potential method, respectively, for the 7s–7p, 7p–8s, 8s–8p, 6d–7p, 7p–7d and 7d–8p transition arrays in singly ionized radium. Very recently, the 7s–7p electric dipole

Table 9. Comparison of lifetimes of low-lying states of Ra I.

Level	E (cm^{-1})	Type	This work	MBPT[a]	MCDHF[b]	RHF[c]	MCDF[d]	RPP[e]	EXP[f]
6d7s ^{3}D$_1$	13 715.85	E1	694 μ s	654 μ s		617 μ s			
6d7s ^{3}D$_2$	13 993.97	E2	3.0 s	3.3 s	4 s	15 s			
7s7p ^{3}P$_1^\circ$	13 999.38	E1	281 ns	362 ns		505 ns	250 ns	420 ns	422(20) ns
7s7p ^{3}P$_2^\circ$	16 688.54	E1	6.4 μ s	5.55 μ s		5.2 μ s			
6d7s ^{1}D$_2$	17 081.45	E1	-*	129 μ s		38 ms			
7s7p ^{1}P$_1^\circ$	20 715.71	E1	5.2 ns	5.53 ns		5.5 ns			

[a] Many-body perturbation theory (Dzuba & Ginges 2006). [b] Multiconfiguration Dirac-Hartree-Fock (Bieron et al. 2004). [c] Relativistic Hartree-Fock (Dzuba et al. 2000). [d] Multiconfiguration Dirac-Fock (Bruneau 1984). [e] Relativistic pseudo-potential (Hafner & Schwarz 1978). [f] Experiment (Scielzo et al. 2006). * Affected by severe cancellation effects.

and 7s–6d electric quadrupole matrix elements in Ra$^+$ were evaluated by Safronova (2007) using a relativistic coupled-cluster method in which single, double and partial triple excitations of Dirac-Fock wavefunctions were included to all orders of perturbation theory. The theoretical lifetimes taken from this study for 7p$_{1/2}$ (τ = 8.94 ns), 7p$_{3/2}$ (τ = 4.84 ns), 6d$_{3/2}$ (τ = 0.669 s) and 6d$_{5/2}$ (τ = 0.334 s) are in excellent agreement (within a few percents) with the values deduced from the present work, i.e. τ = 9.48 ns, 4.97 ns, 0.611 s and 0.316 s, respectively.

In the case of actinium, the only available result for comparison is the one published by Sen & Puri (1989a) for the 7s^2 ^{1}S$_0$–7s7p ^{1}P$_1^\circ$ transition in Ac II. The oscillator strength computed by these authors ($\log gf$ = 0.45) is considerably larger than the result obtained in the present work ($\log gf$ = −0.21). This is probably due to the fact that the quite simple model used by Sen & Puri (1989a) underestimated the strong mixing between the 7s7p ^{1}P$_1^\circ$ and 6d7p ^{3}D$_1^\circ$ states. In fact, for the level at 33 388.61 cm^{-1}, classified as 7s7p ^{1}P$_1^\circ$ in the NIST tables (Moore 1971), our calculations gave a mixing of 61% 6d7p ^{3}D$_1^\circ$ + 23% 7s7p ^{1}P$_1^\circ$, in very good agreement with the composition (60% + 28%) obtained by Blaise & Wyart (1992) using the parametric Slater-Condon method. Moreover, it is interesting to note that, when performing a very simple HFR calculation, including only 7s^2 and 7s7p configurations, we could obtain an oscillator strength ($\log gf$ = 0.40) in good agreement with the one published by Sen & Puri (1989a).

Table 10. Partition functions in Ra I, Ra II, Ac I and Ac II.

T (K)	Ra I	Ra II	Ac I	Ac II
3000	1.03	2.02	6.31	1.99
3500	1.07	2.05	6.96	2.50
4000	1.15	2.10	7.72	3.09
4500	1.26	2.16	8.64	3.73
5000	1.43	2.25	9.73	4.42
5500	1.66	2.35	11.01	5.16
6000	1.95	2.46	12.50	5.94
6500	2.31	2.59	14.21	6.75
7000	2.76	2.73	16.16	7.60
7500	3.30	2.89	18.37	8.49
8000	3.97	3.05	20.86	9.42
8500	4.76	3.22	23.67	10.38
9000	5.70	3.39	26.81	11.39
9500	6.81	3.57	30.32	12.44
10 000	8.10	3.77	34.22	13.53
10 500	9.58	3.96	38.54	14.67
11 000	11.26	4.17	43.31	15.87
11 500	13.17	4.38	48.54	17.12
12 000	15.30	4.61	54.28	18.42
12 500	17.67	4.84	60.52	19.79
13 000	20.29	5.09	67.29	21.22
13 500	23.15	5.36	74.62	22.73
14 000	26.26	5.63	82.51	24.30

5. Partition functions

The calculation of ionization equilibrium in stellar atmospheres using Saha equation requires the evaluation of the partition functions for neutral and ionized species. The values computed in the present work for radium and actinium are given in Table 10 for temperatures from 3000 to 14 000 K. These results were obtained, for each element, using the available experimental levels completed with all the calculated values deduced from the theoretical models described in Sect. 3. This corresponds to total numbers of levels equal to 539, 78, 1722 and 539 for Ra I, Ra II, Ac I and Ac II, respectively. In order to estimate the detrimental effect of missing experimental levels on the partition functions, the latter were also computed using only the available experimental energies. When doing so, it was found that the partition functions reported in Table 10 were almost unaffected for T = 3000 K while they were decreased by a factor of 2.06, 1.04, 2.73 and 1.06 for T = 14 000 K in the case of Ra I, Ra II, Ac I and Ac II, respectively.

6. Astrophysical applications

As pointed out by Cowley et al. (2004), Gopka et al. (2004) and Bidelman (2005), the lines of radioactive elements can be identified in the spectra of Przybylski's star (HD 101065) and of HR 465. Yushchenko et al. (2007) tried to estimate the abundances of actinides, forcing all oscillator strengths to zero. Using the new atomic data obtained in the present work for radium and actinium, we investigated the astrophysical spectra of these two stars.

Some of the wavelengths reported in Tables 5–8 being shorter than 3000 Å, we first used observed IUE spectra from INES archive, namely LWR06999HL for the Przybylski's star and LWP14571HL, LWP14572HL, LWR03984HS, LWR03987HS, LWR07217HL, LWR14522HL, LWR14526HL for HR 465. The spectral resolution (R) of IUE spectra is about 0.1 Å while the signal to noise ratio (S/N) is in the range extending from 10 up to 30. Observed spectrum of Przybylski's star at longer wavelengths (from 3040 to 10 350 Å) was taken from VLT archives (Bagnulo et al. 2002). This spectrum is characterized by a resolution of 80 000 and a S/N ratio greater than 300. For HR 465, we used two spectra for wavelengths longer than 3000 Å. The first one (λ = 4000–6800 Å, R = 40 000, S/N = 70–100), registered in 1996 with the 1.93 meter telescope of Haute-Provence Observatory (France), was extracted from the archives of this observatory

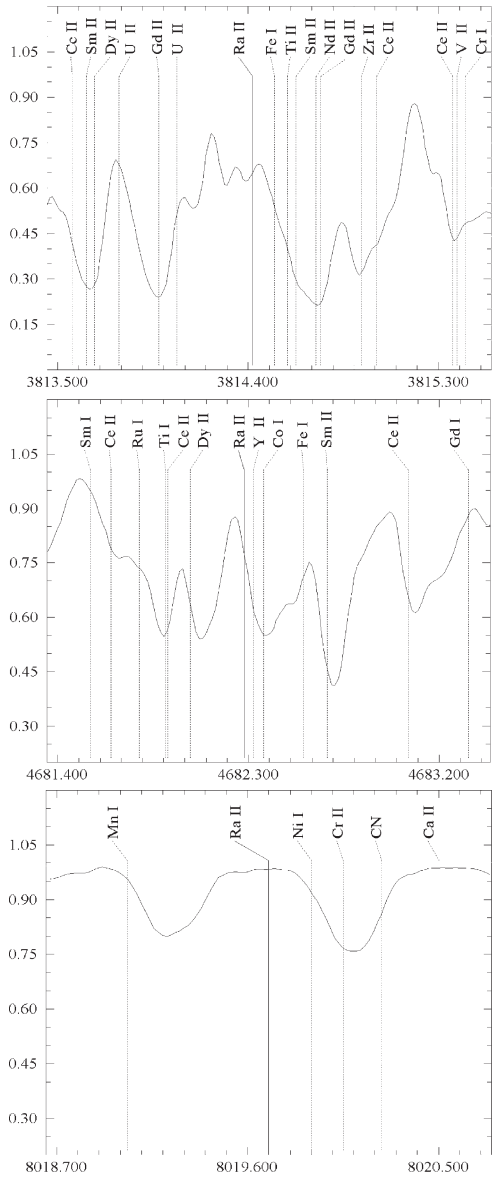

Fig. 1. Three Ra II lines in the spectrum of Przybylski's star. Tentative identifications have also been performed for neighbouring lines but they are very uncertain in some cases. The *x*- and *y*-axis correspond to wavelengths (in Å) and intensities (in arbitrary units), respectively.

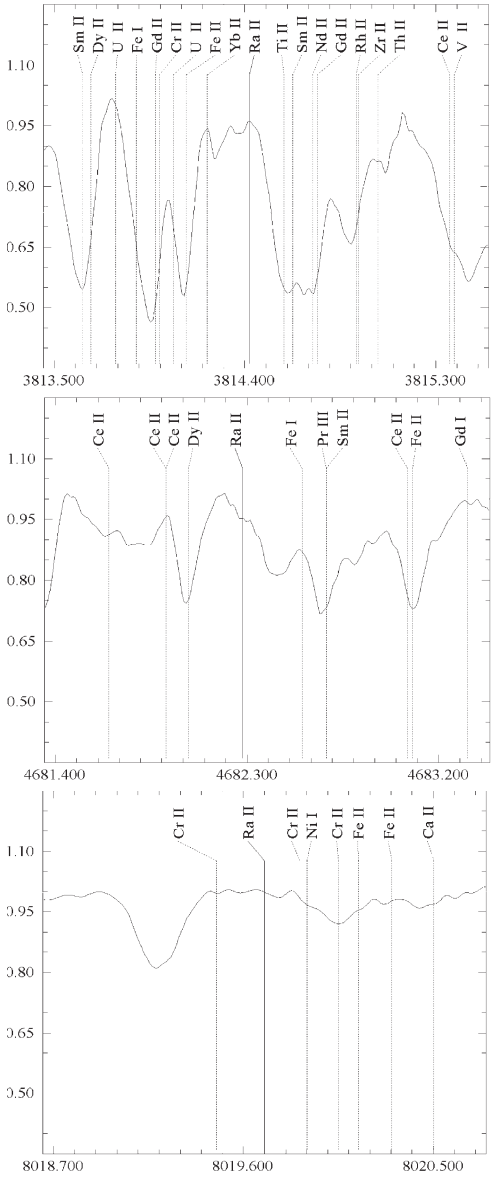

Fig. 2. Same as Fig. 1 for the HR 465 star.

(Prugniel & Soubiran 2001). The second spectrum (λ = 3780–9500 Å, R = 80 000, $S/N > 100$) was observed in 2004 with the 1.8 m telescope of Bohuynsan Observatory (Korea). It should be mentioned that, due to the strong variability of spectral lines in HR 465 with a period of 22–24 years (Preston & Wolff 1970), the first spectrum shows enhanced chromium lines while the second one shows enhanced lanthanide lines.

Both HD 101065 and HR 465 stars have very complicated spectra with a significant part of spectral lines being unidentified. Yushchenko et al. (2007) showed that strong stratification of chemical elements could exist in the atmosphere of Przybylski's star but, unfortunately, there is presently no accurate atmospheric model susceptible to describe the observed spectrum of this star correctly. Consequently, we restrict ourselves, in the present paper, to a short discussion of possible identifications of some lines of radium and actinium in the spectra of these two stars.

6.1. Radium lines

The Ra II line at 2708.96 Å is in the blue wing of the strong λ2709.056 Fe II line and the influence of the strong λ2708.957 Ce II line can explain the observations of Przybylski's star spectrum. The line at 2813.76 Å is faint and located in crowded spectral region. The strongest contribution of the absorption feature at this wavelength in the spectrum of Pzrybylski's star is due to the Os I line at 2813.762 Å. Ultraviolet spectra show numerous absorption lines but the S/N ratio of IUE spectra being only about 10–30, it is very difficult to express any definitive conclusion about possible presence of radium lines in this spectral region. In the visible region, the two Ra II lines at 3649.55 and 4340.64 Å are very close to H I Balmer lines H_{62} (3649.543 Å) and H_γ (4340.462 Å). The lines at 4436.27, 4533.11 and 5813.63 Å are too faint to be detected or are contaminated by lines of other elements.

In fact only three Ra II lines could be used to estimate the upper limit of radium abundance in the atmospheres of the

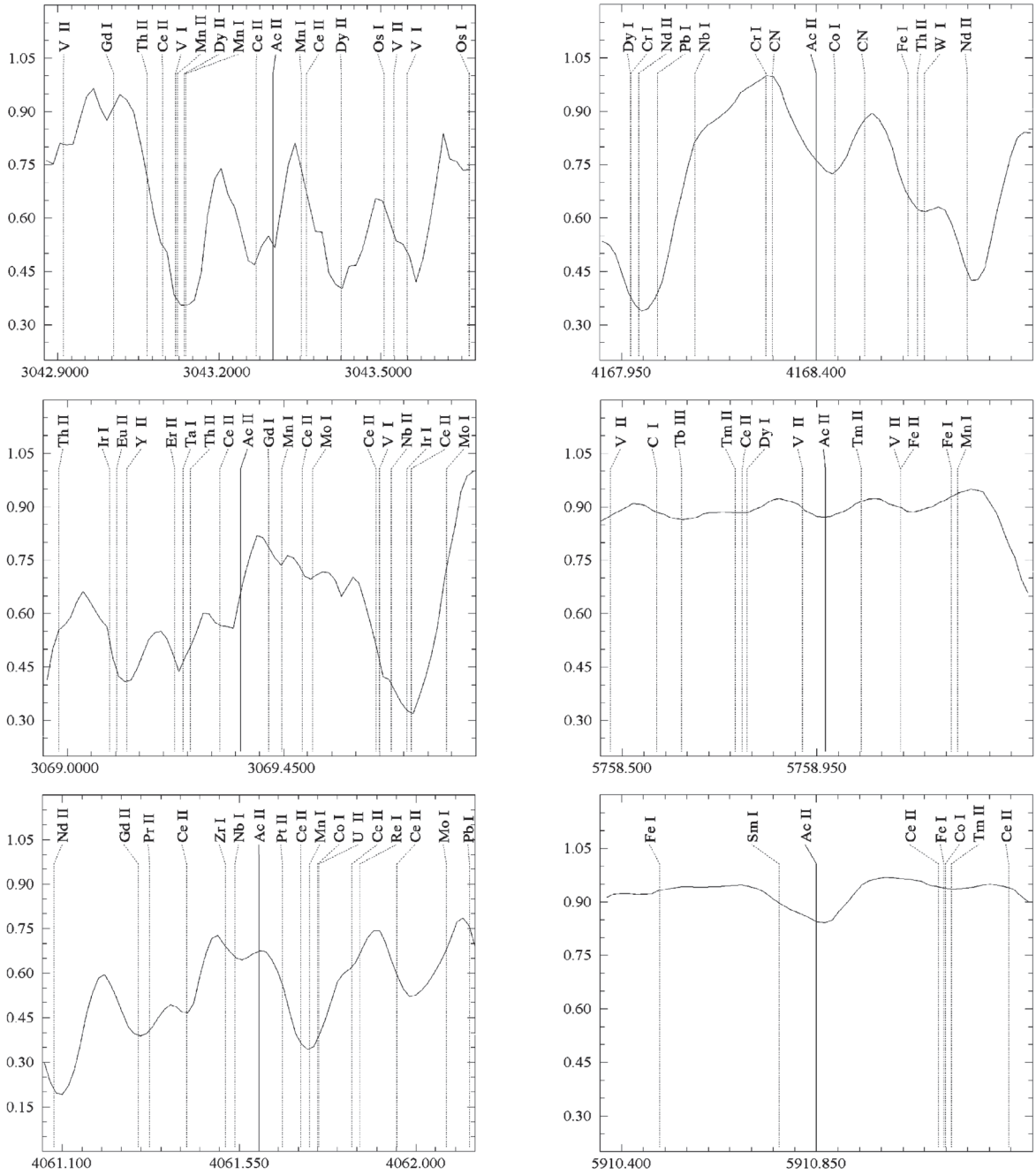

Fig. 3. The six spectral regions around possible Ac II lines in the spectrum of Pzrybylski's star. The *x*- and *y*-axis correspond to wavelengths (in Å) and intensities (in arbitrary units), respectively.

investigated stars if dedicated stellar models were available. These lines, located at 3814.42, 4682.28 and 8019.70 Å, are shown in Figs. 1 and 2 for HD 101065 and HR 465 stars, respectively. For the first line (λ = 3814.42 Å), the observed wavelength is 3814.40 Å in Przybylski's star and 3814.39 Å in HR 465. This line is free of strong blending. For the line at 4682.28 Å, we found no counterparts in the observed spectra. The Y II line at 4682.324 Å is the strongest blending line in the spectra of both stars while the Os I line at 4682.06 Å should influence the spectrum of Przybylski's star only. Ra II line at 8019.70 Å is too weak and could not be identified. The spectral region around this wavelength could be used for determining an upper limit to the stellar content of radium.

6.2. Actinium lines

The search for actinium lines in the HR 465 spectrum was not successful. For most of the lines, the appearance of the observed spectrum can be explained by lines of other elements. In contrast, actinium lines could possibly be present in the spectrum of Przybylski's star. Figure 3 shows the observed spectra of HD 101065 and identifications of the strongest lines. For the Ac II line at 3043.30 Å, the observed wavelength is 3043.01 Å. Some blends could be due to Ce II (λ3043.268) and Tb III (λ3043.324) lines but the influence of these lines is not expected to be important. For the line at 3069.36 Å, the observed wavelength at 3069.345 Å is free from strong blending but the Ce II line at 3069.318 Å should however be taken into account.

The Ac II line at 4061.60 Å, observed at 4061.556 Å in the HD 101065 spectrum, could be blended with Nb I (λ4061.539) and Zr I (λ4061.515) lines. The line at 4168.40 Å, observed at 4168.436 Å, is one of the best lines for which actinium can make the largest input to the absorption feature, the lines of other elements being weak except the Co I contribution at λ4068.443. Finally, the Ac II lines at 5758.97 and 5910.85 Å (observed at 5758.97 and 5910.865 Å) are not expected to be affected by strong blends and the identification of these lines as due to actinium is plausible according to the available linelists.

7. Conclusion

Oscillator strengths have been calculated for strong lines in neutral and singly ionized radium (Ra I–II) and actinium (Ac I–II). For most of the transitions considered in the present work, f-values are reported for the first time. These new results are intended to provide astrophysicists with some of the data they need for quantitative investigations of stellar spectra where such radiaoactive elements are expected to be observed. The two cases of HD 101065 and HR 465 are considered. A close examination of the spectra indicates that some absorption features observed in the spectra of these stars could possibly be due to Ra II and Ac II. A more quantitative analysis however is awaiting the availability of accurate models describing the atmospheres of these stars.

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Table 1. Comparison between experimental and calculated energy levels in Ra I.

Designation[a]	J	$E^a_{\rm exp}$ (cm^{-1})	$E^b_{\rm calc}$ (cm^{-1})	ΔE^c (cm^{-1})	g^d	Composition[e]
Even parity						
7s^2 ^{1}S	0	0.00	0	0		96% 7s^2 ^{1}S
6d7s ^{3}D	1	13 715.85	13 695	21	0.499	100% 6d7s ^{3}D
6d7s ^{3}D	2	13 993.97	14 022	−28	1.163	97% 6d7s ^{3}D
6d7s ^{3}D	3	14 707.35	14 701	6	1.334	100% 6d7s ^{3}D
6d7s ^{1}D	2	17 081.45	17 080	1	1.004	88% 6d7s ^{1}D + 5% 7p^2 ^{1}D
7s8s ^{3}S	1	26 754.05	26 754	0	2.002	100% 7s8s ^3S
	0		27 714			83% 7s8s ^{1}S + 6% 6d^2 ^{1}S
	2		29 476		0.765	74% 6d^2 ^{3}F + 16% 6d^2 ^{1}D
	0		29 778			42% 6d^2 ^{3}P + 36% 7p^2 ^{3}P + 11% 7s8s ^{1}S
	3		30 832		1.084	99% 6d^2 ^{3}F
	2		30 893		1.046	24% 6d^2 ^{1}D + 22% 6d^2 ^{3}F + 16% 6d^2 ^{3}P
7p^2 ^{3}P	1	31 248.61	31 035	214	1.501	61% 6d^2 ^{3}P + 39% 7p^2 ^{3}P
	4		31 915		1.238	95% 6d^2 ^{3}F
7s7d ^{3}D	2	31 993.41	31 935	59	1.184	44% 7s7d ^{1}D + 20% 6d^2 ^{3}P + 19% 7s7d ^{3}D
7s7d ^{3}D	1	32 000.82	32 042	−41	0.499	95% 7s7d ^{3}D
7s7d ^{3}D	3	32 197.28	32 216	−19	1.334	97% 7s7d ^{3}D
7p^2 ^{1}D	2	32 214.84	32 154	61	1.177	76% 7s7d ^{3}D + 11% 7s7d ^{1}D + 6% 6d^2 ^{3}P
7p^2 ^{3}P	2	32 941.13	33 180	−239	1.163	34% 6d^2 ^{1}D + 24% 6d^2 ^{3}P + 14% 7s7d ^{1}D
	0		34 041			47% 7s9s ^{1}S + 24% 6d^2 ^{1}S + 15% 7p^2 ^{1}S
7s9s ^{3}S	1	34 475.78	34 476	0	2.002	100% 7s9s ^{3}S
	4		34 741		1.012	92% 6d^2 ^{1}G
	0		35 775			51% 7s9s ^{1}S + 21% 6d^2 ^{1}S + 12% 7p^2 ^{1}S
Odd parity						
7s7p ^{3}P°	0	13 078.44	13 145	−67		99% 7s7p ^{3}P°
7s7p ^{3}P°	1	13 999.38	13 924	75	1.472	93% 7s7p ^{3}P°
7s7p ^{3}P°	2	16 688.54	16 691	−3	1.501	98% 7s7p ^{3}P°
7s7p ^{1}P°	1	20 715.71	20 732	−16	1.028	78% 7s7p ^{1}P° + 14% 6d7p ^{1}P° + 6% 7s7p ^{3}P°
6d7p ^{3}F°	2	28 038.05	28 276	−238	0.739	78% 6d7p ^{3}F° + 19% 6d7p ^{1}D°
6d7p ^{3}F°	3	30 117.78	30 175	−57	1.089	95% 6d7p ^{3}F°
6d7p ^{1}D°	2	30 918.14	30 862	56	1.025	65% 6d7p ^{1}D° + 17% 6d7p ^{3}F° + 13% 6d7p ^{3}P°
7s8p ^{3}P°	0	31 085.88	31 452	−366		90% 7s7p ^{3}P° + 9% 6d7p ^{3}P°
7s8p ^{3}P°	1	31 563.29	31 071	493	0.969	41% 6d7p ^{3}D° + 20% 7s8p ^{3}P° + 14% 6d7p ^{3}P°
7s8p ^{3}P°	2	31 874.44	31 958	−84	1.436	79% 7s8p ^{3}P° + 7% 6d7p ^{1}D° + 6% 6d7p ^{3}P°
6d7p ^{3}D°	1	32 229.97	31 774	456	1.212	69% 7s8p ^{3}P° + 28% 6d7p ^{3}D°
6d7p ^{3}F°	4	32 367.78	32 138	230	1.251	96% 6d7p ^{3}F°
6d7p ^{3}D°	2	32 506.59	32 619	−112	1.214	81% 6d7p ^{3}D° + 11% 7s8p ^{3}P° + 6% 6d7p ^{3}P°
7s8p ^{1}P°	1	32 857.68	32 954	−96	0.903	58% 7s8p ^{1}P° + 24% 6d7p ^{3}D° + 10% 6d7p ^{1}P°
6d7p ^{3}D°	3	33 197.46	33 452	−254	1.204	60% 6d7p ^{3}D° + 22% 6d7p ^{1}F° + 13% 7s5f ^{1}F°
6d7p ^{3}P°	0	33 782.41	33 731	52		86% 6d7p ^{3}P° + 9% 7s8p ^{3}P°
6d7p ^{3}P°	1	33 823.70	33 865	−41	1.407	75% 6d7p ^{3}P° + 9% 7s8p ^{1}P° + 7% 7s8p ^{3}P°
6d7p ^{3}P°	2	34 382.91	34 439	−56	1.423	69% 6d7p ^{3}P° + 12% 6d7p ^{3}D° + 8% 6d7p ^{1}D°
	3		34 551		1.110	50% 7s5f ^{1}F° + 32% 6d7p ^{3}D° + 14% 6d7p ^{1}F°
7s5f ^{3}F°	2	35 255.65	35 232	23	0.666	98% 7s5f ^{3}F°
7s5f ^{3}F°	3	35 268.02	35 257	11	1.084	98% 7s5f ^{3}F°
7s5f ^{3}F°	4	35 294.40	35 299	−5	1.251	97% 7s5f ^{3}F°
	1		35 631		1.063	77% 7s9p ^{1}P° + 9% 7s9p ^{3}P°
	0		35 748			97% 7s9p ^{3}P°
	1		35 850		1.445	88% 7s9p ^{3}P° + 9% 7s9p ^{1}P°
	2		36 006		1.500	96% 7s9p ^{3}P°
	3		36 685		1.012	34% 7s5f ^{1}F° + 32% 6d7p ^{1}F° + 22% 7s6f ^{1}F°
	2		37 906		0.666	99% 7s6f ^{3}F°
7s6f ^{3}F°	3	37 922.26	37 917	5	1.084	99% 7s6f ^{3}F°
7s6f ^{3}F°	4	37 929.64	37 932	−2	1.251	99% 7s6f ^{3}F°
	3		38 386		1.002	72% 7s6f ^{1}F° + 13% 6d7p ^{1}F° + 7% 7s7f ^{1}F°
	2		39 353		0.666	99% 7s7f ^{3}F°
7s7f ^{3}F°	3	39 360.96	39 360	1	1.084	99% 7s7f ^{3}F°
7s7f ^{3}F°	4	39 366.98	39 367	0	1.251	99% 7s7f ^{3}F°

Table 1. continued.

Designation[a]	J	$E^a_{\rm exp}$ (cm^{-1})	$E^b_{\rm calc}$ (cm^{-1})	ΔE^c (cm^{-1})	g^d	Composition[e]
	1		39 540		1.003	43% 6d7p ^{1}P° + 21% 6d8p ^{1}P° + 9% 7s9p ^{1}P°
	3		39 546		1.001	86% 7s7f ^{1}F°
7s8f ^{3}F°	2	40 219.50	40 217	2	0.666	90% 7s8f ^{3}F° + 8% 7s9f ^{3}F°
7s8f ^{3}F°	3	40 219.50	40 223	–4	1.083	92% 7s8f ^{3}F° + 7% 7s9f^{3}F°
7s8f ^{3}F°	4	40 231.58	40 229	2	1.251	94% 7s8f ^{3}F° + 5% 7s9f^{3}F°
	3		40 280		1.000	64% 7s8f ^{1}F° + 36% 7s9f ^{1}F°

[a] From Moore (1971). [b] Semi-empirical HFR calculations (present work). [c] $\Delta E = E_{\rm exp} - E_{\rm calc}$. [d] Landé factor as calculated in the present work. [e] Only the first three components ≥5% are given. See Sect. 3.1 for explanations concerning the differences between the designations from Moore (1971) and the calculated compositions.

Table 2. Experimental energy levels and calculated Landé g-factors in Ra II. For this ion, the differences $\Delta E = E_{\rm exp} - E_{\rm calc} = 0$ cm^{-1} and the eigenvector purities are equal to 100% for all the levels (see the text).

Designation[a]	J	$E^a_{\rm exp}$ (cm^{-1})	g^b
Even parity			
7s ^{2}S	1/2	0.00	2.002
6d ^{2}D	3/2	12 084.38	0.800
6d ^{2}D	5/2	13 743.11	1.200
8s ^{2}S	1/2	43 405.01	2.002
7d ^{2}D	3/2	48 744.04	0.800
7d ^{2}D	5/2	49 240.48	1.200
9s ^{2}S	1/2	59 165.23	2.002
8d ^{2}D	3/2	61 734.88	0.800
8d ^{2}D	5/2	61 973.82	1.200
5g ^{2}G	7/2	64 150.65	0.889
5g ^{2}G	9/2	64 150.65	1.111
10s ^{2}S	1/2	66 837.88	2.002
9d ^{2}D	3/2	68 264.07	0.800
9d ^{2}D	5/2	68 394.86	1.200
6g ^{2}G	7/2	69 560.85	0.889
6g ^{2}G	9/2	69 560.85	1.111
11s ^{2}S	1/2	71 172.92	2.002
10d ^{2}D	3/2	72 043.06	0.800
10d ^{2}D	5/2	72 123.78	1.200
7g ^{2}G	7/2	72 824.37	0.889
7g ^{2}G	9/2	72 824.37	1.111
12s ^{2}S	1/2	73 863.1	2.002
11d ^{2}D	3/2	74 434.04	0.800
11d ^{2}D	5/2	74 488.51	1.200
8g ^{2}G	7/2	74 941.91	0.889
8g ^{2}G	9/2	74 941.91	1.111
12d ^{2}D	3/2	[76047]	0.800
12d ^{2}D	5/2	76 080.74	1.200
9g ^{2}G	7/2	76 393.12	0.889
9g ^{2}G	9/2	76 393.12	1.111
10g ^{2}G	7/2	77 431.31	0.889
10g ^{2}G	9/2	77 431.31	1.111
11g ^{2}G	7/2	78 195.21	0.889
11g ^{2}G	9/2	78 195.21	1.111
Odd parity			
7p ^{2}P°	1/2	21 351.20	0.666
7p ^{2}P°	3/2	26 208.86	1.334
5f ^{2}F°	5/2	48 987.98	0.857
5f ^{2}F°	7/2	49 272.31	1.143
8p ^{2}P°	1/2	50 606.01	0.666
8p ^{2}P°	3/2	52 392.05	1.334
6f ^{2}F°	5/2	59 515.48	0.857
6f ^{2}F°	7/2	59 815.59	1.143
9p ^{2}P°	1/2	[62 977]	0.666
9p ^{2}P°	3/2	63 410.41	1.334
7f ^{2}F°	5/2	66 521.86	0.857
7f ^{2}F°	7/2	66 691.22	1.143

[a] From Moore (1971). Energies between brackets are calculated values obtained in the present work. [b] Landé factor as calculated in the present work.

Table 3. Comparison between experimental and calculated energy levels in Ac I.

Designation[a]	J	$E^a_{\rm exp}$ (cm^{-1})	$E^b_{\rm calc}$ (cm^{-1})	ΔE^c (cm^{-1})	g^d	Composition[e]
Even parity						
6d7s^2 ^{2}D	3/2	0.00	0	0	0.799	90% 6d7s^2 ^{2}D
6d7s^2 ^{2}D	5/2	2231.43	2231	0	1.200	89% 6d7s^2 ^{2}D + 5% 6d^2(^{1}D)7s ^{2}D
6d^2(^{3}F)7s ^{4}F	3/2	9217.28	9204	13	1.679	95% 6d^2(^{3}F)7s ^{4}F
6d^2(^{3}F)7s ^{4}F	5/2	9863.59	9879	−15	1.031	94% 6d^2(^{3}F)7s ^{4}F
6d^2(^{3}F)7s ^{4}F	7/2	10 906.02	10 910	−4	1.237	97% 6d^2(^{3}F)7s ^{4}F
6d^2(^{3}F)7s ^{4}F	9/2	12 078.07	12 072	6	1.329	97% 6d^2(^{3}F)7s ^{4}F
Odd parity						
	1/2		9465		0.663	84% 7s^{2}7p ^{2}P° + 10% 6d7s(^{3}D)7p ^{2}P°
	3/2		13 173		1.334	78% 7s^{2}7p ^{2}P° + 12% 6d7s(^{3}D)7p ^{2}P°
6d7s(^{3}D)7p ^{4}F°	3/2	13 712.90	15 193	–1480	0.465	84% 6d7s(^{3}D)7p ^{4}F° + 8% 6d7s(^{3}D)7p ^{2}D°
6d7s(^{3}D)7p ^{4}F°	5/2	14 940.72	16 290	–1349	1.071	70% 6d7s(^{3}D)7p ^{4}F° + 10% 6d7s(^{3}D)7p ^{2}D° + 8% 6d7s(^{1}D)7p ^{2}D°
6d7s(^{3}D)7p ^{4}D°	1/2	17 199.71	17 561	–361	0.058	93% 6d7s(^{3}D)7p ^{4}D°
6d7s(^{3}D)7p ^{4}F°	7/2	17 683.87	18 852	–1168	1.239	94% 6d7s(^{3}D)7p ^{4}F°
6d7s(^{3}D)7p ^{2}D°	3/2	17 736.26	18 237	–501	1.157	81% 6d7s(^{3}D)7p ^{4}D° + 5% 6d7s(^{1}D)7p ^{2}D°
6d7s(^{3}D)7p ^{2}D°	5/2	17 950.71	19 063	–1112	1.223	27% 6d7s(^{3}D)7p ^{4}D° + 24% 6d7s(^{3}D)7p ^{4}F°
6d7s(^{3}D)7p ^{4}D°	3/2	19 012.46	20 158	–1146	0.992	35% 6d7s(^{3}D)7p ^{2}D° + 24% 6d7s(^{1}D)7p ^{2}D° + 21% 6d7s(^{3}D)7p ^{4}P°
6d7s(^{3}D)7p ^{4}D°	5/2	21 195.87	19 957	1239	1.373	61% 6d7s(^{3}D)7p ^{4}D° + 18% 6d7s(^{3}D)7p ^{4}P° + 10% 6d7s(^{3}D)7p ^{2}D°
	9/2		21 559		1.334	98% 6d7s(^{3}D)7p ^{4}F°
6d7s(^{3}D)7p ^{4}P°	1/2	22 401.52	20 944	1457	2.596	95% 6d7s(^{3}D)7p ^{4}P°
6d7s(^{3}D)7p ^{4}P°	3/2	22 801.10	21 415	1386	1.511	67% 6d7s(^{3}D)7p ^{4}P° + 9% 6d7s(^{3}D)7p ^{4}D° + 8% 6d7s(^{1}D)7p ^{2}D°
6d7s(^{3}D)7p ^{4}D°	7/2	23 475.94	21 222	2254	1.402	88% 6d7s(^{3}D)7p ^{4}D° + 5% 6d7s(^{3}D)7p ^{2}F°
6d7s(^{3}D)7p ^{4}P°	5/2	23 898.86	22 787	1112	1.317	55% 6d7s(^{3}D)7p ^{4}P° + 23% 6d7s(^{1}D)7p ^{2}F° + 5% 6d7s(^{1}D)7p ^{2}D°
6d7s(^{3}D)7p ^{2}F°	5/2	23 916.84	23 914	3	1.048	31% 6d7s(^{1}D)7p ^{2}F° + 17% 6d7s(^{3}D)7p ^{4}P° + 14% 6d7s(^{3}D)7p ^{2}F°
6d7s(^{3}D)7p ^{2}F°	7/2	24 969.30	26 001	–1032	1.164	53% 6d7s(^{1}D)7p ^{2}F° + 27% 6d7s(^{3}D)7p ^{2}F° + 7% 6d7s(^{3}D)7p ^{4}D°
6d7s(^{3}D)7p ^{2}P°	1/2	25 729.03	26 821	–1092	0.661	40% 6d7s(^{1}D)7p ^{2}P° + 31% 6d7s(^{3}D)7p ^{2}P° + 10% 6d^2(^{1}D)7p ^{2}P°
6d7s(^{1}D)7p ^{2}D°	3/2	26 066.04	25 192	874	0.857	35% 6d7s(^{3}D)7p ^{2}D° + 35% 6d7s(^{1}D)7p ^{2}D° + 16% 6d^2(^{3}F)7p ^{2}D°
6d7s(^{1}D)7p ^{2}D°	5/2	26 533.16	25 296	1237	0.919	55% 6d7s(^{3}D)7p ^{2}F° + 17% 6d7s(^{1}D)7p ^{2}F° + 8% 6d7s(^{3}D)7p ^{2}D°
6d7s(^{1}D)7p ^{2}F°	5/2	26 836.20	28 619	–1783	1.161	33% 6d7s(^{3}D)7p ^{2}D° + 32% 6d7s(^{1}D)7p ^{2}D° + 16% 6d^2(^{3}F)7p ^{2}D°
6d7s(^{3}D)7p ^{2}P°	3/2	27 009.84	27 227	–217	1.295	70% 6d7s(^{1}D)7p ^{2}P° + 11% 6d^2(^{1}D)7p ^{2}P° + 7% 6d7s(^{1}D)7p ^{2}D°
6d7s(^{1}D)7p ^{2}F°	7/2	28 568.40	27 050	1518	1.148	44% 6d7s(^{3}D)7p ^{2}F° + 22% 6d7s(^{1}D)7p ^{2}F° + 10% 5f7s^2 ^{2}F°
	1/2		29 062		0.683	39% 6d7s(^{1}D)7p ^{2}P° + 26% 6d7s(^{3}D)7p ^{2}P° + 19% 7s^{2}8p ^{2}P°
6d7s(^{1}D)7p ^{2}P°	3/2	30 396.61	30 103	294	1.325	43% 6d7s(^{3}D)7p ^{2}P° + 35% 7s^{2}8p ^{2}P° + 6% 7s^{2}7p ^{2}P°
6d^2(^{3}F)7p ^{4}G°	5/2	31 494.68	31 068	427	0.614	85% 6d^2(^{3}F)7p ^{4}G°
6d^2(^{3}F)7p ^{4}G°	7/2	32 219.62	33 007	–787	0.993	93% 6d^2(^{3}F)7p ^{4}G°
6d^2(^{3}F)7p ^{4}G°	9/2	32 867.39	35 080	–2213	1.168	94% 6d^2(^{3}F)7p ^{4}G°
6d^2(^{3}F)7p ^{4}G°	11/2	33 429.76	37 381	–3951	1.264	92% 6d^2(^{3}F)7p ^{4}G°

[a] From Blaise & Wyart (1992). [b] Semi-empirical HFR calculations (present work). [c] $\Delta E = E_{\rm exp} - E_{\rm calc}$. [d] Landé factor as calculated in the present work. [e] Only the first three components ≥5% are given.

Table 4. Comparison between experimental and calculated energy levels in Ac II.

Designation[a]	J	$E^a_{\rm exp}$ (cm^{-1})	$E^b_{\rm calc}$ (cm^{-1})	ΔE^c (cm^{-1})	g^d	Composition[e]
Even parity						
7s^2 ^{1}S	0	0.00	0	0		95% 7s^2 ^{1}S
6d7s ^{3}D	1	4739.63	4688	51	0.499	99% 6d7s ^{3}D
6d7s ^{3}D	2	5267.16	5352	−84	1.150	89% 6d7s ^{3}D + 9% 6d7s ^{1}D
6d7s ^{3}D	3	7426.52	7404	23	1.334	99% 6d7s ^{3}D
6d7s ^{1}D	2	9087.54	9352	−265	1.007	67% 6d7s ^{1}D + 18% 6d^2 ^{1}D + 10% 6d7s ^{3}D
6d^2 ^{3}F	2	13 236.46	13 134	102	0.692	92% 6d^2 ^{3}F + 6% 6d7s ^{1}D
6d^2 ^{3}F	3	14 949.21	14 970	−21	1.084	99% 6d^2 ^{3}F
6d^2 ^{3}F	4	16 756.90	16 839	−82	1.230	91% 6d^2 ^{3}F + 8% 6d^2 ^{1}G
6d^2 ^{3}P	0	17 737.10	17 767	−30		91% 6d^2 ^{3}P + 6% 6d^2 ^{1}S
6d^2 ^{3}P	1	19 015.32	19 055	−40	1.501	98% 6d^2 ^{3}P
6d^2 ^{1}D	2	19 203.02	19 137	66	1.312	62% 6d^2 ^{3}P + 25% 6d^2 ^{1}D + 7% 6d7s ^{1}D
6d^2 ^{1}G	4	20 848.23	20 838	10	1.021	90% 6d^2 ^{1}G + 8% 6d^2 ^{3}F
6d^2 ^{3}P	2	22 199.45	22 122	77	1.173	52% 6d^2 ^{1}D + 35% 6d^2 ^{3}P + 8% 6d7s ^{1}D
	0		28 072			82% 6d^2 ^{1}S + 7% 6d^2 ^{3}P
	0		51 281			83% 7p^2 ^{3}P + 8% 7p^2 ^{1}S
	2		51 348		1.079	41% 6d8s ^{3}D + 35% 6d8s ^{1}D + 13% 7s7d ^{1}D
7s8s ^3S	1	51 680.55	51 470	211	1.989	94% 7s8s ^3S
	1		51 574		0.510	90% 6d8s ^{3}D
	3		52 816		0.809	46% 5f7p ^{3}G + 31% 6d7d ^{3}G + 12% 5f7p ^{1}F
7s8s ^{1}S	0	53 374.01	53 304	70		94% 7s8s ^{1}S
Odd parity						
7s7p ^{3}P°	0	20 956.40	20 980	−24		98% 7s7p ^{3}P°
7s7p ^{3}P°	1	22 180.52	22 147	34	1.463	90% 7s7p ^{3}P° + 5% 7s7p ^{1}P°
7s7p ^{3}P°	2	26 446.96	26 446	1	1.494	95% 7s7p ^{3}P°
6d7p ^{3}F°	2	28 201.11	27 555	646	0.714	55% 6d7p ^{3}F° + 32% 5f7s ^{3}F° + 10% 6d7p ^{1}D°
6d7p	1	29 250.40	29 289	−39	0.892	36% 6d7p ^{1}P° + 30% 6d7p ^{3}D° + 22% 7s7p ^{1}P°
5f7s ^{1}F°	3	29 881.09	29 753	128	1.067	46% 5f7s ^{3}F° + 33% 6d7p ^{3}F° + 16% 5f7s ^{1}F°
6d7p	3	31 174.60	31 409	−234	1.042	44% 5f7s ^{1}F° + 28% 6d7p ^{1}F° + 17% 6d7p ^{3}F°
6d7p ^{1}D°	2	31 878.87	32 064	−185	0.961	64% 6d7p ^{1}D° + 23% 5f7s ^{3}F° + 6% 6d7p ^{3}P°
5f7s ^{3}F°	4	32 965.55	32 902	64	1.251	62% 5f7s ^{3}F° + 38% 6d7p ^{3}F°
6d7p ^{3}D°	2	33 304.96	33 485	−180	1.184	83% 6d7p ^{3}D° + 7% 6d7p ^{3}P°
6d7p ^{3}D°	1	33 388.61	33 271	118	0.684	61% 6d7p ^{3}D° + 23% 7s7p ^{1}P° + 11% 6d7p ^{1}P°
6d7p ^{3}D°	3	35 144.35	35 903	−759	1.289	80% 6d7p ^{3}D° + 10% 5f7s ^{1}F° + 6% 5f6d ^{3}D°
6d7p	2	35 397.12	35 729	−332	0.741	37% 5f7s ^{3}F° + 36% 6d7p ^{3}F° + 11% 5f6d ^{3}F°
6d7p ^{3}P°	0	36 780.01	36 787	−7		85% 6d7p ^{3}P° + 13% 5f6d ^{3}P°
6d7p ^{3}P°	1	36 855.50	36 948	−92	1.445	78% 6d7p ^{3}P° + 12% 5f6d ^{3}P° + 6% 7s7p ^{1}P°
6d7p	3	36 972.94	37 288	−315	1.084	40% 6d7p ^{3}F° + 38% 5f7s ^{3}F° + 16% 5f6d ^{3}F°
6d7p ^{3}P°	2	38 371.64	38 364	8	1.407	68% 6d7p ^{3}P° + 12% 6d7p ^{1}D° + 11% 5f6d ^{3}P°
6d7p ^{3}F°	4	39 119.02	38 958	161	0.852	81% 5f6d ^{3}H° + 13% 5f6d ^{1}G°
5f6d ^3H°	4	39 807.14	39 640	167	1.206	41% 6d7p ^{3}F° + 26% 5f7s ^{3}F° + 23% 5f6d ^{3}F°
5f6d ^{3}F°	2	41 578.57	41 608	−29	0.739	68% 5f6d ^{3}F° + 20% 5f6d ^{1}D°
5f6d ^{1}G°	4	41 627.79	41 554	74	1.004	79% 5f6d ^{1}G° + 10% 5f6d ^3H° + 6% 6d7p ^{3}F°
6d7p ^{1}F°	3	41 937.05	41 686	251	1.016	47% 6d7p ^{1}F° + 22% 5f6d ^{1}F° + 21% 5f7s ^{1}F°
	6		43 001		1.167	100% 5f6d ^3H°
5f6d ^{3}F°	3	43 275.85	43 419	−143	1.083	83% 5f6d ^{3}F° + 9% 6d7p ^{3}F° + 6% 5f7s ^{3}F°
6d7p	1	44 199.94	44 233	−33	1.014	30% 5f6d ^{1}P° + 30% 7s7p ^{1}P°
5f6d ^{1}D°	2	44 705.33	44 672	33	0.944	70% 5f6d ^{1}D° + 19% 5f6d ^{3}F°
5f6d ^{3}F°	4	45 040.30	45 283	−242	1.238	74% 5f6d ^{3}F° + 13% 6d7p ^{3}F° + 8% 5f7s ^{3}F°
5f6d ^{3}G°	3	45 807.06	45 948	−141	0.759	96% 5f6d ^{3}G°
5f6d ^{3}G°	4	47 427.67	47 422	6	1.050	99% 5f6d ^{3}G°
5f6d ^{3}D°	1	48 518.41	48 507	11	0.552	87% 5f6d ^{3}D°
5f6d ^{3}G°	5	49 151.54	48 994	157	1.198	99% 5f6d ^{3}G°
5f6d ^{3}D°	2	49 479.05	49 583	−104	1.170	90% 5f6d ^{3}D° + 5% 6d7p ^{3}D°
5f6d ^{3}P°	0	49 780.60	49 932	−151		85% 5f6d ^{3}P° + 12% 6d7p ^{3}P°
5f6d ^{3}D°	3	50 059.70	50 151	−91	1.280	79% 5f6d ^{3}D° + 11% 5f6d ^{1}F°
5f6d ^{3}P°	1	50 235.60	50 012	224	1.439	78% 5f6d ^{3}P° + 10% 6d7p ^{3}P°
5f6d ^{3}P°	2	51 257.51	51 208	50	1.481	82% 5f6d ^{3}P° + 11% 6d7p ^{3}P°

Table 4. continued.

Designation[a]	J	$E^a_{\rm exp}$ (cm^{-1})	$E^b_{\rm calc}$ (cm^{-1})	ΔE^c (cm^{-1})	g^d	Composition[e]
5f6d ^{1}F°	3	53 255.30	53 095	160	1.048	62% 5f6d ^{1}F° + 14% 5f6d ^{3}D° + 10% 6d7p ^{1}F°
	5		55 784		1.002	97% 5f6d ^{1}H°
5f6d ^{1}P°	1	56 152.2	56 320	–168	1.014	48% 5f6d ^{1}P° + 15% 7s8p ^{1}P° + 11% 6d8p ^{1}P°

[a] From Blaise & Wyart (1992). [b] Semi-empirical HFR calculations (present work) [c] $\Delta E = E_{\rm exp} - E_{\rm calc}$. [d] Landé factor as calculated in the present work. [e] Only the first three components ≥5% are given.