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Transition probabilities in Gd III

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Abstract. Theoretical lifetimes, calculated with inclusion of core-polarization effects, have been determined for five $4f^76p$ levels of doubly ionized gadolinium. They agree quite well with recent experimental values measured by time-resolved laser-induced fluorescence spectroscopy. From this agreement, the accuracy of a first set of Gd III transition probabilities, calculated for $4f^75d$–$4f^76p$ and $4f^76s$–$4f^76p$ transitions of astrophysical interest, has been assessed.

Key words. atomic data – stars: chemically peculiar

1. Introduction

Singly ionized gadolinium is well represented in the solar spectrum and its abundance is, according to the latest determinations, in good agreement with the meteoritic value (Bergström et al. 1988; Anders & Grevesse 1989). Gd II has been also identified in many other stars of different types: as a few examples, let us mention the Hg-Mn stars (Adelman 1989), the Ap stars *HR465* and *HR7575* (Hartoog et al. 1973), the Mira variables (Grudzinska 1985), the Ba stars (Lambert 1985) or the Am star *32 Aqr* (Magazzu & Cowley 1986). Strong lines of lanthanides, including Gd II, have been observed in the spectrum of a cool rapidly rotating Ap star (roAp) i.e. the Przybylski's star (*HD101065*, *V816 Cen*) (Cowley et al. 2000). Gd II lines have also been analyzed in the K giant star *CS 22892-052* by Sneden et al. (1996) who found an abundance result corresponding to a scaled solar system *r*-process value.

In general, the abundances of the lanthanide rare-earths (RE), deduced in magnetic Ap stars and in metallic line A stars, exceed considerably the solar system values and are generally larger, by about one order of magnitude, in the first than in the second group. In many magnetic Ap stars however, the effective temperatures imply that most of the atoms should be doubly ionized. Until recently, abundance values in such stars were mostly obtained from the non-dominant ionization stage (i.e. the second spectrum) due to the fact that transition probabilities for doubly ionized RE elements were unavailable or that the strongest lines of the third spectra fall outside of the accessible spectral region (Cowley 1980). The situation has now changed and there has been, in recent years, a revival of interest for the doubly ionized species of the lanthanides. In particular, we have started a systematic investigation of the line intensities in these spectra within the framework of the DREAM project (for more details, see `http://www.umh.ac.be/~astro/dream.shtml`) and extensive tables of transition probabilities, tested in many cases by comparison with laser lifetime measurements, have been obtained for most of the doubly ionized elements of the group (Biémont et al. 1999, 2001a,b,c,d, 2002; Fedchak et al. 2000; Li et al. 2001; Palmeri et al. 2000; Zhang et al. 2001a, 2002a,b,c). The case of Gd III has not been considered so far and, for this reason, the first results are presented in the present paper.

2. The spectrum of Gd III

Gadolinium ($Z = 64$) has seven isotopes (152, 154, 155, 156, 157, 158 and 160) of which Gd 155, 156, 157, 158 and 160 are represented, in the solar system, by nearly equal amounts (15, 20, 16, 25 and 22%, respectively). These isotopes are essentially produced by the *r*-process, small amounts of the first four isotopes being due to the s-process.

Among the third RE spectra, doubly ionized gadolinium has the most complex electronic structure. This is due to the fact that the lowest configurations of this ion are characterized by a half-filled 4f subshell with the presence of an additional valence electron. As a result of this complexity, Gd III has been the subject of very few investigations in the past although lines of this ion have been observed in some astrophysical spectra such as those of the stars $\alpha^2 CVn$ (Cohen et al. 1969) and *HR465* (Bidelman et al. 1995). A search of the third spectra of RE, including Gd III, in IUE spectra of chemically peculiar stars has also been reported by Cowley & Greenberg (1988).

According to the NIST compilation (Martin et al. 1978), only 25 energy levels belonging to the $4f^8$, $4f^7(^8S^\circ)5d$, $4f^7(^8S^\circ)6s$, $4f^7(^8S^\circ)6p$ and $4f^7(^8S^\circ)7s$ configurations have been determined experimentally. These levels were deduced from

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Table 1. Adopted parameters for HFR calculations in Gd III.

Config.	Parameter	Ab initio (cm^{-1})	Adopted (cm^{-1})	Ratio
Even parity				
4f^{7}5d	E_{av}	97683	96777	
	F^2(4f, 4f)	116091	98677	0.850*f*
	F^4(4f, 4f)	72815	61893	0.850*f*
	F^6(4f, 4f)	52379	44522	0.850*f*
	$\zeta_{4\mathrm{f}}$	1582	1582	1.000*f*
	$\zeta_{5\mathrm{d}}$	1034	957	0.926
	F^2(4f, 5d)	25640	21794	0.850*f*
	F^4(4f, 5d)	12246	10409	0.850*f*
	G^1(4f, 5d)	11662	8227	0.705∗
	G^3(4f, 5d)	9358	6601	0.705∗
	G^5(4f, 5d)	7105	5011	0.705∗
4f^{7}6s	E_{av}	104059	102080	
	F^2(4f, 4f)	116684	99182	0.850*f*
	F^4(4f, 4f)	73216	62234	0.850*f*
	F^6(4f, 4f)	52675	44774	0.850*f*
	$\zeta_{4\mathrm{f}}$	1588	1588	1.000*f*
	G^3(4f, 6s)	2749	2083	0.758
4f^{7}5d – 4f^{7}6s	R^2(4f, 5d; 4f, 6s)	−214	−182	0.850*f*
	R^2(4f, 5d; 4f, 6s)	2162	1838	0.850*f*
Odd parity				
4f^{7}6p	E_{av}	139046	138527	
	F^2(4f, 4f)	116761	99247	0.850*f*
	F^4(4f, 4f)	73267	62277	0.850*f*
	F^6(4f, 4f)	52712	44805	0.850*f*
	$\zeta_{4\mathrm{f}}$	1589	1589	1.000*f*
	$\zeta_{6\mathrm{p}}$	2469	3026	1.226
	F^2(4f, 6p)	7447	6330	0.850*f*
	G^2(4f, 6p)	1881	1762	0.937∗
	G^4(4f, 6p)	1689	1582	0.937∗
4f^8	E_{av}	84926	65548	
	F^2(4f, 4f)	108539	92258	0.850*f*
	F^4(4f, 4f)	67727	57568	0.850*f*
	F^6(4f, 4f)	48620	41327	0.850*f*
	$\zeta_{4\mathrm{f}}$	1466	1359	0.927
4f^{7}6p – 4f^8	R^2(4f, 6p; 4f, 4f)	−4099	−3484	0.850*f*
	R^4(4f, 6p; 4f, 4f)	−2509	−2133	0.850*f*

f Fixed parameter (see the text).
∗ Fixed ratio (see the text).

Table 2. Comparison between calculated radiative lifetimes, τ in ns, obtained in the present work without (HFR) and with ($HFR + CP$) core-polarization contributions and experimental results for 4f^{7}6p levels of Gd III.

E(cm^{-1})	J	HFR	$HFR + CP$	Experiment∗
43019.99	3	1.41	1.87	1.9 ± 0.2
43611.69	4	1.49	1.97	1.9 ± 0.2
47233.93	5	1.06	1.41	1.4 ± 0.2
48339.14	4	1.24	1.65	1.5 ± 0.2
48859.62	3	1.32	1.75	1.5 ± 0.2

∗ Zhang et al. (2001b).

observations due to Callahan (1963), Johansson & Litzén (1973), Kielkopf (1976) and Wyart (1976). More precisely, from his analyis of the 4f^7(^{8}S$^\circ$)5d–6p and 4f^7(^{8}S$^\circ$)6s–6p transitions in the region 2043–3177 Å, Callahan (1963) was able to classify 42 lines and to deduce the 4f^{7}5d, 6s and 6p levels. The five known levels of the 4f^8 ^{7}F term were obtained by Johansson & Litzén (1973) from the ^{7}F–^{7}D$^\circ$ multiplet observed in the infrared region (1.43–2.56 μm). Kielkopf (1976) has reevaluated the levels on the basis of his own observations and his levels were adopted by Martin et al. (1978) with the exception of the two 4f^7(^{8}S$^\circ$)7s levels taken from Wyart (1976).

Concerning the transition rates, neither theoretical nor experimental transition probabilities have been determined so far. Natural radiative lifetimes of five 4f^{7}6p levels in Gd III were measured for the first time by Zhang et al. (2001b) using time-resolved laser-induced fluorescence in a laser-produced plasma. No additional results were available for comparison.

3. Calculations and discussion of the results

In the present work, we report on the first theoretical investigation of transition rates in Gd III. The new results were calculated in the framework of the relativistic Hartree-Fock (HFR) method coded in Cowan's (1981) suite of computer programs in which we have incorporated the core-polarization (CP) effects by means of a model potential and a correction to the electric dipole operator. The method is similar to that previously described (see e.g. Biémont et al. 2001a,b,c,d) and, consequently, the details will not be repeated here. The configurations retained in the physical model were 4f^{7}5d, 4f^{7}6s for the odd parity and 4f^{7}6p, 4f^8 for the even parity. This model is clearly simple but the consideration of additional configurations was prevented by the computer capabilities available. However, the lifetime values deduced in the present work (see further) justify a posteriori the model used. The core-polarization contributions were estimated using the static dipole polarizability computed by Fraga et al. (1976) for Gd IV, i.e. $\alpha_{\mathrm{d}} = 6.81\ \mathrm{a}_0^3$, and the cut-off radius, $r_{\mathrm{c}} = 1.55\ \mathrm{a}_0$, which corresponds to the average HFR value $<r>$ for the outermost core orbital (5p^6). A least-squares optimization procedure of the radial parameters was followed in order to minimize the differences between the calculated levels and the experimental values compiled by the NIST (Martin et al. 1978). In view of the scarcity of these experimental levels, we were able to adjust only a few parameters. More precisely, since only the ^{8}S$^\circ$ parent term is known in the 4f^7*nl* (*nl* = 5d, 6s, 6p) configurations, only the parameters E_{av}, ζ_{nl} and G^k(4f,*nl*) were allowed to vary with the constraint that the ratios $G^1/G^3/G^5$ and G^2/G^4 were kept fixed during the fitting process concerning the 4f^{7}5d and 4f^{7}6p configurations, respectively. For 4f^8, only E_{av} and $\zeta_{4\mathrm{f}}$ could be adjusted due to the fact that only the ^{7}F multiplet is determined experimentally in this configuration. All the other electrostatic parameters, not optimized semi-empirically, were scaled down by a factor equal to 0.85. The mean deviations between fitted and observed levels in the odd and even parities were found to be equal to 25 cm^{-1} (12 levels) and 8 cm^{-1} (11 levels), respectively. The numerical values of the radial parameters adopted in the HFR calculations are reported in Table 1.

Table 3. Calculated oscillator strengths (log gf) and transition probabilities (gA) for 4f^{7}5d–4f^{7}6p and 4f^{7}6s–4f^{7}6p transitions in Gd III. $A(+B)$ stands for $A \times 10^B$.

λ(Å)[a]	Lower level			Upper level			log gf	$gA(s^{-1})$
	Config.	J	E(cm^{-1})	Config.	J	E(cm^{-1})		
2032.085[b]	4f^{7}5d	2.0	0	4f^{7}6p	2.0	49195	−2.36	6.98(+6)
2043.698	4f^{7}5d	3.0	279	4f^{7}6p	2.0	49195	−2.21	9.81(+6)
2046.029	4f^{7}5d	2.0	0	4f^{7}6p	3.0	48860	−1.06	1.38(+8)
2057.792	4f^{7}5d	3.0	279	4f^{7}6p	3.0	48860	−1.37	6.69(+7)
2075.524[b]	4f^{7}5d	4.0	694	4f^{7}6p	3.0	48860	−2.29	7.96(+6)*
2080.080	4f^{7}5d	3.0	279	4f^{7}6p	4.0	48339	−0.88	2.05(+8)
2098.204	4f^{7}5d	4.0	694	4f^{7}6p	4.0	48339	−0.63	3.57(+8)
2125.683	4f^{7}5d	5.0	1310	4f^{7}6p	4.0	48339	−0.74	2.72(+8)
2148.034	4f^{7}5d	4.0	694	4f^{7}6p	5.0	47234	−0.83	2.13(+8)
2176.844	4f^{7}5d	5.0	1310	4f^{7}6p	5.0	47234	−0.17	9.64(+8)
2223.943	4f^{7}5d	6.0	2283	4f^{7}6p	5.0	47234	0.31	2.76(+9)
2307.031	4f^{7}5d	3.0	279	4f^{7}6p	4.0	43612	−0.57	3.38(+8)
2323.783	4f^{7}5d	2.0	0	4f^{7}6p	3.0	43020	−0.17	8.27(+8)
2329.347	4f^{7}5d	4.0	694	4f^{7}6p	4.0	43612	−0.20	7.84(+8)
2338.973	4f^{7}5d	3.0	279	4f^{7}6p	3.0	43020	−0.21	7.50(+8)
2361.913	4f^{7}5d	4.0	694	4f^{7}6p	3.0	43020	−0.46	4.17(+8)
2363.261	4f^{7}5d	5.0	1310	4f^{7}6p	4.0	43612	−0.08	9.86(+8)
2520.389	4f^{7}6s	4.0	9195	4f^{7}6p	3.0	48860	−0.45	3.73(+8)
2551.560	4f^{7}5d	3.0	10015	4f^{7}6p	2.0	49195	−0.58	2.69(+8)
2553.904	4f^{7}6s	4.0	9195	4f^{7}6p	4.0	48339	0.09	1.27(+9)
2554.045	4f^{7}5d	4.0	9718	4f^{7}6p	3.0	48860	−0.17	6.93(+8)
2564.469	4f^{7}5d	5.0	9356	4f^{7}6p	4.0	48339	0.04	1.12(+9)
2565.959	4f^{7}5d	2.0	10234	4f^{7}6p	2.0	49195	−0.36	4.45(+8)
2573.573	4f^{7}5d	3.0	10015	4f^{7}6p	3.0	48860	−0.27	5.42(+8)
2576.068	4f^{7}5d	1.0	10387	4f^{7}6p	2.0	49195	−0.40	3.99(+8)
2588.221	4f^{7}5d	2.0	10234	4f^{7}6p	3.0	48860	−0.68	2.08(+8)
2588.467	4f^{7}5d	4.0	9718	4f^{7}6p	4.0	48339	−0.43	3.74(+8)
2608.530	4f^{7}5d	3.0	10015	4f^{7}6p	4.0	48339	−1.13	7.33(+7)
2628.108	4f^{7}6s	4.0	9195	4f^{7}6p	5.0	47234	0.60	3.86(+9)
2639.299	4f^{7}5d	5.0	9356	4f^{7}6p	5.0	47234	−1.72	1.85(+7)
2655.599	4f^{7}6s	3.0	11550	4f^{7}6p	2.0	49195	0.25	1.70(+9)
2664.722	4f^{7}5d	4.0	9718	4f^{7}6p	5.0	47234	−2.43	3.48(+6)
2679.449	4f^{7}6s	3.0	11550	4f^{7}6p	3.0	48860	0.33	1.97(+9)
2717.357	4f^{7}6s	3.0	11550	4f^{7}6p	4.0	48339	0.30	1.80(+9)
2904.726	4f^{7}6s	4.0	9195	4f^{7}6p	4.0	43612	0.27	1.46(+9)
2918.398	4f^{7}5d	5.0	9356	4f^{7}6p	4.0	43612	−0.52	2.35(+8)
2949.512	4f^{7}5d	4.0	9718	4f^{7}6p	4.0	43612	−1.17	5.24(+7)
2955.534	4f^{7}6s	4.0	9195	4f^{7}6p	3.0	43020	0.29	1.49(+9)
2975.594	4f^{7}5d	3.0	10015	4f^{7}6p	4.0	43612	−1.99	7.75(+6)
3001.918	4f^{7}5d	4.0	9718	4f^{7}6p	3.0	43020	−1.36	3.21(+7)
3028.936	4f^{7}5d	3.0	10015	4f^{7}6p	3.0	43020	−1.55	2.05(+7)
3049.241	4f^{7}5d	2.0	10234	4f^{7}6p	3.0	43020	−2.02	6.81(+6)
3118.041	4f^{7}6s	3.0	11550	4f^{7}6p	4.0	43612	0.00	6.90(+8)
3176.662	4f^{7}6s	3.0	11550	4f^{7}6p	3.0	43020	−0.54	1.90(+8)

[a] From Callahan (1963) except when otherwise indicated.

[b] Deduced from the experimental energy levels (Martin et al. 1978).

* Transition probability possibly affected by cancellation effects.

The radiative lifetimes calculated in the present work, without (HFR) and with ($HFR + CP$) core-polarization corrections and with the fitted parameters, are compared in Table 2 with the available (uncertainties of about 10–15%) laser measurements of Zhang et al. (2001b) published for five 4f^{7}6p levels of Gd III. As seen from this table, the agreement between our $HFR + CP$ results and the experimental values is excellent, the mean ratio $\tau_{\rm exp}/\tau_{HFR+CP}$ being equal to 0.95 ± 0.06 where the uncertainty represents the standard deviation of the mean.

Calculated oscillator strengths and transition probabilities are reported in Table 3 for 44 4f^{7}5d–6p and 4f^{7}6s–6p transitions in the spectral range 2000–3200 Å. In view of the close

Table 4. Calculated Lande factors for low-lying levels of Gd III.

$E(\mathrm{cm}^{-1})$	J	Lande factor
0.00	2	2.653
279.32	3	2.071
694.37	4	1.839
1310.13	5	1.725
2282.83	6	1.663
2381.24	6	1.495
3996.71	5	1.496
5015.20	4	1.497
5789.97	3	1.497
6334.17	2	1.498
9195.04	4	1.995
9356.30	5	1.600
9717.70	4	1.651
10014.75	3	1.750
10234.49	2	1.997
10387.30	1	2.984
11549.50	3	1.992
43019.99	3	2.196
43611.69	4	1.863
47233.93	5	1.796
48339.14	4	1.819
48859.62	3	1.935
49194.70	2	2.321

agreement between theoretical and observed lifetime values, the theoretical transition probabilities were not renormalized with the experimental data. Such a procedure would change the final data by only a few % and could be easily applied if needed. It is clear also that the agreement between the theoretical and experimental lifetime values is a necessary but not sufficient condition to definitely assess the accuracy of the final transition probabilities. Measurement of accurate branching fractions would be necessary as an additional step but such measurements have not been performed so far. However, in view of the accuracy reached in other doubly ionized elements of the same group (see the DREAM database and the relevant publications) and of the fact that most of the transitions considered in the present paper are rather strong, uncertainties of the order of 10–20% are probably to be expected for most of the transitions quoted in Table 3. Only one transition of Table 3 (λ2075.524) is likely to be affected by cancellation effects.

In view of their intrinsic interest for the analysis of the spectra of magnetic stars, we report in Table 4 the calculated Lande factors for 23 low-lying levels of Gd III.

4. Conclusions

A first set of transition probabilities has been obtained in Gd III for 44 $4f^7 5d$–$6p$ and $4f^7 6s$–$6p$ transitions of astrophysical interest appearing in the spectral range 2000–3200 Å. These results will help provide a quantitative analysis of UV spectra of chemically peculiar stars and will allow the astrophysicists to deduce the chemical composition of some stars from the lines emitted by the dominant (doubly ionized) species of this atom.

Due to the lack of experimental energy levels in Gd III, the set of oscillator strengths reported in the present paper is limited to lines appearing in the near ultraviolet region, which means that they are restricted to observations made from space. In order to extend the study of radiative properties in the visible range for the interpretation of ground-based spectra, new term analysis of this ion would be very welcome.

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