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Experimental and theoretical radiative lifetimes, branching fractions and oscillator strengths in Lu II

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ABSTRACT

By a combination of radiative lifetimes measured using the fast-beam-laser method and experimental branching ratios deduced from Fourier transform spectrometer spectra, it has been possible to derive experimental *f*-values for Lu II lines observed in the visible and near-ultraviolet regions. These data are compared with relativistic Hartree–Fock calculations, taking core polarization effects into account, and a set of additional oscillator strengths of astrophysical interest is presented.

Key words: atomic data – atomic processes.

1 INTRODUCTION

Rare-earth elements are important in astrophysics in relation with nucleosynthesis and star formation. They have been observed in many Ap stars, particularly in the Cr–Eu–Sr subgroup, and also in Am stars (Jaschek & Brandi 1972; Jaschek & Jaschek 1995). As an example, some Lu II lines have been identified recently in the spectrum of the extreme peculiar star HD 101065 (Przybylski's star; Cowley & Mathys 1998). Many of the transitions observed, however, give rise to medium strong or weak lines which are blended with contributions originating from the most abundant elements (e.g. those of the iron group). Accurate transition probabilities are therefore needed to disentangle the blends and to determine more accurately the possible overabundances of these elements when compared with the cosmic values. Lu II is also observed in the solar spectrum (Grevesse & Blanquet 1969; Den Hartog et al. 1998; Bord, Cowley & Mirijanian 1999), and the refinement of the photospheric abundance value is strongly dependent upon accurate oscillator strengths.

Very few experimental values exist in the literature for the radiative lifetimes of Lu II energy levels, these essentially being limited to the Aarhus beam-foil data (Andersen & Sorensen 1974). The notable exceptions are the very recent precision measurement by Den Hartog et al. (1998) of the lifetime of 6s6p $^3P_1^\circ$ level using laser-induced fluorescence (LIF) of a slow atomic beam and measurements based on a laser-produced plasma followed by pulsed laser excitation and time-resolved detection (Li & Lundberg 1998). As beam-foil excitation is highly non-selective, there is always the danger that lifetimes measured using that technique may be subject to cascade-related errors. We have therefore undertaken a series of experiments using LIF of a fast ion beam, with the aim of extending the experimental data bank to include cascade-free measurements of the lifetimes of Lu II levels of the 5d6p configuration. We have also combined these measurements with some new branching ratio measurements to obtain individual experimental *f*-values for 11 transitions in Lu II. Finally, these *f*-values are compared with the results of a new relativistic Hartree–Fock (HFR) calculation taking core-polarization effects into account and a new set of oscillator strengths is proposed for 105 transitions.

2 LIFETIME MEASUREMENTS

In order to provide a test of the HFR calculation described below, the lifetimes of four energy levels in Lu II were measured using the fast-beam-laser method. Lu^+ ions from a Danfysik 911 ion source were accelerated through a potential difference of 300 kV and made to intersect frequency-doubled radiation from an excimer-pumped Hyperdye 500 laser from Lumonics Inc. (105 Schneider Road, Kanata, Ontario K2 K1Y3, Canada. Tuning the laser radiation into resonance with a selected transition in Lu II then excited the level to be studied. The only *LS* coupling allowed ground-state transition in Lu II above 200 nm is to the 6s6p $^1P^o$ term. Unfortunately the lifetime of this level was found to be too short to be measured in this experiment. Consequently, it was necessary to study levels that could be excited from one of the 5d6s metastable levels, which contain only a few per cent of the total ion beam. This problem was made even worse by the presence in the Lu spectrum of very large hyperfine structures.

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This resulted in laser resonances with widths much larger than that of the exciting laser radiation and hence only a fraction of the ions in the given metastable state could actually be excited, corresponding to maybe 1 per cent of the total ion beam. Clearly, it was necessary to operate with as intense an ion beam as possible to obtain a useful fluorescence signal. However, this inevitably gave rise to a large beam background signal, because of excitation of the ions by the residual gas atoms in the target chamber, even when the pressure in the target chamber was held below 5×10^{-7} torr. A final experimental difficulty arose from the relatively low vapour pressure of Lu metal at the temperatures attainable in our ion source, which limited the ion current to typically 0.5 μA. This combination of experimental problems inevitably reduced the accuracy of the final results, the final uncertainties being somewhat larger than the 1–3 per cent range normally obtained in such measurements.

The intensity of the LIF radiation was measured as a function of distance along the ion beam, and hence as a function of elapsed time from the excitation region, using a solar-blind photomultiplier (Hamamatsu Model 431S – Hamamatsu Corp., 325–6 Sunoyama-Cho, Hamamatsu City, Shizuoka Prefecture, 430 Japan) operated in a charge-integration mode to avoid signal pile-up (Ansbacher, Li & Pinnington 1989). Decay curves were recorded by moving the detection system along the target chamber, alternately parallel and antiparallel to the direction of the ion beam, in steps of 0.25 mm. Comparison of data recorded in the two directions gave a routine test for possible drifts in laser wavelength or power. The signal at each point was normalized to the ion beam current. Three signals were recorded at each position along the beam, these corresponding to the total signal (T), the beam background (B) with the laser off and the scattered laser light (L) with the ion beam off. Typically 10 sweeps were then superimposed to give a final decay curve. The individual data points were then given weights equal to $1/(T + B + L)$ in the fitting algorithm. At the velocity of the Lu^+ at 300 kV, one lifetime corresponded to about 2 mm along the beam. As the width of the excitation region itself was about 2 mm and the LIF signals were not strong (for the reasons discussed above), it was necessary to include the excitation region in the decay and in the fitting function. Details of this procedure have been given previously (Pinnington et al. 1997). Because of the various problems discussed above, it was necessary to record a large number (typically 25) of decay curves for each level studied. Full details of the experimental procedures are available elsewhere (Ansbacher et al. 1989; Biémont et al. 1997; Pinnington et al. 1997).

The experimental lifetime values obtained in the present work are reported in Table 1, where they are compared with previous measurements (Andersen & Sorensen 1974; Andersen et al. 1975; Den Hartog et al. 1998; Li & Lundberg 1998).

3 BRANCHING FRACTION MEASUREMENTS

Branching fractions for Lu II in the visible and near-ultraviolet (UV) were measured using the 1.0-m Fourier transform spectrometer (FTS) at the US National Solar Observatory (NSO) on Kitt Peak in Arizona (Brault 1976). Branching fractions in the deep UV were measured using a 1.0-m focal length Acton Research Corp. (PO Box 2215, Acton, MA 01720, USA) grating spectrometer equipped with a 2400 groove mm^{-1} holographic grating and 1024-element photodiode array. A pair of commercially available Lu hollow cathode lamps were used as emission sources. One of the lamps has a neon fill and the other has an argon fill. Both lamps have fused silica windows.

The advantages of a FTS for branching fraction measurements are well known: (1) a limit of resolution as small as or smaller than the Doppler width of spectral lines, (2) wavenumber accuracy to about 1 part in 10^8, (3) a very high rate of data collection, (4) broad spectral coverage from the UV to the infrared, and (5) a simultaneous measurement across all spectral resolution elements. The last advantage means that branching fraction measurements using a FTS are not sensitive to small drifts in light source performance. Seven FTS spectra were used in this work; the grating spectrometer was used only for deep UV measurements where the NSO FTS does not have adequate sensitivity.

Hollow cathode lamps operate far from local thermodynamic equilibrium (LTE) because of relatively low buffer gas pressures. The lack of LTE is not a concern in branching fraction measurements. Accurate transition probabilities can be determined from branching fractions as long as a radiative lifetime is available for

Table 1. Theoretical and experimental lifetime values, τ, in ns, and Landé g-factors in Lu II.

Level[a]	E(cm^{-1})[a]	τ (Experiment)		τ (Theory)		g-factors	
		Previous	This work	Previous[e]	This work[f]	Experiment[a]	This work[f]
6s6p $^3P_0^\circ$	27 264.40	61 ± 5[b]			69.66	0.00	0.00
6s6p $^3P_1^\circ$	28 503.16	37 ± 4[b]			37.60	1.51	1.47
		37.4 ± 1.9[c]					
6s6p $^3P_2^\circ$	32 453.26	42 ± 6[b]			46.47	1.66	1.50
5d6p $^3F_2^\circ$	41 224.96	3.7 ± 0.4[d]		5.18	5.31	0.71	0.77
5d6p $^3F_3^\circ$	44 918.68	3.8 ± 0.5[d]	5.09 ± 0.18	4.21	4.45	1.08	1.10
5d6p $^1D_2^\circ$	45 458.56	2.8 ± 0.3[d]		3.92	3.86	0.94	1.00
5d6p $^3D_1^\circ$	45 532.33	3.1 ± 0.2[b]		2.51	2.81	0.43	0.57
		2.4 ± 0.3[d]					
5d6p $^3D_2^\circ$	46 904.38	3.8 ± 0.5[d]		3.01	3.05	1.13	1.14
5d6p $^3F_4^\circ$	48 536.83	4.2 ± 0.4[d]	3.96 ± 0.16	3.25	3.45	1.25	1.25
5d6p $^3D_3^\circ$	48 733.19	4.0 ± 0.5[d]	3.80 ± 0.18	2.91	3.06	1.30	1.27
5d6p $^3P_1^\circ$	50 049.20	3.4 ± 0.5[d]		1.94	2.07	1.43	1.43
5d6p $^1F_3^\circ$	53 079.33		4.50 ± 0.22		3.96	1.02	1.05

[a] From Martin et al. (1978).
[b] Li & Lundberg (1998): time-resolved-laser spectroscopy.
[c] Den Hartog et al. (1998): laser-induced fluorescence.
[d] Andersen & Sorensen (1974), Andersen et al. (1975): beam-foil spectroscopy.
[e] Bord et al. (1998): HXR calculations.
[f] HFR + CP results.

each upper level of interest. The low collision rates of hollow cathode lamps provide a major advantage in studies of complex spectra because emission line shapes are usually dominated only by Doppler broadening. Far fewer line blends occur in hollow cathode spectra than occur in spectra from LTE sources. Possible blends of Lu lines with buffer gas lines were identified and corrected using two different buffer gases. Possible effects of radiation trapping were identified and corrected using spectra recorded at different lamp currents.

Three FTS spectra of the Lu–Ar hollow cathode lamp were recorded at lamp currents of 15, 12, and 10 mA during a 1997 June observing run at the NSO. These spectra had only four coadds (coherently added interferograms). Two additional FTS spectra of the Lu–Ar hollow cathode lamp at 30 mA current with 16 and 64 coadds were recorded during a 1998 June observing run. Signal-to-noise ratios on weaker lines were improved by higher lamp currents and additional coadds. Two FTS spectra of the Lu–Ne hollow cathode lamp at currents of 25 and 15 mA, each with eight coadds, were recorded during a 1998 June observing run. The UV beam splitter and 'Super Blue' photodiode detectors were used to record all spectra. These spectra cover the region from 35 000 to 8000 cm^{-1} with a limit of resolution of 0.053 cm^{-1}.

All the FTS data were analysed by using an interactive personal computer program that displays the spectra on a computer console. The Lu^+ energy levels tabulated by Martin, Zalubas & Hagan (1978) were used to calculate the wavenumbers of all possible transitions that satisfy parity and $J \leqslant 1$ selection rules. Lines were found, as expected, well within 0.05 cm^{-1} of the calculated positions, but most of the lines have substantial hyperfine structure. Apparent line intensities were determined using numerical integration across the line profile of the Lu II and selected Ar I and Ar II transitions. Even with the very high spectral resolving power of the FTS, the broad hyperfine structure of Lu II causes some spectral blends. The blend of the 16 706.92 cm^{-1} line from the $^3P_1$ level at 28 503.16 cm^{-1} is an example that has been discussed in earlier work (Den Hartog et al. 1998).

Apparent line intensities for selected sets of Ar I and Ar II lines were used to determine the relative efficiency as a function of wavenumber for each spectrum. Adams & Whaling (1981) identified and measured a set of Ar I and Ar II branching ratios for relative spectral efficiency calibration in the region from 4300 to 35 000 cm^{-1}. The lines selected are not prone to radiation trapping and are strong in typical hollow cathode emission spectra. Danzmann & Kock (1982) and Hashiguchi & Hasikuni (1985) have independently remeasured the selected Ar I and Ar II branching ratios. Whaling, Carle & Pitt (1993) recently provided a refined set of measurements. The apparent intensity of subsets of Ar I and Ar II lines from a common upper level divided by the branching ratios of the lines provided overlapping subsets of points which were used to construct a plot of the relative quantum efficiency of the FTS as a function of wavenumber. This (relative) spectroradiometric calibration procedure automatically includes the effects of variations in the window transmittance and/or reflectance of the back of the hollow cathode lamp.

The apparent line intensity for each Lu II line, when divided by the relative quantum efficiency of the FTS, yields the branching ratio for that line. These branching ratios were normalized to the dominant line from their respective upper levels. Weighting factors based on the signal-to-noise ratio of each line in each spectrum were used to compute the weighted mean branching ratio of the line. The mean branching ratios for lines from each upper level were converted to branching fractions by rescaling the ratios so that they sum to 1.0. The sensitivity of the NSO FTS is now rather poor in the deep UV above 35 000 cm^{-1} (its deep UV sensitivity was better in earlier years). The grating spectrometer mentioned above has good sensitivity in the deep UV, but much lower spectral resolving powers and inferior wavenumber accuracy to the FTS. Only the deep UV lines from the $^3D_3$ level

Table 2. Theoretical and experimental branching fractions obtained in this work for Lu II.

λ_{air}	Upper odd level		Lower even level		Branching fraction	
(Å)	E(cm^{-1})	J	E(cm^{-1})	J	Expt	HFR + CP
6463.11	27 264.40	0	11 796.24	1	1.000 ± 1%	1.000
3507.38	28 503.16	1	0.00	0	0.469 ± 7%	0.454
5983.89	28 503.16	1	11 796.24	1	0.160 ± 7%	0.167
6221.89	28 503.16	1	12 435.32	2	0.371 ± 7%	0.376
4839.62	32 453.26	2	11 796.24	1	0.017 ± 10%	0.017
4994.13	32 453.26	2	12 435.32	2	0.178 ± 3%	0.178
5476.68	32 453.26	2	14 199.08	3	0.797 ± 1%	0.791
3397.07	41 224.96	2	11 796.24	1	0.441 ± 5%	0.482
3472.48	41 224.96	2	12 435.32	2	0.420 ± 5%	0.353
4184.26	41 224.96	2	17 332.58	2	0.124 ± 8%	0.146
8459.16	41 224.96	2	29 406.70	2	0.015 ± 20%	0.019
3077.61	44 918.68	3	12 435.32	2	0.631 ± 3%	0.646
3254.31	44 918.68	3	14 199.08	3	0.307 ± 5%	0.271
3623.98	44 918.68	3	17 332.58	2	0.057 ± 11%	0.049
2911.39	48 536.83	4	14 199.08	3	0.957 ± 4%	0.963
2754.17	48 733.19	3	12 435.32	2	0.350 ± 3%	0.365
2894.84	48 733.19	3	14 199.08	3	0.631 ± 2%	0.527
2571.23	53 079.33	3	14 199.08	3	0.175 ± 5%	0.223
2796.63	53 079.33	3	17 332.58	2	0.798 ± 2%	0.594

Table 3. Experimental and theoretical (HFR + CP) oscillator strengths as deduced in the present work. Only transitions involving upper levels below 70 000 cm^{-1} with wavelengths shorter than 1 μm and $gf \geqslant 0.001$ are quoted.

λ^a	Lower level			Upper level			gf	
(Å)	E (cm^{-1})^b	J		E (cm^{-1})^b	J		HFR + CP^c	Expt^d
1691.41	0.00	0	(e)	59 122.40	1	(o)	0.475	
1998.03	0.00	0	(e)	50 049.20	1	(o)	0.031	
2141.25	12 435.32	2	(e)	59 122.40	1	(o)	0.005	
2195.56	0.00	0	(e)	45 532.33	1	(o)	0.155	
2392.20	17 332.58	2	(e)	59 122.40	1	(o)	0.957	
2459.64	12 435.32	2	(e)	53 079.33	3	(o)	0.007	
2469.27	28 503.16	1	(o)	68 988.80	0	(e)	0.033	
2536.96	11 796.24	1	(e)	51 201.66	2	(o)	0.055	
2571.23	14 199.08	3	(e)	53 079.33	3	(o)	0.391	0.270 ± 7%
2578.79	12 435.32	2	(e)	51 201.66	2	(o)	0.577	
2613.40	11 796.24	1	(e)	50 049.20	1	(o)	0.648	
2615.41	0.00	0	(e)	38 223.49	1	(o)	1.394	
2619.26	11 796.24	1	(e)	49 963.58	0	(o)	0.488	
2657.80	12 435.32	2	(e)	50 049.20	1	(o)	0.766	
2701.71	14 199.08	3	(e)	51 201.66	2	(o)	1.341	
2738.17	27 264.40	0	(o)	63 774.30	1	(e)	0.217	
2754.17	12 435.32	2	(e)	48 733.19	3	(o)	0.953	0.734 ± 6%
2796.63	17 332.58	2	(e)	53 079.33	3	(o)	1.231	1.456 ± 5%
2834.35	28 503.16	1	(o)	63 774.30	1	(e)	0.593	
2847.51	11 796.24	1	(e)	46 904.38	2	(o)	0.592	
2894.84	14 199.08	3	(e)	48 733.19	3	(o)	1.517	1.461 ± 5%
2900.30	12 435.32	2	(e)	46 904.38	2	(o)	0.771	
2911.39	14 199.08	3	(e)	48 536.83	4	(o)	3.196	2.766 ± 6%
2951.68	17 332.58	2	(e)	51 201.66	2	(o)	0.482	
2963.32	11 796.24	1	(e)	45 532.33	1	(o)	0.580	
2969.81	11 796.24	1	(e)	45 458.56	2	(o)	0.263	
3020.54	12 435.32	2	(e)	45 532.33	1	(o)	0.455	
3027.29	12 435.32	2	(e)	45 458.56	2	(o)	0.002	
3055.66	17 332.58	2	(e)	50 049.20	1	(o)	0.003	
3056.72	14 199.08	3	(e)	46 904.38	2	(o)	0.543	
3077.61	12 435.32	2	(e)	44 918.68	3	(o)	1.449	1.233 ± 5%
3183.73	17 332.58	2	(e)	48 733.19	3	(o)	0.036	
3191.82	32 453.26	2	(o)	63 774.30	1	(e)	0.916	
3198.11	14 199.08	3	(e)	45 458.56	2	(o)	0.402	
3249.48	38 223.49	1	(o)	68 988.80	0	(e)	0.568	
3254.31	14 199.08	3	(e)	44 918.68	3	(o)	0.680	0.671 ± 6%
3364.26	29 406.70	2	(e)	59 122.40	1	(o)	0.002	
3380.63	17 332.58	2	(e)	46 904.38	2	(o)	0.016	
3397.07	11 796.24	1	(e)	41 224.96	2	(o)	0.781	
3472.48	12 435.32	2	(e)	41 224.96	2	(o)	0.601	
3507.38	0.00	0	(e)	28 503.16	1	(o)	0.067	0.069 ± 9%^{e}
3545.12	17 332.58	2	(e)	45 532.33	1	(o)	0.001	
3554.42	17 332.58	2	(e)	45 458.56	2	(o)	1.533	
3623.98	17 332.58	2	(e)	44 918.68	3	(o)	0.154	0.154 ± 11%
3782.90	11 796.24	1	(e)	38 223.49	1	(o)	0.001	
3876.65	12 435.32	2	(e)	38 223.49	1	(o)	0.082	
3912.66	38 223.49	1	(o)	63 774.30	1	(e)	0.032	
4184.26	17 332.58	2	(e)	41 224.96	2	(o)	0.360	
4223.10	29 406.70	2	(e)	53 079.33	3	(o)	0.016	
4259.51	35 652.10	0	(e)	59 122.40	1	(o)	0.001	
4262.02	45 532.33	1	(o)	68 988.80	0	(e)	0.044	
4342.03	36 098.18	2	(e)	59 122.40	1	(o)	0.253	
4430.33	36 557.05	1	(e)	59 122.40	1	(o)	0.002	
4433.48	41 224.96	2	(o)	63 774.30	1	(e)	0.002	
4505.22	30 889.09	3	(e)	53 079.33	3	(o)	0.022	
4586.93	29 406.70	2	(e)	51 201.66	2	(o)	0.019	
4785.43	17 332.58	2	(e)	38 223.49	1	(o)	0.012	
4839.62	11 796.24	1	(e)	32 453.26	2	(o)	0.007	
4843.02	29 406.70	2	(e)	50 049.20	1	(o)	0.027	
4858.74	32 503.62	4	(e)	53 079.33	3	(o)	0.039	
4865.42	38 574.94	2	(e)	59 122.40	1	(o)	0.256	
4921.69	30 889.09	3	(e)	51 201.66	2	(o)	0.064	
4994.13	12 435.32	2	(e)	32 453.26	2	(o)	0.072	
5172.81	29 406.70	2	(e)	48 733.19	3	(o)	0.002	
5278.47	50 049.20	1	(o)	68 988.80	0	(e)	0.010	
5458.27	45 458.56	2	(o)	63 774.30	1	(e)	0.018	
5476.68	14 199.08	3	(e)	32 453.26	2	(o)	0.383	
5480.34	45 532.33	1	(o)	63 774.30	1	(e)	0.001	

Table 3 – *continued*

λ^a	Lower level			Upper level			*gf*	
(Å)	E (cm^{-1})^b	J		E (cm^{-1})^b	J		HFR + CP^c	Expt^d
5602.54	30 889.09	3	(e)	48 733.19	3	(o)	0.015	
5664.88	30 889.09	3	(e)	48 536.83	4	(o)	0.040	
5713.46	29 406.70	2	(e)	46 904.38	2	(o)	0.030	
5887.25	36 098.18	2	(e)	53 079.33	3	(o)	0.033	
5926.07	46 904.38	2	(o)	63 774.30	1	(e)	0.004	
5983.89	11 796.24	1	(e)	28 503.16	1	(o)	0.072	0.069 ± 9%^{e}
6159.89	32 503.62	4	(e)	48 733.19	3	(o)	1.167	
6199.59	29 406.70	2	(e)	45 532.33	1	(o)	0.463	
6221.89	12 435.32	2	(e)	28 503.16	1	(o)	0.175	0.173 ± 9%^{e}
6228.09	29 406.70	2	(e)	45 458.56	2	(o)	0.088	
6235.33	32 503.62	4	(e)	48 536.83	4	(o)	0.527	
6242.31	30 889.09	3	(e)	46 904.38	2	(o)	0.759	
6444.85	29 406.70	2	(e)	44 918.68	3	(o)	0.030	
6463.11	11 796.24	1	(e)	27 264.40	0	(o)	0.089	
6611.63	17 332.58	2	(e)	32 453.26	2	(o)	0.008	
6619.16	36 098.18	2	(e)	51 201.66	2	(o)	0.102	
6826.57	36 557.05	1	(e)	51 201.66	2	(o)	0.071	
6861.77	30 889.09	3	(e)	45 458.56	2	(o)	0.008	
6892.56	38 574.94	2	(e)	53 079.33	3	(o)	0.085	
6943.93	35 652.10	0	(e)	50 049.20	1	(o)	0.073	
7125.83	30 889.09	3	(e)	44 918.68	3	(o)	0.389	
7165.96	36 098.18	2	(e)	50 049.20	1	(o)	0.088	
7238.76	49 963.58	0	(o)	63 774.30	1	(e)	0.017	
7283.91	50 049.20	1	(o)	63 774.30	1	(e)	0.045	
7409.68	36 557.05	1	(e)	50 049.20	1	(o)	0.081	
7457.00	36 557.05	1	(e)	49 963.58	0	(o)	0.095	
7912.34	36 098.18	2	(e)	48 733.19	3	(o)	0.062	
7917.54	38 574.94	2	(e)	51 201.66	2	(o)	0.240	
7951.59	51 201.66	2	(o)	63 774.30	1	(e)	0.067	
8052.52	32 503.62	4	(e)	44 918.68	3	(o)	0.007	
8459.16	29 406.70	2	(e)	41 224.96	2	(o)	0.186	
8712.77	38 574.94	2	(e)	50 049.20	1	(o)	0.035	
8949.63	17 332.58	2	(e)	28 503.16	1	(o)	0.003	
9661.68	36 557.05	1	(e)	46 904.38	2	(o)	0.051	
9672.39	30 889.09	3	(e)	41 224.96	2	(o)	0.001	
9841.52	38 574.94	2	(e)	48 733.19	3	(o)	0.011	
9926.01	28 503.16	1	(o)	38 574.94	2	(e)	0.001	

[a] Wavelengths are deduced from the experimental energy levels compiled by Martin et al. (1978).They are given in vacuum below 2000 Å and in air above that limit.
[b] From Martin et al. (1978).
[c] This work: see the text (Section 4).
[d] This work: the *gf*-values are obtained from the combination of the experimental radiative lifetimes of Table 1 with the measured branching fractions reported in Table 2.
[e] Deduced using the 6s6p $^3P_1^\circ$ lifetime measured by Den Hartog et al. (1998).
(o) odd parity level; (e) even parity level.

at 48 733 cm^{-1} and $^1F_3$ level at 53 079 cm^{-1} were measured using the grating spectrometer. A deuterium lamp with a NIST (National Institute of Standards and Technology) traceable calibration as a standard of spectral irradiance was used to determine the relative quantum efficiency of the grating spectrometer as a function of wavenumber.

Uncertainties in the branching fractions were determined in a multistep process. In the first step a standard deviation for the weighted mean branching ratio, referenced to the dominant line from the upper level, was computed. Up to five independently calibrated measurements contributed to this standard deviation. For a few lines, which had poor signal-to-noise ratios, or which appeared in only two or three spectra, the standard deviation of the weighted mean was replaced by a larger number based on a fractional uncertainty estimated as the inverse of the signal-to-noise ratios combined in quadrature. The second step involved combining in quadrature twice the preceding standard deviation with a radiometric calibration uncertainty estimated as 0.001 per cent per cm^{-1} of separation between the line of interest and the dominant line from the upper level. This radiometric calibration uncertainty includes the effect of possible errors in the Ar I and Ar II branching ratios. The resulting number is the branching ratio uncertainty. In the third step, branching ratio uncertainties were combined using a standard error propagation formula to determine a branching fraction uncertainty. Error propagation to the branching fractions affects lines differently; for example, a level that decays on two nearly equally strong lines with a ±10 per cent uncertainty for the single branching ratio will have ±5 per cent uncertainty for two branching fractions. A level that decays primarily on a single dominant line, but also has some weak lines, yields a different result: the largest uncertainties 'migrate' to the branching fractions of the weaker lines from the upper level, while the branching fraction of the dominant line has a small uncertainty. Branching fractions of weak lines which have large final uncertainties are dropped from the table, but are kept in the branching fraction calculation. The sum of the branching fractions from an upper level in the table is less than 1 in some cases because of those branches that were dropped. The possibility of

other missing branches to currently unknown lower levels is not a concern because of the simplicity of Lu II.

The experimental branching fractions obtained in the present work are given in Table 2, where they are compared with the HFR data obtained by following the procedure described in Section 4.

The first three FTS spectra discussed above were used by Den Hartog et al. (1998) to determine branching fractions from the $^3P_1$ level at 27 530 cm^{-1}. Our branching fractions for lines from this level agree with Den Hartog et al. (1998) to within a small fraction of the uncertainties, and the differences are caused by our averaging of measurements from additional spectra into our final results.

4 HFR CALCULATIONS

For heavy ions such as Lu II, accurate calculations of atomic structure should allow for both intravalence and core–valence correlation. Migdalek & Baylis (1978) have suggested an approach in which the largest part of the intravalence correlation is represented within a configuration interaction scheme, while core–valence correlation is represented approximately by a core-polarization model potential. For atoms with n valence electrons, the one-particle operator of this potential can be written as

$$V_{\rm P1} = -\frac{1}{2}\alpha_{\rm d}\sum_{i=1}^{n}\frac{r_i^2}{(r_i^2+r_{\rm c}^2)^3}, \tag{1}$$

where $\alpha_{\rm d}$ is the dipole polarizability of the core and $r_{\rm c}$ is the cut-off radius, which is arbitrarily chosen as a measure of the size of the ionic core. This latter parameter is usually taken as the expectation value of r for the outermost core orbitals.

In addition, the interaction between the modified electric fields experienced by the valence electrons gives rise to a two-particle term given by

$$V_{\rm P2} = -\alpha_{\rm d}\sum_{i>j}\frac{\boldsymbol{r}_i\cdot\boldsymbol{r}_j}{[(r_i^2+r_{\rm c}^2)(r_j^2+r_{\rm c}^2)]^{3/2}}. \tag{2}$$

A further correction, introduced by Hameed, Herzenberg & James (1968) and Hameed (1972) to allow for more accurate treatment of the penetration of the core by the valence electrons, corresponds in the present formalism to the addition to the integral

$$\int_0^\infty P_{nl}(r)\frac{r}{(r^2+r_{\rm c}^2)^{3/2}}P_{n'l'}(r)\,{\rm d}r \tag{3}$$

in (2) of the core-penetration term

$$\frac{1}{r_{\rm c}^3}\int_0^{r_{\rm c}} P_{nl}(r)rP_{n'l'}(r)\,{\rm d}r. \tag{4}$$

When including the core polarization and core penetration in the Hamiltonian, the dipole-moment operator in the transition matrix element has also to be modified for consistency. The dipole radial integral

$$\int_0^\infty P_{nl}(r)rP_{n'l'}(r)\,{\rm d}r \tag{5}$$

has to be replaced by

$$\int_0^\infty P_{nl}(r)r\left[1-\frac{\alpha_{\rm d}}{(r^2+r_{\rm c}^2)^{3/2}}\right]P_{n'l'}(r)\,{\rm d}r - \frac{\alpha_{\rm d}}{r_{\rm c}^3}\int_0^{r_{\rm c}} P_{nl}(r)rP_{n'l'}(r)\,{\rm d}r. \tag{6}$$

In the present work, the wavefunctions were obtained by the HFR method described by Cowan & Griffin (1976) using the suite of computer codes written by Cowan (1981), in which we have incorporated the core-polarization and core-penetration corrections (CP) as described above. Outer correlation was considered among the configurations $4f^{14}6s^2$, $4f^{14}5d6s$, $4f^{14}5d7s$, $4f^{14}5d6d$, $4f^{14}6s6d$, $4f^{14}6s7s$, $4f^{14}5d^2$, $4f^{14}6p^2$ and $4f^{14}6d^2$ for the even parity and $4f^{14}5d6p$, $4f^{14}5d7p$, $4f^{14}6s6p$, $4f^{14}6s7p$, $4f^{14}6p6d$, $4f^{14}5d5f$, $4f^{14}5d6f$, $4f^{14}6s5f$ and $4f^{14}6s6f$ for the odd parity. The dipole polarizability of the ionic core, $\alpha_{\rm d}$, has been chosen equal to $5.20a_0^3$, which corresponds to the value reported by Fraga, Karwowski & Saxena (1976) in the case of Lu IV. For the cut-off radius, $r_{\rm c}$, we have used the average value $\langle r\rangle$ for the outermost core orbitals ($5p^6$) as calculated by the Cowan's code, i.e. $r_{\rm c} = 1.387a_0$. Using a well-established least-squares fitting procedure (Cowan 1981), the radial parameter values have been adjusted to obtain the best agreement between the calculated and the experimental energy levels compiled by Martin et al. (1978). For the configurations for which no experimental energy levels are available, the Slater integrals have been scaled down by a factor 0.85 while the ab initio values of the spin-orbit parameters have been used without scaling.

5 DISCUSSION

The HFR + CP lifetime values calculated in the present work agree well with the laser measurements also obtained in this work. The mean ratio $\tau_{\rm exp}/\tau_{\rm HFR}$ is 1.17 ± 0.05 and this ratio is remarkably constant for the four levels considered. The HFR + CP lifetimes for 6s6p $^3P^\circ_{0,1,2}$ are in close agreement with the recent laser measurements of Den Hartog et al. (1998) and Li & Lundberg (1998).

From Table 2, it also appears that theoretical branching ratios agree with experiment (within the errors) for most of the transitions quoted. The HFR + CP oscillator strengths calculated in the present work are reported in Table 3. We also give in the same table the experimental oscillator strengths derived from the laser measurements as well as the experimental branching ratios measured in this work.

The theoretical Landé g-factors obtained in the present work (some of which are quoted in the last column of Table 1) agree well (generally within 10 per cent) with the experimental values compiled by NIST (Martin et al. 1978) and taken from Anderson (1956) and Pinnington (1963a). They differ more substantially (15–35 per cent) for four levels (36 098.18, 38 574.94, 45 532.33 and 59 122.4 cm^{-1}). It should be emphasized that the values measured for the first three of these levels may not be accurate, as they were determined from Zeeman patterns that were incompletely resolved (Anderson 1956). Furthermore, in all four cases the result may have been affected by hyperfine structure. It is worth noting that many levels in Lu I and Lu II show unusually large hyperfine structures (Pinnington 1963a,b).

The solar abundance of Lu has been recently rediscussed by Bord et al. (1999) and Den Hartog et al. (1998). The present work entirely confirms the result obtained by Den Hartog et al. concerning the agreement between photospheric and meteoritic chemical compositions.

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