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Landé g-factors along the sixth row of the periodic table

É Biémont[1,2], P Palmeri[1] and P Quinet[1,2]

[1] Astrophysique et Spectroscopie, Université de Mons, 20 Place du Parc, B-7000 Mons, Belgium
[2] IPNAS, Université de Liège, B15 Sart Tilman, B-4000 Liège, Belgium

E-mail: E.Biemont@ulg.ac.be

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Abstract
Landé g-factors are calculated, in intermediate coupling, for 2084 levels belonging to atoms or ions of the sixth row of the periodic table. Extensive configuration interaction and relativistic effects are included in the framework of the relativistic Hartree–Fock approximation including core-polarization effects. The results have been refined using least-squares fittings of the Hamiltonian eigenvalues to the observed energy levels (when available). The new results fill in some gaps in the existing data for a large number of levels belonging to ions of astrophysical interest and are expected to be useful for investigating magnetic fields in CP stars.

1. Introduction

In astrophysics, strong magnetic fields have been detected in hot stars of types O, B and A. Definite spectropolarimetric detections have been reported, e.g. for Ap, Be or β Cephei stars, the field strength reaching in some cases several tens of kG (Mathys 1999). In the case of magnetic Ap stars extensively studied over the past few years, the oblique rotator model is accepted as the plausible explanation of the observed characteristics, which include spectral variations correlated with the rotation period and the magnetic-field modifications. More precisely, magnetic fields have been detected and measured from the observation of their circular polarization signatures in spectral lines (see e.g. Hubrig *et al* 2009; Elkin *et al* 2008; Freyhammer *et al* 2008). Detailed investigations of these magnetic fields require the knowledge of accurate Landé g-factors. Many of these g-factors are unknown or inadequately known, particularly for the heavy elements of the sixth row of the periodic table. The gaps in the atomic data concern the neutral atoms but also the low-charged ions (in the first three ionization stages) whose lines are now currently identified in the available high-resolution stellar spectra. In the past, some experimental data have been published in successive NIST compilations (see e.g. Moore 1958, 1971) but data for many levels (even of low excitation energy) are still lacking or, when they exist, their accuracy frequently suffers from the limitations inherent in old laboratory analyses.

Theoretical work on g-factors in heavy atoms or ions is still very scarce in view of the complexity of the calculations. *Ab initio* calculations however (MCDF approach) have been reported for the lowest $4f^N6s^2$ configurations of neutral rare-earth atoms (Cheng and Childs 1985).

These considerations have motivated us to undertake a systematic investigation of the Landé g-factors of the sixth-row elements and of their first ions using a theoretical approach combined with a least-squares fitting (LSF) procedure of calculated values to the experimental ones (when available) in order to refine the accuracy of the predicted values.

2. Basic considerations

The Landé g-factor of an atomic level is related to the energy shift of the sublevels having magnetic quantum number M by:

$$\Delta E = gM\mu_0 B \tag{1}$$

where B is the magnetic field intensity and μ_0 the Bohr magneton.

In pure LS coupling, the g-factor is given by:

$$g_{LSJ} = 1 + (g_S - 1) \times \frac{J(J+1) - L(L+1) + S(S+1)}{2J(J+1)} \tag{2}$$

where g_S is the g-value for a pure electron spin (S level), a value of 2 for g_S yielding the Landé formula.

In intermediate coupling, the Landé g-factor is given by

$$g_{\gamma J} = \sum_{\alpha LS} g_{LSJ} |\langle \alpha LSJ | \gamma J \rangle|^2 \tag{3}$$

where the summation is extended over the same set of quantum numbers as for the wavefunction $|\gamma J M\rangle$ of the M sublevel of a level γJ. $|\gamma J M\rangle$ is expressed in terms of LS basis states $|\alpha L S J M\rangle$ by:

$$|\gamma J M\rangle = \sum_{\alpha L S} |\alpha L S J M\rangle \langle \alpha L S J | \gamma J \rangle. \quad (4)$$

Calculations in heavy ions, such as those considered here, are not obvious and their accuracy basically suffers from the limited configuration interaction (CI) one is able to introduce in the calculations. These limitations are discussed in detail in section 5.

Of course, experimental approaches are also used for investigating the Landé factors in heavy atoms and ions and these values are most welcome in assessing the accuracy of the theoretical models. Most of the experimental results, however, have been published a long time ago (see e.g. the different NIST compilations (Moore 1958, 1971) for more details). More recent efforts have also been attempted and can be mentioned (see e.g. Zhang *et al* 2008). We will not, however, further discuss the experimental methods in the present context but systematically show comparisons between theoretical and experimental results in the different figures and tables of this paper.

3. Context of the present work

In the recent past, our group has been involved in large-scale determination of radiative properties (e.g. transition probabilities, f-values, branching fractions, and lifetimes) of heavy atoms and ions. Many results obtained for the lanthanides (atoms and ions in the first two ionization stages) are stored in the database DREAM (**D**atabase for **R**are-**EA**rth at **M**ons University), accessible at the URL address http://www.umh.ac.be/∼astro/dream.shtml). More details can be found in Biémont and Quinet (2005). Similar results for the neutral, singly or multiply ionized elements belonging to the sixth row of the periodic table are stored in the database DESIRE (**D**atabas**E** on the **SI**xth **R**ow **E**lements) accessible at http://www.umh.ac.be/∼astro/desire.shtml. To date, DESIRE contains results for the following ions: Ta I, W II, W III, Re I, Re II, Os I, Os II, Ir I, Ir II, Au I, Au II, Tl I, Pb I and Bi II, but is regularly updated. More details can be found in Fivet *et al* (2007).

All the results available in these two databases were obtained from theoretical calculations, using a relativistic Hartree–Fock method (Cowan 1981) including core-polarization effects (HFR+CPOL approach), eventually combined with an LSF adjustment of the Hamiltonian eigenvalues to the observed energy levels. The accuracy of the calculations was systematically tested through detailed and extensive comparisons with experimental data, essentially lifetimes measured using the time-resolved laser-induced fluorescence (TR-LIF) spectroscopy or branching fractions (BF) determined by Fourier transform spectroscopy. These systematic comparisons allowed us to assess the reliability of the calculations on a firm basis. For more details, see the relevant papers quoted on the above URL addresses.

In the same context, we also calculated Landé g-factors for a number of atoms and ions, particularly the doubly ionized lanthanides atoms (Quinet and Biémont 2004), for which there was a definite requirement in astrophysics. In the present work, we describe a large-scale determination of Landé factors for selected ions of the sixth-row elements also needed by astrophysicists. Samples of the results obtained so far are shown in the present paper, and extensive comparisons with the available experimental data are also made. These must be considered as a first step toward a thorough investigation of the Landé factors for neutral elements, and of the low-charged ions of this group.

4. HFR+CPOL calculations

The calculations reported and discussed in the following sections have been performed with the HFR+CPOL approach. CPOL effects were introduced in the calculations using a method already discussed elsewhere (see e.g. Quinet *et al* 1999; Biémont and Quinet 2003; Biémont 2005). Most of the intravalence correlation is represented within a CI scheme, while core-valence correlation for systems with more than one valence electron is described by a CPOL potential. For an atom with n valence electrons, the one-particle operator of the potential can be expressed as:

$$V_P = -\frac{1}{2}\alpha_{\rm d} \sum_{i=1}^{n} \frac{r_i^2}{\left(r_i^2 + r_{\rm c}^2\right)^3} \quad (5)$$

where $\alpha_{\rm d}$ is the static dipole polarizability of the ionic core and $r_{\rm c}$ is a cut-off radius.

As no experimental data are available for the static dipole polarizabilities of the heavy elements or ions, we have systematically adopted for this parameter the values from Fraga *et al* (1976) while, for the cut-off radius, $r_{\rm c}$, the values retained were the HFR expectation value of $\langle r \rangle$ for the outermost core orbital. The values of the parameters α_d and r_c adopted in the present work are summarized in table 1.

5. Results and discussion

5.1. Ta ($Z = 73$)

In Ta I, the reported calculations (Fivet *et al* Fivet *et al* 2006a) included the configurations $5d^36s^2$, $5d^4ns$ (n = 6–7), $5d^46d$, $5d^5$, $5d^36p^2$, $5d^36s7s$, $5d^36s6d$, $5d^26s^26d$, $5d^26s6p^2$ and $5d^4np$ (n = 6–7), $5d^36snp$ (n = 6–7), $5d^36snf$ (n = 5–6), $5d^26s^26p$, $5d^26s^2nf$ (n = 5–6), the known energy levels having been determined experimentally by Van den Berg *et al* (1952). An LSF procedure was applied using the levels taken from the compilation available (from the web site): http://iep.tu-graz.ac.at/ta.html, which incorporates levels from an analysis by Guthöhrlein *et al* (1995) with more recent updates. The low-lying levels at 11796.14, 14875.70, 21091.53 and 22434.37 cm^{-1} were excluded from the fit for the reasons stated in Fivet *et al* (2006a). The high-energy odd levels (above 38 000 cm^{-1}) were also excluded because, due to strong CI, an unambiguous connection between experimental and calculated levels could not be established, even when

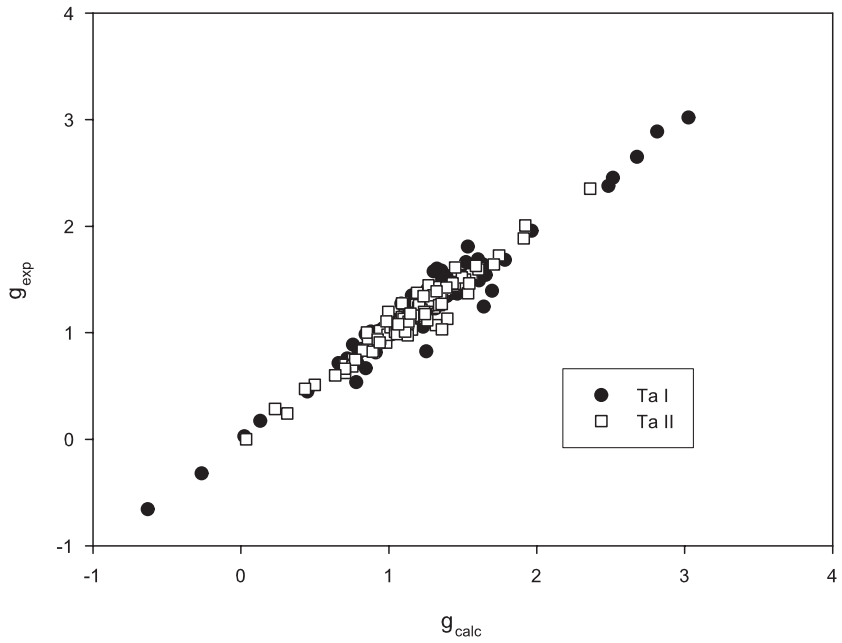

Figure 1. Comparison between the HFR+CPOL(B) Landé factors and the experimental values from Moore (1958, 1971) in Ta I (filled circles). In Ta II (squares) the previous data are taken from Wyart (1978) and Wyart and Blaise (1990).

Table 1. Static dipole polarizability, α_d, and cut-off radius, r_c, adopted for the different ions. All the data are given in a.u. We give also the outermost core orbital corresponding to the calculation of r_c and the ionic core corresponding to the value of α_d.

Ion	α_d^a	r_c^b	Ionic core
Ta I	(A) 6.75	2.20 (5d)	$5p^6$ Ta^{5+}
	(B) 2.81	1.31 (5p)	$5d^3$ Ta^{2+}
Ta II	(A) 3.18	1.30 (5p)	$4f^{14}$ Ta^{5+}
	(B) 6.75	1.95 (5d)	$4f^{14}5d^2$ Ta^{3+}
Ta III	3.18	1.30 (5p)	$4f^{14}$ Ta^{5+}
W II	(A) 2.80	1.26 (5p)	$4f^{14}$ W^{6+}
	(B) 4.59	1.77 (5d)	$4f^{14}5d^2$ W^{4+}
W III	(A) 2.80	1.25 (5p)	$4f^{14}$ W^{6+}
	(B) 4.00	1.66 (5d)	$4f^{14}5d$ W^{5+}
Re I	6.81	1.87 (5d)	$5d^4$ Re^{3+}
Re II	2.58	1.22 (5p)	$4f^{14}$ Re^{7+}
Os I	6.55	1.74 (5d)	$5d^6$ Os^{3+}
Os II	6.55	1.74 (5d)	$5d^6$ Os^{3+}
Ir I	6.48	1.60 (5d)	$5d^6$ Ir^{3+}
Ir II	4.59	1.61 (5d)	$5d^5$ Ir^{4+}
Pt II	4.52	1.55 (5d)	$5d^6$ Pt^{4+}
Au I	8.70	1.58 (5d)	$5d^8$ Au^{3+}
Au II	4.45	1.47 (5d)	$5d^7$ Au^{4+}
Pb I	3.98	1.29 (5d)	$6s^26p^2$ Pb^{4+}
Bi II	(A) 15.05	2.18 (6s)	$5d^66s^2$ Bi^{3+}
	(B) 15.05	2.18 (6s)	$5d^66s^2$ Bi^{3+}
	(C) 3.20	1.22 (5d)	$5d^6$ Bi^{5+}

[a] Data from Fraga *et al* (1976) except when otherwise indicated.
[b] Calculated HFR values: see the text. (A), (B) and (C) correspond to the different models used. See the text for more details.

using the available experimental Landé factors. The standard deviation (s.d.) obtained in the fit was 140 cm^{-1} for the even parity (28 levels) and 266 cm^{-1} for the odd parity (106 levels). The Landé factors calculated for 142 Ta I levels are reported in the DESIRE database. They are compared with available results (Moore 1958, 1971) in figure 1.

In Ta II, the g-factors were reported and discussed recently (Quinet *et al* 2009) and, consequently, no more details will be given in the present paper. For a comparison with the previous data of Wyart (1977) and Wyart and Blaise (1990), see figure 1.

The extensive calculations performed in Ta III (Fivet *et al* 2008) were based on the following configuration sets: $5d^3 + 5d^26s + 5d^26d + 5d6s^2 + 5d6p^2 + 5d6d^2 + 5d5f^2 + 5d6f^2 + 5d6s6d + 5d6pnf$ (n = 5–6) + $5d5f6f + 6s^26d + 6s6p^2 + 6p^26d + 6s6d^2 + 6d^3 + 6s5f^2 + 6d5f^2 + 6s6f^2 + 6d6f^2$ and $5d^26p + 5d^2nf$ (n = 5–6) + $5d6s6p + 5d6snf$ (n = 5–6) + $5d6p6d + 5d6dnf$ (n = 5–6) + $6s^26p + 6s^2nf$ (n = 5–6) + $6p^2nf$ (n = 5–6) + $6p^3 + 6p6d^2 + 6d^2nf$ (n = 5–6) + $6p5f^2 + 6p6f^2 + 5f^26f + 5f6f^2$. In the LSF procedure, we used all Azarov *et al*'s experimentally established levels (2003), i.e. 37 even levels and 68 odd levels. The s.d. in the fitting procedures was 145 and 191 cm^{-1} for the even and odd parities, respectively. The calculated Landé factors reported in DESIRE for 105 levels are in reasonable agreement with the results of Azarov *et al* (2003).

5.2. *W* ($Z = 74$)

In singly ionized tungsten (W II), a $4f^{14}5d^2$ Yb-like ionic core surrounded by three electrons was adopted in the calculations of Nilsson *et al* (2008). For the valence–valence interactions, we included in the vectorial basis the configurations $5d^5$, $5d^4ns$ (n = 6–8), $5d^36sns$ (n = 6–8), $5d^46d$, $5d^36s6d$, $5d^26s^26d$ and $5d^36p^2$ (even parity) and $5d^4np$ (n = 6–8), $5d^36snp$ (n = 6–8), $5d^26s^26p$ and $5d^26p^3$ (odd parity). The HFR+CPOL approach was then combined with an LSF minimizing the discrepancies between calculated and experimental energy

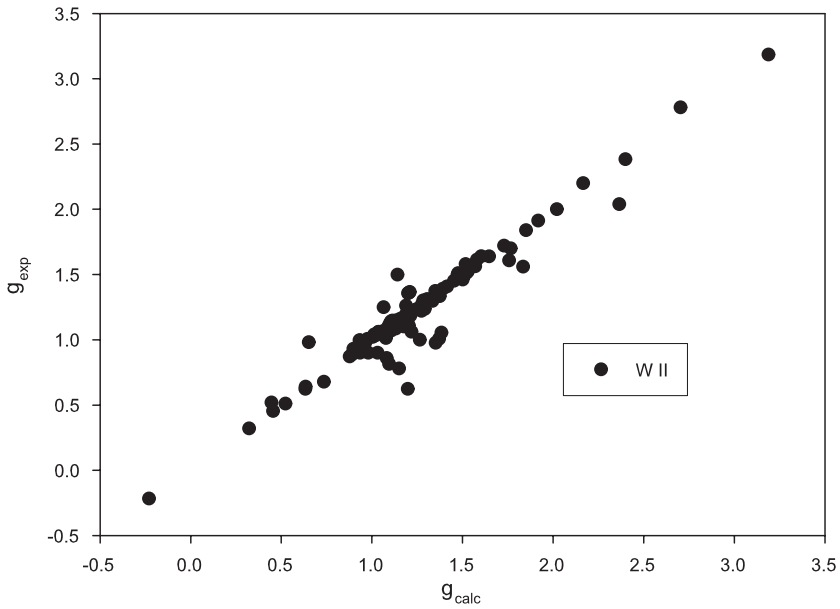

Figure 2. Comparison between the HFR+CPOL(B) Landé factors and the results compiled by Kramida and Shirai (2006) for W II.

levels from Kramida and Shirai's compilation (2006). 263 levels were included in the fitting process and the s.d. of the fits was found to be 99 cm^{-1} and 138 cm^{-1} for the even and odd parities respectively. The results are reported in table 2 and they are compared in figure 2 with the g-values taken from Kramida and Shirai (2006). For 29 of the 34 levels common to both works, the agreement is excellent (a few per cent). Somewhat larger discrepancies are observed for five levels.

Two sets of calculations were reported for W III (Palmeri *et al* 2008). In the first one, an Er-like ionic core ($4f^{14}$) surrounded by four valence electrons was adopted. In the second model, we adopted a $4f^{14}5d$ Tm-like ionic core surrounded by three valence electrons. In both cases, the following configurations were included in the vectorial basis: $5d^4 + 5d^3ns$ ($n = 6$–8) + $5d^26sns$ ($n = 6$–8) + $5d^36d$ + $5d^26s6d + 5d6s^26d + 5d^26p^2$ and $5d^3np$ ($n = 6$–8) + $5d^26snp$ ($n = 6$–8) + $5d6s^26p$. All the 235 experimentally known levels, belonging to the $5d^4$, $5d^36s$, $5d^26s^2$, $5d^36p$ and $5d^26s6p$ configurations (Iglesias *et al* 1989), were included in the LSF process. The s.d. in the fits was found to be 122 and 241 cm^{-1} for the two parities. The new Landé factors are stored in the database DESIRE (235 levels). There are no data available for comparison.

5.3. *Re* ($Z = 75$)

Calculations of f values and radiative lifetimes in Re I have been reported by Palmeri *et al* (2006). The following configurations were considered in the theoretical model: $5d^6ns$ ($n = 6$–8), $5d^56sns$ ($n = 6$–8), $5d^7$, $5d^66d$, $5d^56s6d$, $5d^46s^26d$, $5d^56p^2$, $5d^46s6p^2$ and $5d^6np$ ($n = 6$–8), $5d^56snp$ ($n = 6$–8), $5d^46s^26p$, $5d^46p^3$. An LSF procedure minimizing the discrepancies between the calculated eigenvalues and the experimental levels of Klinkenberg *et al* (1957) and Wyart (1978) was applied. 54 even-parity levels below 36 000 cm^{-1} and 97 odd-parity levels, below 50 000 cm^{-1} and belonging to the $5d^66s$, $5d^56s^2$, $5d^7$, $5d^66p$ and $5d^46s^26p$ configurations, were retained for the adjustment procedure. The s.d. of the fits was found equal to 88 and 176 cm^{-1} for the even and odd parities respectively. The calculated and the experimental Landé g-factors (Klinkenberg *et al* 1957) reported in DESIRE (160 levels), generally agree within 10% (see figure 3). For the levels for which the discrepancy is larger, incorrect correspondence between calculated and observed levels cannot be ruled out.

In Re II, the results were discussed in detail by Palmeri *et al* (2005) with respect to the valence–valence correlations. The interactions between the following configurations were considered: $5d^5ns$ ($n = 6$–8), $5d^46sns$ ($n = 6$–8), $5d^6$, $5d^56d$, $5d^46s6d$, $5d^36s^26d$, $5d^46p^2$ and $5d^36s6p^2$ for the even parity and $5d^5np$ ($n = 6$–8), $5d^46snp$ ($n = 6$–8), $5d^36s^26p$ for the odd parity. As far as the LSF was concerned, the experimental levels of Meggers *et al* (1958), Wyart (1977) and Wahlgren *et al* (1997) were adopted. 44 even-parity and 55 odd-parity levels were retained leading to an s.d. of 135 and 192 cm^{-1} for even and odd levels respectively. Five low-energy even levels were excluded from the fit in agreement with Wyart (1977) and, similarly, all the odd levels above 70 000 cm^{-1}, as well as five levels below that limit, were not included in the LSF. An excellent agreement is observed between the HFR+CPOL results and the values measured by Meggers *et al* (1958) (see figure 3).

5.4. *Os* ($Z = 76$)

In Os I and Os II, atomic structure calculations have been reported by Quinet *et al* (2006).

In the Os I HFR+CPOL calculations, CI was retained among $5d^66s^2$, $5d^66p^2$, $5d^66s7s$, $5d^66s6d$, $5d^7ns$ ($n = 6$–7), $5d^76d$, $5d^56s^27s$, $5d^56s^26d$ and $5d^8$ for the even parity and $5d^66snp$ ($n = 6$–7), $5d^66s5f$, $5d^7np$ ($n = 6$–7), $5d^75f$ and

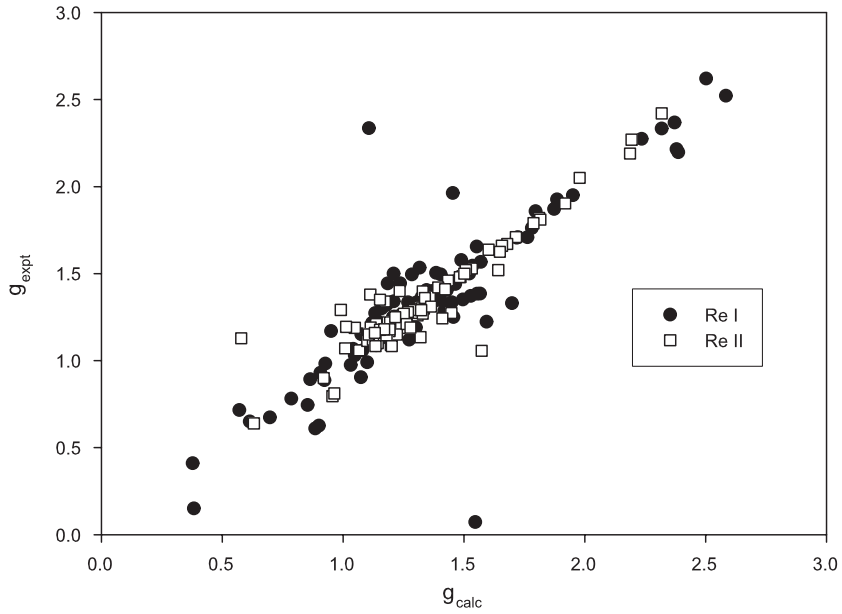

Figure 3. Comparison between the theoretical Landé factors and the results published by Klinkenberg *et al* (1958) for Re I and Meggers *et al* (1958) for Re II.

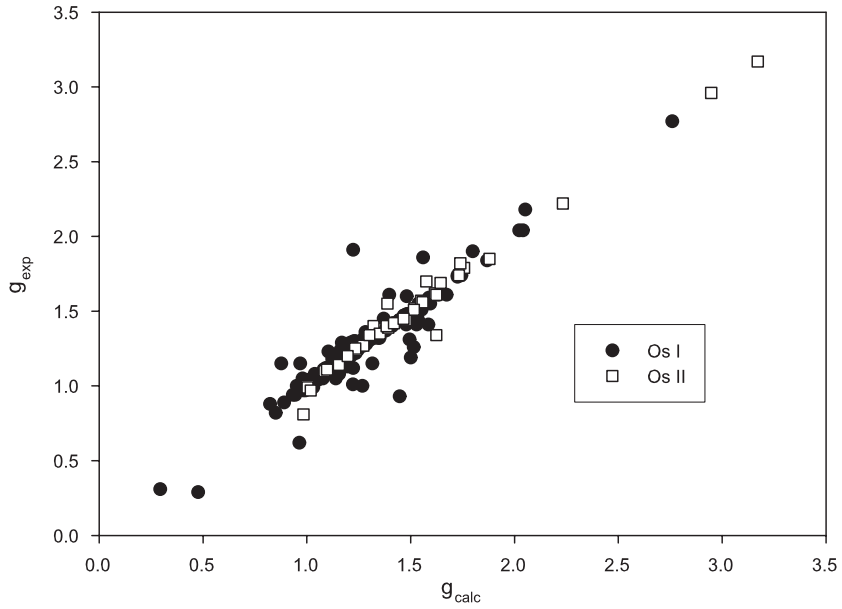

Figure 4. Comparison between the theoretical Landé factors and the experimental results of Van Kleef and Klinkenberg (1961) for Os I and Os II.

$5d^5 6s^2 6p$ for the odd parity. The energy levels used in the fit were taken from Van Kleef and Klinkenberg (1961). They belong to the configurations $5d^6 6s^2$, $5d^7 6s$, $5d^6 6s6p$ and $5d^7 6p$. Only the 46 even-parity experimental levels below 32 000 cm^{-1} and the 95 odd-parity levels, for which a spectroscopic designation is given by the latter authors, were included in the fit. The s.d. was found to be 78 and 230 cm^{-1} for the even and odd parities respectively.

In Os II, a similar approach was adopted, considering the configurations $5d^6 ns$ (n = 6–7), $5d^6 6d$, $5d^5 6s^2$, $5d^5 6p^2$, $5d^5 6s6d$ and $5d^7$ and also $5d^6 np$ (n = 6–7), $5d^6 5f$, $5d^5 6s6p$, $5d^5 6s5f$. Only 22 and 21 experimental levels of Os II belonging to $5d^6 6s$, $5d^5 6s^2$, $5d^7$ and $5d^6 6p$, $5d^5 6s6p$ configurations were reported by Van Kleef and Klinkenberg (1961) (on a total of 119 and 597 possible levels). Consequently, a reasonable semi-empirical fit could not be achieved and only the average energies were adjusted in the calculations.

The numerical values of the Landé factors for both Os I (144 levels) and Os II (34 levels) can be found in the database DESIRE. A comparison between theory and experience (Van Kleef and Klinkenberg 1961) for Os I and Os II is shown in figure 4. The agreement is excellent for Os II. A somewhat larger dispersion of the points is observed for a few levels of Os I.

Table 2. Experimental and calculated Landé g-factors in singly ionized tungten (W II).

$E^a_{Exp.}$ (cm^{-1})	Parity	J	$g^b_{Calc.}$	$g^c_{Exp.}$	$E^a_{Exp.}$ (cm^{-1})	Parity	J	$g^b_{Calc.}$	$g^c_{Exp.}$
0	(e)	0.5	3.188	3.186	25209.233	(e)	4.5	1.140	
1518.829	(e)	1.5	1.850	1.839	25672.099	(e)	2.5	0.980	0.900
3172.473	(e)	2.5	1.646	1.639	26158.581	(e)	4.5	1.171	
4716.278	(e)	3.5	1.570	1.563	26226.897	(e)	2.5	1.013	1.040
6147.085	(e)	4.5	1.528	1.522	26526.710	(e)	0.5	2.202	
7420.261	(e)	2.5	1.918	1.913	26929.008	(e)	5.5	0.995	
8711.274	(e)	1.5	0.633	0.624	27273.753	(e)	3.5	1.045	
8832.728	(e)	0.5	2.399	2.383	28118.836	(e)	2.5	1.399	
10592.485	(e)	1.5	1.474	1.471	28187.578	(e)	6.5	1.091	
11301.024	(e)	2.5	1.101	1.084	28377.585	(e)	5.5	1.204	
13173.337	(e)	0.5	0.455	0.455	28490.920	(e)	1.5	1.091	
13411.939	(e)	3.5	1.196	1.186	28631.688	(e)	3.5	1.149	
13434.070	(e)	2.5	1.530	1.526	29341.426	(e)	4.5	1.181	
14634.336	(e)	1.5	1.185	1.183	30223.744	(e)	1.5	1.353	
14857.160	(e)	4.5	1.245	1.234	30618.045	(e)	2.5	0.977	
14967.745	(e)	2.5	1.077	1.013	30632.927	(e)	4.5	1.022	
15146.977	(e)	3.5	0.877	0.872	31100.286	(e)	5.5	0.955	
16234.715	(e)	2.5	0.935	0.995	31347.087	(e)	6.5	1.078	
16553.087	(e)	4.5	1.135	1.137	31446.928	(e)	3.5	1.251	
16589.603	(e)	3.5	1.163	1.153	31538.785	(e)	2.5	1.226	
17436.932	(e)	5.5	1.194	1.181	32486.525	(e)	1.5	1.149	
18000.627	(e)	3.5	1.098	1.098	32950.226	(e)	1.5	0.863	
18990.929	(e)	1.5	0.934	0.900	32950.460	(e)	3.5	1.018	
19070.550	(e)	4.5	1.110	1.102	33910.548	(e)	5.5	1.076	
19276.431	(e)	2.5	0.932	0.997	34090.867	(e)	4.5	1.174	
19403.991	(e)	0.5	0.634	0.640	34447.663	(e)	2.5	1.183	
19442.466	(e)	6.5	1.216		35315.585	(e)	3.5	1.160	
19637.309	(e)	2.5	1.176	1.102	35826.644	(e)	4.5	1.159	
20039.682	(e)	3.5	1.120	1.107	35925.336	(e)	2.5	1.143	
20455.888	(e)	1.5	0.523	0.510	36165.356	(o)	0.5	0.735	0.678
20534.191	(e)	5.5	1.204	1.197	37312.218	(e)	3.5	1.201	
20780.358	(e)	4.5	1.061	1.065	37971.528	(o)	1.5	0.118	
22139.861	(e)	2.5	1.037	1.060	38576.313	(o)	0.5	1.580	1.614
22194.031	(e)	3.5	1.122	1.119	39129.460	(o)	1.5	1.146	1.147
22502.951	(e)	1.5	1.208	1.220	39936.842	(o)	2.5	0.892	0.889
22535.610	(e)	0.5	2.166	2.200	41583.988	(e)	4.5	1.078	
23046.724	(e)	3.5	1.081	0.860	42049.478	(o)	2.5	1.296	1.292
23234.778	(e)	4.5	1.064	1.249	42298.223	(o)	1.5	1.472	1.498
23450.418	(e)	2.5	1.307	1.297	42390.287	(o)	3.5	1.158	1.161
23803.702	(e)	3.5	1.135		44354.784	(o)	2.5	1.391	1.390
23955.349	(e)	5.5	1.090	1.100	44455.212	(o)	0.5	−0.230	−0.217
24804.612	(e)	3.5	1.099	1.100	44758.095	(o)	4.5	1.275	1.270
24991.591	(e)	1.5	1.031	0.900	44877.209	(o)	3.5	1.287	1.277
25045.238	(e)	0.5	0.322	0.320	44911.659	(o)	1.5	1.273	1.221
25169.877	(e)	1.5	1.603	1.640	45457.066	(o)	0.5	0.446	0.519

5.5. Ir ($Z = 77$)

Lifetime measurements and calculations in Ir I and Ir II were reported by Xu *et al* (2007).

In Ir I, the configurations considered in the physical model were: $5d^76s^2$, $5d^76p^2$, $5d^76d^2$, $5d^76s7s$, $5d^76s6d$, $5d^66s^27s$, $5d^66s^26d$, $5d^66s6p^2$, $5d^8ns$ (n = 6–7), $5d^86d$, $5d^9$ (even) and $5d^76snp$ (n = 6–7), $5d^76snf$ (n = 5–6), $5d^66s^26p$, $5d^8np$ (n = 6–7), $5d^8nf$ (n = 5–6) (odd). For the even parity, the 30 experimental levels belonging to the 'low even group' reported by Van Kleef (1957) were adopted while, for the odd parity, the 86 lowest levels situated below 50 000 cm^{-1} were retained for the fit. The s.d. in the LSF was found to be equal to 111 and 192 cm^{-1} (for the even and odd parities), respectively.

In Ir II, the model included the configurations $5d^7ns$ (n = 6–7), $5d^76d$, $5d^66s^2$, $5d^66p^2$, $5d^66s7s$, $5d^66s6d$, $5d^56s^27s$, $5d^56s^26d$, $5d^8$ and $5d^7np$ (n = 6–7), $5d^75f$, $5d^66snp$ (n = 6–7), $5d^66s5f$, and $5d^56s^26p$. 35 even-parity levels reported by Van Kleef and Metsch (1978) and 21 odd-parity levels situated below 60 000 cm^{-1}, belonging to the configurations $5d^76s$, $5d^66s^2$, $5d^8$, $5d^76p$ and $5d^66s6p$, were considered for adjusting the parameters.

Landé factors were reported by Xu *et al* (2007) but only for Ir II. Additional values for Ir I are available in the database DESIRE (116 levels). A theory–experiment comparison is illustrated in figure 5. The experimental data are taken from Van Kleef (1957) (Ir I) and from Van Kleef and Metsch (1978) (Ir II). There is some scatter in the points, particularly for the highly excited levels (E > 45 000 cm^{-1}). There is no clear

Table 2. (Continued.)

$E^a_{Exp.}$ (cm^{-1})	Parity	J	$g^b_{Calc.}$	$g^c_{Exp.}$	$E^a_{Exp.}$ (cm^{-1})	Parity	J	$g^b_{Calc.}$	$g^c_{Exp.}$
45553.652	(o)	1.5	1.020	1.033	54498.608	(o)	3.5	1.358	
46175.395	(o)	3.5	1.453	1.452	54704.585	(o)	2.5	1.198	0.623
46355.404	(o)	2.5	1.291	1.236	54958.573	(o)	5.5	1.106	1.141
46493.356	(o)	4.5	1.305	1.311	55022.932	(o)	3.5	1.281	
46625.281	(o)	0.5	1.766	1.700	55162.390	(o)	2.5	1.264	1.000
47179.941	(o)	1.5	0.976	1.007	55392.446	(o)	4.5	1.218	1.061
47413.270	(o)	2.5	1.203	1.111	55488.134	(o)	1.5	1.804	
47588.647	(o)	1.5	2.020	2.000	56084.326	(o)	1.5	1.004	1.021
48284.498	(o)	2.5	1.209	1.366	56376.569	(o)	5.5	1.209	
48332.758	(o)	5.5	1.322		56413.649	(o)	4.5	1.201	
48830.701	(o)	3.5	1.371	1.008	56439.643	(o)	6.5	1.146	
48982.939	(o)	1.5	1.729	1.720	56544.508	(o)	2.5	1.636	
49124.508	(o)	3.5	1.141	1.499	56612.836	(o)	3.5	1.219	1.220
49154.484	(o)	0.5	2.703	2.780	56768.602	(o)	3.5	1.114	1.147
49181.034	(o)	4.5	1.415	1.409	56874.983	(o)	2.5	1.095	0.815
49242.042	(o)	2.5	1.520	1.510	56932.345	(o)	1.5	1.037	1.060
50292.354	(o)	2.5	1.374	1.334	57089.482	(o)	4.5	1.066	
50430.999	(o)	1.5	0.898	0.930	57252.138	(o)	2.5	0.928	
50863.106	(o)	4.5	1.188	1.194	57729.994	(o)	3.5	1.212	1.184
51045.292	(o)	3.5	1.408		57856.759	(o)	2.5	1.205	1.360
51254.429	(o)	1.5	1.517	1.580	57986.939	(o)	4.5	1.101	
51438.064	(o)	2.5	1.283	1.301	58007.690	(o)	1.5	1.211	1.200
51495.054	(o)	5.5	1.384	1.054	58308.799	(o)	0.5	0.579	
51536.621	(o)	0.5	2.439		58337.096	(o)	2.5	1.227	
51862.999	(o)	3.5	0.951	0.937	58537.630	(o)	3.5	1.418	
52087.110	(o)	2.5	1.260		58687.965	(o)	4.5	1.235	
52275.291	(o)	3.5	1.334	1.297	58709.614	(o)	3.5	1.152	
52355.250	(o)	0.5	0.652	0.981	58748.042	(o)	1.5	1.150	0.780
52567.276	(o)	4.5	1.331		58891.742	(o)	5.5	1.134	1.144
52593.766	(o)	0.5	1.834	1.560	59276.854	(o)	3.5	1.131	1.102
52803.012	(o)	1.5	1.505		59370.490	(o)	1.5	0.833	
52901.794	(o)	3.5	1.350	1.374	59399.339	(o)	4.5	1.192	1.179
53113.533	(o)	2.5	1.189	1.262	59443.051	(o)	2.5	1.464	
53329.762	(o)	1.5	1.199	1.357	59816.385	(o)	1.5	1.128	
53338.075	(o)	3.5	0.961	0.968	59869.150	(o)	3.5	1.099	1.125
53370.011	(o)	4.5	1.132	1.086	59933.692	(o)	3.5	1.157	
53423.050	(o)	1.5	1.352	0.976	59992.379	(o)	2.5	1.123	
53440.213	(o)	0.5	2.365	2.038	60219.015	(o)	5.5	1.144	1.130
53641.254	(o)	6.5	1.365		60256.547	(o)	3.5	1.394	
54026.309	(o)	2.5	1.203		60278.726	(o)	4.5	1.110	
54056.594	(o)	4.5	1.131	1.123	60424.237	(o)	3.5	1.112	
54137.225	(o)	1.5	1.757	1.608	60474.732	(o)	2.5	1.079	
54229.082	(o)	5.5	1.358		60656.540	(o)	2.5	1.107	
54375.859	(o)	2.5	1.476	1.510	60665.356	(o)	1.5	1.320	
54485.701	(o)	0.5	1.501	1.460	60901.023	(o)	2.5	0.937	0.920

explanation for these discrepancies, but they could be due to incorrect designation of the levels.

5.6. *Pt* ($Z = 78$)

HFR+CPOL calculations were performed in Pt II by Quinet *et al* (2008). Two different models were adopted. In the first, the configurations were: $5d^9$, $5d^8ns$ ($n = 6$–7), $5d^8nd$ ($n = 6$–7), $5d^76s^2$, $5d^76p^2$, $5d^76d^2$, $5d^76s6d$, $5d^76s7s$, $5d^76d7s$, $5d^66s^27s$, $5d^66s^26d$ (even) and $5d^8np$ ($n = 6$–7), $5d^8nf$ ($n = 5$–6), $5d^76snp$ ($n = 6$–7), $5d^76p7s$, $5d^76p6d$, $5d^76s6f$, $5d^66s^26p$ (odd). 71 even experimental levels were adopted from the analysis by Blaise and Wyart (1992), the two levels at 119 057.05 and 121 651.19 cm^{-1} being excluded. The s.d. was 44 cm^{-1}. For the odd parity, all the experimental levels reported by Wyart *et al* (1995) below 110 000 cm^{-1}, i.e. 180 levels, were considered in the LSF procedure and the s.d. was found to be 108 cm^{-1}. The second model included the same configurations as the first, but the $5d^66s^27s$ and $5d^66s^26d$ even configurations and the $5d^66s^26p$ odd configurations were not included. 71 even levels and 150 odd levels (below 104 600 cm^{-1}) were included in the fit, leading to mean deviations of 44 and 203 cm^{-1}. The Landé factors corresponding to the second theoretical model (considered the best) are stored in the database DESIRE (250 levels). There are no experimental data available for comparison.

5.7. *Au* ($Z = 79$)

Atomic structure calculations in neutral and singly ionized gold were reported by Fivet *et al* (2006b), the main purpose of their paper being the determination of transition probabilities

Table 2. (Continued.)

$E^{a}_{Exp.}$ (cm^{-1})	Parity	J	$g^{b}_{Calc.}$	$g^{c}_{Exp.}$	$E^{a}_{Exp.}$ (cm^{-1})	Parity	J	$g^{b}_{Calc.}$	$g^{c}_{Exp.}$
61055.849	(o)	4.5	1.150		65684.866	(o)	5.5	1.087	
61117.662	(o)	1.5	0.662		66026.803	(o)	3.5	1.020	
61240.813	(o)	5.5	1.136	1.120	66144.496	(o)	2.5	0.960	
61326.281	(o)	3.5	1.092		66271.003	(o)	4.5	1.091	
61360.578	(o)	4.5	1.121		66703.457	(o)	5.5	1.097	
61550.649	(o)	3.5	1.116		66816.290	(o)	4.5	1.124	
61566.854	(o)	2.5	1.106	1.070	66898.059	(o)	3.5	1.132	
61589.457	(o)	5.5	1.135	1.149	67028.654	(o)	4.5	1.163	
61602.268	(o)	6.5	1.206		67173.555	(o)	2.5	1.020	
62131.107	(o)	0.5	0.545		67847.271	(o)	4.5	1.043	
62330.855	(o)	4.5	1.107		68012.627	(o)	5.5	1.112	
62333.247	(o)	2.5	1.090		68079.006	(o)	6.5	1.020	
62437.086	(o)	4.5	1.239		68362.322	(o)	3.5	1.080	
62454.559	(o)	1.5	1.186		68443.785	(o)	2.5	1.223	
62561.090	(o)	3.5	1.131		68499.486	(o)	1.5	1.043	
62714.675	(o)	6.5	1.136		68619.990	(o)	3.5	1.195	
62716.159	(o)	4.5	1.421		68734.663	(o)	4.5	1.007	
62724.690	(o)	1.5	1.201		69035.063	(o)	6.5	1.144	
62966.514	(o)	5.5	1.095		69060.711	(o)	2.5	1.106	
62989.639	(o)	2.5	1.009		69105.775	(o)	4.5	1.065	
63087.934	(o)	6.5	1.116		69481.712	(o)	2.5	1.002	
63134.773	(o)	1.5	1.192		69580.334	(o)	3.5	1.138	
63266.459	(o)	3.5	0.981		69587.792	(o)	5.5	1.130	
63788.242	(o)	3.5	1.087		70000.529	(o)	6.5	1.143	
63875.361	(o)	7.5	1.183		70211.800	(o)	3.5	1.099	
63880.265	(o)	2.5	0.996		70674.184	(o)	3.5	1.093	
64030.511	(o)	2.5	1.256		70845.790	(o)	7.5	1.152	
64207.585	(o)	4.5	1.102		70902.470	(o)	4.5	1.110	
64255.162	(o)	1.5	1.027		71164.174	(o)	5.5	1.171	
64310.114	(o)	2.5	1.111		71220.067	(o)	6.5	1.108	
64356.750	(o)	3.5	1.178		71245.032	(o)	4.5	1.077	
64516.226	(o)	4.5	1.193		71785.392	(o)	4.5	1.092	
64804.173	(o)	1.5	1.117		72180.632	(o)	5.5	1.141	
64896.325	(o)	3.5	1.057		72401.581	(o)	4.5	1.077	
64969.172	(o)	5.5	1.123		72557.895	(o)	4.5	1.104	
64990.383	(o)	2.5	1.083		72597.303	(o)	3.5	1.065	
65003.292	(o)	4.5	1.051		72821.142	(o)	7.5	1.132	
65299.715	(o)	1.5	1.276		73266.317	(o)	5.5	1.093	
65326.546	(o)	5.5	1.174		73427.537	(o)	3.5	1.161	
65455.496	(o)	3.5	0.950		73705.965	(o)	4.5	1.031	
65481.012	(o)	2.5	1.690		74446.931	(o)	4.5	1.178	
65643.968	(o)	3.5	1.182						

[a] Kramida and Shirai (2006).
[b] HFR values: this work.
[c] Kramida and Shirai (2006).

and lifetimes. An extension of their work to the transitions emitted from 6d and 7s configurations of Au II is due to Biémont *et al* (2007).

In Au I, the configurations included in the model were $5d^{10}ns$ (n = 6–11), $5d^{10}nd$ (n = 6–11), $5d^{9}6s^{2}$, $5d^{9}6p^{2}$, $5d^{9}6d^{2}$, $5d^{9}5f^{2}$, $5d^{9}6f^{2}$, $5d^{9}6s7s$, $5d^{9}6s6d$, $5d^{9}6p6f$, $5d^{8}6s^{2}6d$, $5d^{8}6s6p^{2}$ (even parity) and $5d^{10}np$ (n = 6–11), $5d^{10}nf$ (n = 5–11), $5d^{9}6snp$ (n = 6–11), $5d^{9}6snf$ (n = 5–6), $5d^{9}6p6d$, $5d^{9}6dnf$ (n = 5–6), $5d^{8}6s^{2}6p$, $5d^{8}6s^{2}nf$ (n = 5–6) (odd parity). The experimental levels were due to Platt and Sawyer (1941), Ehrhardt and Davis (1971), Brown and Ginter (1978) and George *et al* (1988). For the even parity, all the levels below the first ionization limit were included in the fit, but three even levels were excluded. The s.d. was 47 cm^{-1} and 113 cm^{-1} (for even and odd parities respectively).

In Au II (Fivet *et al* 2006b), the configurations considered were for the even and odd parities, respectively: $5d^{10}$, $5d^{9}ns$ (n = 6–7), $5d^{9}nd$ (n = 6–7), $5d^{8}6s^{2}$, $5d^{8}7s^{2}$, $5d^{8}6p^{2}$, $5d^{8}7p^{2}$, $5d^{8}6s7s$, $5d^{8}6s6d$, $5d^{7}6s^{2}6d$, $5d^{7}6s6p^{2}$ and $5d^{9}np$ (n = 6–7), $5d^{9}nf$ (n = 5–6), $5d^{8}6s6p$, $5d^{8}6s7p$, $5d^{8}6s5f$, $5d^{8}6s6f$, $5d^{7}6s^{2}6p$, $5d^{7}6s^{2}5f$ and $5d^{7}6s^{2}6f$. 37 even levels and 84 odd levels determined experimentally by Rosberg and Wyart (1997) were used for the LSF resulting in an s.d. of 66 and 194 cm^{-1} (for even and odd parities respectively).

The g-factors for Au I (43 levels) and Au II (119 levels) are reported in the database DESIRE. A theory–experiment comparison is illustrated in figure 6. There is an excellent agreement between the measurements of Symons and Daley (1929) and Green and Maxwell (1955) in Au I if we exclude the level at 56 105.580 cm^{-1}. A somewhat larger

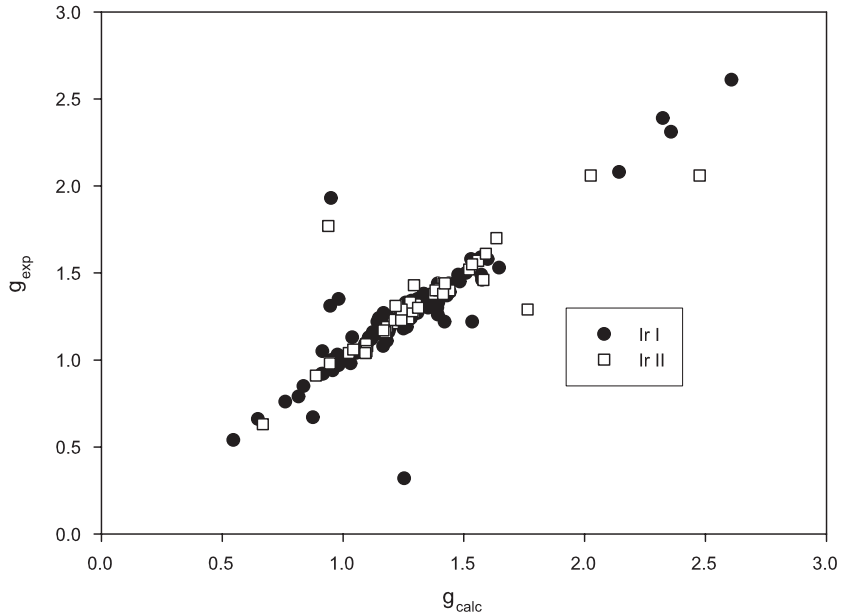

Figure 5. Comparison between the theoretical Landé factors and the experimental results of Van Kleef (1957) (Ir I) and of Van Kleef and Metsch (1978) (Ir II).

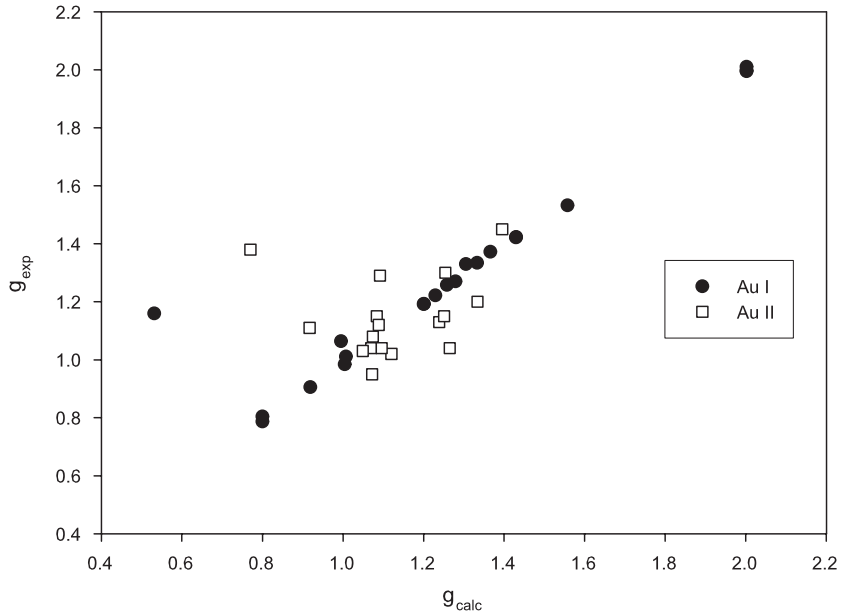

Figure 6. Comparison between the HFR+CPOL Landé factors and the experimental results of Symons and Daley (1929) and Green and Maxwell (1955) (Au I) and of Moore (1958, 1971) (Au II).

scatter is observed in Au II (values reported by Moore 1958, 1971).

5.8. Pb ($Z = 82$)

In the computations reported by Biémont *et al* (2000), extensive configuration interaction was considered by retaining the configurations $6s^26p^2 + 6s^26pnp$ ($n = 7$–13) + $6s^26pnf$ ($n = 5$–13) + $6p^4 + 6s6p^2ns$ ($n = 7$–10) and $6s^26pns$ ($n = 7$–13) + $6s^26pnd$ ($n = 6$–13) + $6s6p^3 + 6s6p^2np$ ($n = 7$–10). The polarization parameters are reported in table 1. The levels used for the fit were taken from Wood and Andrew (1968), Brown *et al* (1977) and Hasegawa and Suzuki (1996). This led to an s.d. of 41 cm^{-1} (65 even levels) and 65 cm^{-1} (50 odd levels). For the numerical values, see the corresponding table in DESIRE (115 levels). In figure 7 the HFR+CPOL results are compared to the experimental results reported by Moore (1958, 1971). The agreement is excellent for the 11 levels for which experimental data are available.

5.9. Bi ($Z = 83$)

In Bi II, three sets of calculations were reported by Palmeri *et al* (2001). The configuration sets adopted were: $6p^2$, $6pnp$ ($n = 7$–10), $6pnf$ ($n = 5$–10) (even) and $6s6p^3$, $6pns$

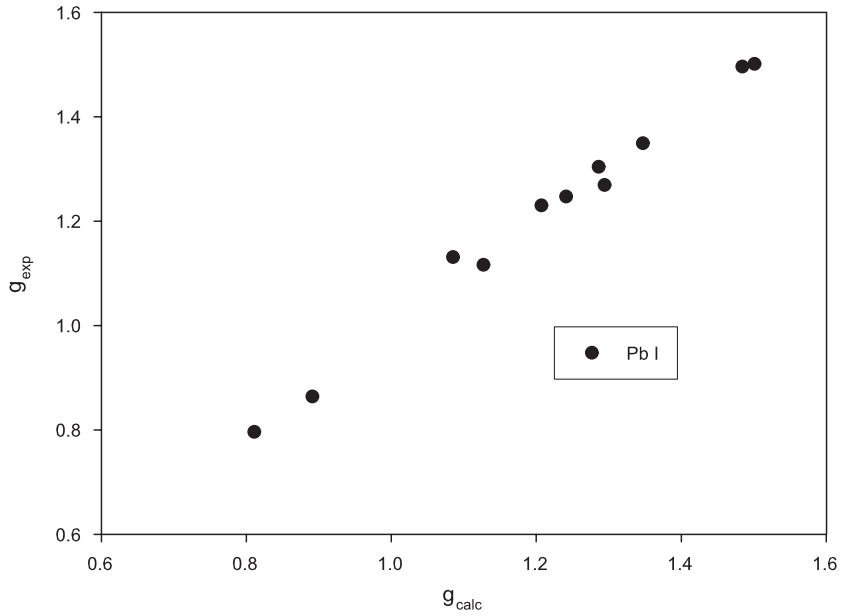

Figure 7. Comparison between the HFR+CPOL Landé factors and the experimental results reported by Moore (1958, 1971) for Pb I.

(n = 7–10), 6pnd (n = 6–10) (odd) (calculation A); $6p^2$, 6pnp (n = 7–10), 6pnf (n = 5–10), $6p^4$, $6s6p^2ns$ (n = 7–10) (even) and $6s6p^3$, 6pns (n = 7–10), 6pnd (n = 6–10), $6s6p^2np$ (n = 7–10) (odd) (calculation B) and finally $6p^2$, 6pnp (n = 7–10), 6pnf (n = 5–10), $6p^4$, $6s6p^2ns$ (n = 7–10), $6s6p^2nd$ (n = 6–10), $7s^2$, 6d7s, $6d^2$, $7p^2$ (even) and $6s6p^3$, 6pns (n = 7–10), 6pnd (n = 6–10), $6s6p^2np$ (n = 7–10), $6s6p^2nf$ (n = 5–10), 7s7p, 6d7p, 6d5f, 6d6f (odd) (calculation C). For the adjustment of the parameters, the energy levels were taken from Moore (1958, 1971) as there are no recent term analyses for this ion. The s.d. of the fit reached 58 cm^{-1} (for 24 experimental even levels, the two levels at 106 447 and 105 269 cm^{-1} having been excluded) and 89 cm^{-1} (for 23 odd levels). The Landé factors corresponding to the best theoretical model (model C) are reported in the DESIRE database for 47 levels. There are no results available for comparison.

6. Conclusions

Landé factors have been obtained in the present work for 2084 levels of the sixth-row elements and ions, and are stored in a database called DESIRE, recently posted on a Mons University website. They are expected to help astrophysicists in quantitative investigations of the magnetic fields in stars. Recent stellar observations of hot stars (e.g. by Kochukhov *et al* 2004) using Zeeman–Doppler imaging techniques have confirmed the oblique rotator model of the magnetic Ap stars. It has been shown that the inhomogeneous distribution of the elements over the stellar surface is correlated with the star's magnetic field. Although there is a qualitative agreement with predictions of diffusion theory, more quantitative investigations are needed, and such analyses require refined atomic data including Landé factors (see e.g. Alecian and Stift 2004, 2006, 2007). The present determination of g-factors along the sixth-row period of the periodic table is a first step in the direction of a systematic investigation of heavy elements characterized by relatively low cosmic abundances and for which, in many cases, the atomic data are still scarce or even completely missing.

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