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Résumé. — Des niveaux d'énergie récemment établis qui appartiennent aux sous-configurations 4 $f^6(^7F)$ 5 d du samarium ionisé une fois (Sm II), 4 $f^8(^7F)$ 5 d du gadolinium ionisé une fois (Gd II) et 4 $f^8(^7F)$ 5 d 6 s^2 du terbium neutre ont été utilisés pour obtenir des valeurs pour les six paramètres électrostatiques (Slater) et les deux de spin orbite autour de la demi-couche 4 f^7. Il y a 57 niveaux dans chaque atome ; 54 de Sm^+, 45 de Gd^+ et 27 de Tb sont optimisés avec une erreur de 168 cm^{-1} (1,24 % du domaine étudié) 239 cm^{-1} (1,76 %) et 152 cm^{-1} (1,76 %) respectivement. Les niveaux peuvent être désignés en utilisant les notations du couplage *L-S*, malgré quelques mélanges. Des vecteurs propres notablement différents de ceux publiés précédemment ainsi que des prévisions pour les niveaux manquants sont présentés. Environ 70 raies de Gd II sont classées.

Abstract. — The newly established levels of the subconfigurations 4 $f^6(^7F)$ 5 d of singly ionized samarium (Sm II), 4 $f^8(^7F)$ 5 d of singly ionized gadolinium (Gd II) and 4 $f^8(^7F)$ 5 d 6 s^2 of neutral terbium (Tb I) are used to obtain reliable values for the six electrostatic (Slater) and two spin-orbit interaction parameters around the half filled 4 f shell. Out of 57 possible levels in each case, 54 of Sm^+, 45 of Gd^+ and 27 of Tb are fitted with an *rms* error of 168 cm^{-1} (1.24 % of total width), 239 cm^{-1} (1.76 %) and 152 cm^{-1} (1.76 %) respectively. *L-S* coupling notations can be used for level designations despite some heavy admixtures. Eigenvectors differing significantly from previously given ones, as well as predictions for missing levels are tabulated. About 70 Gd II lines are classified.

I. Introduction. — Our knowledge of the 4 f-5 d interactions around the middle of the 4 f shell has, until now, been limited to cases based on a single state of a 4 f electron. The reason is that only configurations of the type 4 $f^7(^8S_{3\frac{1}{2}})$ *nln' l'* have been observed in the spectra europium and gadolinium. The high symmetry of the 4 f^7 core configuration results in the vanishing of the coefficients of the direct Slater parameters F_2 and F_4 for these configurations. Thus, observed term splittings in Eu I, Eu II, Gd I and Gd II depend only on the single exchange integral $G = G_1 + 4\,G_3 + 22\,G_5$. Values for the individual G_k's as well as for the F_k's needed for a full understanding of the 4 f-5 d interaction around the half-filled 4 f shell could not, thus, be derived.

Recently we [1] have observed levels belonging to the 4 $f^8(^7F)$ 5 d subconfiguration of Gd II. Similar observations, including Zeeman effect data, were made by Blaise and Van Kleef [2]. Blaise et al. [3] also observed levels of 4 $f^6(^7F)$ 5 d in Sm II. Klinkenberg et al. [4] have improved on some of their previously published levels of 4 $f^8(^7F)$ 5 d 6 s^2 of Tb I.

This recent accumulation of observational material seemed to us well worthy of a theoretical interpretation. The high number of fully observed terms warrants the convergence of a least squares calculations involving the radial electrostatic parameters. In Gd II and Sm II we were able to obtain reliable values for each of the G_k's separately as well as for the F_k's. The latter appear for the first time as independent variables in least squares calculations around the middle of the 4 f shell. We present here the results of our optimization process in Sm^+, Gd^+ and Tb.

II. **Theoretical Calculations.** — The assumption underlying our theoretical treatment of the observed levels is the purity of the ^7F term in *L-S* coupling. This assumption has been carefully established both theoretically and experimentally in various instances and is now commonly accepted. The theoretical predictions of the 4 $f^6(^7F)$ 5 d and 4 $f^8(^7F)$ 5 d levels and their *g*-values involve diagonalizing the energy matrix that is a linear combination of electrostatic and spin orbit interactions. In this section we describe the calculation of the angular coefficients (matrix elements) of this linear combination.

A. THE CALCULATION OF THE ELECTROSTATIC MATRIX ELEMENTS. — The 4 $f^6(^7F)$ 5 d subconfiguration has 10 terms : five sextets and five octets, ^{6,8}PDFGH. Since the f_k's (coefficients of F_k's) are functions of the orbital angular momentum only, they are the same for

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the two multiplicities of each L. For the ^{7}F parent all spins are parallel. There is one electron missing from the half-filled 4 f shell, which in the orbital space, can be considered as a closed shell. Thus the $f^6(^7F)$ d is the almost closed shell conjugate of fd. According to Racah [5] (eq. (74)), therefore, the f_k's for the terms of $f^6(^7F)$ 5 d have simply the same magnitude but the opposite sign of the corresponding ones in fd[6].

For the g_k's we used the procedure outlined in ref. 1, equations (1) to (6). Modifying eq. (6) of ref. 1 to fit our case we obtain :

$$g^{(k)} = \frac{1}{2}[3 + 2(S_f . s_d)]\, C_{32k}\left[\frac{35}{2\,k+1}\,\delta_{Lk} - 7\right]. \qquad (1)$$

Since $2(S_f . s_d) = S(S+1) - \frac{51}{4}$ we can write (1) as :

$$g^{(k)} = \frac{7}{12}\left[S(S+1) - \frac{39}{4}\right] C_{32k}\left[\frac{5}{2\,k+1}\,\delta_{Lk} - 1\right]. \qquad (2)$$

We denote with bars the corresponding expressions for the almost closed shell conjugate of $f^6(^7F)$ d namely $f^8(^7F)$ d. The transition from $f^{(k)}$ to $\bar{f}^{(k)}$ is accomplished by a change of sign. In order to obtain $\bar{g}^{(k)}$ we use the following relation by Judd [7] :

$$\bar{g}^{(k)}(^6L) = \begin{bmatrix} 3 & k & 2 \\ 0 & 0 & 0 \end{bmatrix}^2 + \frac{8}{7}\,g^{(k)}(^6L) \qquad (3)$$

which gives $\bar{g}^{(k)}$ in terms of the $g^{(k)}$'s obtained from eq. (2).

$$\bar{g}^{(k)}(^8L) = -\,7\begin{bmatrix} 3 & k & 2 \\ 0 & 0 & 0 \end{bmatrix}^2 . \qquad (4)$$

The coefficients of the Slater exchange integrals for all octet terms of $f^8(^7F)$ d are independent of the term's L. It is thus seen that the observation of terms with next to higher multiplicity is an essential condition for the independent determination of all three Slater exchange parameters G_1, G_3 and G_5, in f^N d configuration when $N > 7$. As we shall see in Section III this condition is satisfied in Gd II but not in Tb I. For $N < 7$ the condition is not essential since even terms with highest multiplicity contain different linear combinations of all G_k's.

In Table I we give the $f^{(k)}$, $g^{(k)}$ and $\bar{g}^{(k)}$ for the ^{6,8}PDFGH of $f^6(^7F)$ d and $f^8(^7F)$ d.

TABLE I

Electrostatic matrix elements for $f^6(^7F)$ d *and* $f^8(^7F)$ d

	f_2	f_4	g_1	g_3	g_5	$\bar{g}_1$	$\bar{g}_3$	$\bar{g}_5$
^{8}P	− 24	− 66	14	− 84	− 462	− 21	− 84	− 462
D	− 6	99	− 21	− 84	− 462	− 21	− 84	− 462
F	11	− 66	− 21	− 24	− 462	− 21	− 84	− 462
G	15	22	− 21	− 84	− 462	− 21	− 84	− 462
H	− 10	− 3	− 21	− 84	− 252	− 21	− 84	− 462
^{6}P	− 24	− 66	$-\frac{7}{3}$	14	77	$\frac{7}{3}$	− 14	− 308
D	− 6	99	$\frac{7}{2}$	14	77	7	63	$-\frac{231}{2}$
F	11	− 66	$\frac{7}{2}$	4	77	$-\frac{7}{2}$	$-\frac{49}{6}$	$\frac{77}{6}$
G	15	22	$\frac{7}{2}$	14	77	$\frac{91}{6}$	$-\frac{161}{6}$	$\frac{325}{6}$
H	− 10	− 3	$\frac{7}{2}$	14	42	− 14	$\frac{7}{3}$	$\frac{455}{6}$

B. THE CALCULATION OF THE SPIN-ORBIT MATRIX ELEMENTS. — We calculated the coefficients of ζ_f and ζ_d according to the following formulas :

For ζ_f :

$$\left(3\,\tfrac{1}{2}\,S\,32\,LJ \,\middle|\, \sum_i (s_f . l_f) \,\middle|\, 3\,\tfrac{1}{2}\,S'\,32\,L'J\right) =$$
$$= (-1)^{\frac{1}{2}+L'-L-J} \times$$
$$\times\, 14\sqrt{(2\,S+1)(2\,S'+1)(2\,L+1)(2\,L'+1)}$$
$$\times\, W(SLS'L'\,;J\,1)\ W(3\,L\,3\,L'\,;\,21)$$
$$\times\, W(3\,S\,3\,S'\,;\,\tfrac{1}{2}\,1)\,. \qquad (5)$$

For ζ_d :

$$(-1)^{S-S'-J-\frac{1}{2}} \times$$

$$\times 3\sqrt{5(2S+1)(2S'+1)(2L+1)(2L'+1)}$$
$$\times W(\tfrac{1}{2}S\tfrac{1}{2}S';31)\,W(SLS'L':J1)$$
$$\times W(2L2L';31).$$

The matrices for these coefficients are given in the Appendix.

C. — It should be noted that if we assign to the F_k's and G_k's the set of values given in Table II the complete electrostatic energy expression

$$\sum_k f^{(k)} F_k + g^{(k)} G_k + \bar{g}^{(k)} \bar{G}_k$$

vanishes for each term separately. This may serve as a check for the angular coefficients.

TABLE II

Values for checking the electrostatic matrix elements

$F_0 = 3\,465$	$G_1 = -\bar{G}_1 = 297$
$F_2 = 165$	$G_3 = -\bar{G}_3 = 77$
$F_4 = 45$	$G_5 = -\bar{G}_5 = 25$

III. The Observed Levels. — The recent observational material used in the present calculations includes the following :

1. Sm II. — In addition to the group of 28 4 f^6(^{7}F) 5d levels given by Albertson [8] we had a group of 28 new levels, 8 in the range of Albertson's observations and 20 above them, given in ref. 3. All but 4 of these Sm II levels were accompanied by g-values. Russell Saunders designations were used throughout the list.

2. Gd II. — All 4 f^8(^{7}F) 5d levels are the results of recent investigations (ref. 1, 2). The previous work on this atom by Russell [9] contained configurations with 4 f^7 as the only core configuration. As mentioned in ref. 1, the lower levels of 4 f^8(^{7}F) 5d are well isolated from the rest of the even levels, and the higher ones overlap those belonging to 4 f^7(^{8}S) dp and 4 f^7(^{8}S) sp. This overlap, which increases the configuration interaction between the group of even levels results in the breaking of the strict selection rules observed in ref. 1 to govern the pure

$$4\,f^8(^7F)\,5\,d \rightarrow 4\,f^7(^8S)\,5d\,6s$$

transitions involving the isolated part of 4 f^8(^{7}F) 5d. The 16 levels of 4 f^8(^{7}F) 5 d reported in ref. 1 were supplemented by 29 other even levels later selected from Table 1 of ref. 2.

3. Tb I. — The most recent compilation by Klinkenberg et al. [10] gives 27 corrected 4 f^8(^{7}F) 5d 6s^2 levels. Of these all but one are members of the octet system. All are accompanied by L-S designations and g-factors.

IV. **Calculations and results.** — A. Sm II. 4 f^6(^{7}F) 5 d. — We selected 54 levels out of the 56 ones designated as belonging to 4f^6(^{7}F) 5d in ref. 3, and fitted them to the predicted eigenvalves. A preliminary set of predicted positions was obtained using values for the radial parameters that were derived by interpolation from other spectra. In Table III we give the values used in the final diagonalization and those obtained

TABLE III

Parameters for 4 f^6(^{7}F) 5 d *of* Sm II

Name	Diagonalization (in cm^{-1})	Least squares (in cm^{-1})
A	16 600	16 597 ± 36
F_2	138	138 ± 3
F_4	9	8.6 ± 0.7
G_1	183	182 ± 5
G_3	11	10 ± 2
G_5	2.3	2.4 ± 0.2
ζ_f	1 150	1 139 ± 26
ζ_d	400	403 ± 42
rms error		168
in % of total width		1.24 %

after the optimization process (least squares). Since the *rms* error is only 168 cm^{-1} (1.24 % of the total width) and the parameters were invariant — within their definition — to the least squares adjustment we conclude that convergence has been reached.

An interesting outcome is the small value of ζ_d that was also anticipated by Eremin et al. [11].

In Table IV we give the comparison between calculated and observed levels and g-factors, as well as L-S coupling notations. While the ^{8}H and ^{8}D are pure, heavy admixtures are indicated between ^{8}G-^{8}F, ^{8}P-^{6}P, and ^{6}F-^{6}D-^{6}G. Still, L-S notations have a major component that is higher than 50 % in 90 % of the cases and therefore Russell — Saunders scheme is suitable for level designations in this case. There is quite a satisfactory agreement between the observed and calculated levels and g-factors, except for the two levels with $J = 0\frac{1}{2}$ where the observed to calculated correspondance dictated by the positions contradicts the one indicated by the g-factors predictions. At this stage we decided to follow the theoretical predictions for the level positions rather than the g-factor considerations for the following reasons : 1) The interchange would involve a deviation of more than 1 000 cm^{-1} for the ^{6}F$_{0\frac{1}{2}}$. We believe our calculations are better than such a deviation. 2) A change of the parameters causing only a second order change in the prediction of level position will cause a first order correction to the g-factors. This sensitivity of the g-factors to small changes in the

TABLE IV

Calculated positions, g-values and percentages in L-S coupling for the $4f^6(^7F)\,5d$ *levels of* Sm II

Observed designation	J	Percentage composition	Observed level (in cm^{-1})	Calculated level (in cm^{-1})	O-C (in cm^{-1})	$g_{obs.}$	$g_{calc.}$
^8H	$1\frac{1}{2}$	100 % ^8H	7 135	7 348	− 213	− 0.385	− 0.397
^8H	$2\frac{1}{2}$	100 % ^8H	7 525	7 645	− 120	0.70	0.687
^8H	$3\frac{1}{2}$	100 % ^8H	8 046	8 062	− 16	1.055	1.049
^8H	$4\frac{1}{2}$	100 % ^8H	8 679	8 602	77	1.210	1.214
^8H	$5\frac{1}{2}$	100 % ^8H	9 407	9 266	141	1.300	1.302
^8H	$6\frac{1}{2}$	100 % ^8H	10 214	10 056	158	1.35	1.355
^8H	$7\frac{1}{2}$	100 % ^8H	11 094	10 973	121	1.38	1.389
^8H	$8\frac{1}{2}$	100 % ^8H	12 045	12 021	24	1.412	1.412
^8D	$1\frac{1}{2}$	85 % ^8D	8 578	9 069	− 491	2.62	2.727
^8D	$2\frac{1}{2}$	88 % ^8D	9 410	9 531	− 121	2.01	2.030
^8D	$3\frac{1}{2}$	86 % ^8D	10 181	10 071	110	1.79	1.790
^8D	$4\frac{1}{2}$	81 % ^8D	10 960	10 770	190	1.685	1.677
^8D	$5\frac{1}{2}$	79 % ^8D	11 791	11 724	67	1.636	1.617
^8G	$0\frac{1}{2}$	90 % ^8F	10 372	10 413	− 41	0.36	3.536
^8G	$1\frac{1}{2}$	72 % ^8F + 22 % ^8G	10 518	10 588	− 70	1.335	1.769
^8G	$2\frac{1}{2}$	59 % ^8F + 34 % ^8G	10 873	10 897	− 26	1.435	1.580
^8G	$3\frac{1}{2}$	50 % ^8F + 41 % ^8G	11 395	11 345	50	1.465	1.530
^8G	$4\frac{1}{2}$	*41* % ^8F + 46 % ^8G	12 045	11 941	104	1.470	1.512
^8G	$5\frac{1}{2}$	49 % ^8G + 35 % ^8F	12 789	12 675	114	1.47	1.507
^8G	$6\frac{1}{2}$	56 % ^8F + 42 % ^8G	13 605	13 436	169	1.477	1.501
^8G	$7\frac{1}{2}$	96 % ^8G	14 504	14 791	− 287	1.455	1.463
^8F	$0\frac{1}{2}$	90 % ^8G	10 743	10 840	− 97	2.32	− 0.873
^8F	$1\frac{1}{2}$	69 % ^8G + 20 % ^8F	11 155	11 126	29	1.64	1.315
^8F	$2\frac{1}{2}$	55 % ^8G + 31 % ^8F	11 798	11 570	89	1.57	1.504
^8F	$3\frac{1}{2}$	56 % ^8G + 37 % ^8F	12 232	12 115	117	1.532	1.482
^8F	$4\frac{1}{2}$	52 % ^8G + 44 % ^8F	12 842	12 785	57	1.526	1.496
^8F	$5\frac{1}{2}$	*46* % ^8F + 49 % ^8G	13 466	13 518	− 52	1.520	1.501
^8F	$6\frac{1}{2}$	55 % ^8G + 44 % ^8F	14 084	14 220	− 136	1.54	1.490
^6P	$1\frac{1}{2}$	77 % ^6P	11 047	11 071	− 24	2.510	2.310
^6P	$2\frac{1}{2}$	42 % ^6P + 40 % ^8P	11 798	11 490	308	1.99	1.976
^6P	$3\frac{1}{2}$	63 % ^6P + 31 % ^8P	13 777	14 089	− 312	1.78	1.786
^8P	$2\frac{1}{2}$	52 % ^8P + 41 % ^6P	12 567	12 681	− 114	2.16	2.079
^8P	$3\frac{1}{2}$	62 % ^8P + 30 % ^6P	12 987	12 655	332	1.86	1.850
^8P	$4\frac{1}{2}$	94 % ^8P	14 115	14 268	− 153	1.778	1.771
^6F	$0\frac{1}{2}$	86 % ^6D	16 162	16 041	121	0.300	2.835
^6F	$1\frac{1}{2}$	64 % ^6D + 31 % ^6F	16 078	16 147	− 69	1.35	1.596
^6F	$2\frac{1}{2}$	49 % ^6D + 45 % ^6F	16 429	16 420	9	1.355	1.477
^6F	$3\frac{1}{2}$	52 % ^6F + 36 % ^6D	17 005	16 914	91	1.405	1.459
^6F	$4\frac{1}{2}$	55 % ^6F + 34 % ^6D	17 718	17 627	91	—	1.460
	$5\frac{1}{2}$	72 % ^6F		19 102			1.424
^6D	$0\frac{1}{2}$	86 % ^6F		17 105			− 0.165
^6D	$1\frac{1}{2}$	55 % ^6F + 31 % ^6D	17 568	17 449	119	1.183	1.58
^6D	$2\frac{1}{2}$	*30* % ^6F + 42 % ^6D	18 050	17 954	96	1.54	1.345
^6D	$3\frac{1}{2}$	46 % ^6D + 34 % ^6G	18 808	18 574	234	1.52	1.404
^6D	$4\frac{1}{2}$	53 % ^6D + 34 % ^6G	19 400	19 206	194	—	1.444

TABLE IV (contd.)

Observed designation	J	Percentage composition	Observed level (in cm^{-1})	Calculated level (in cm^{-1})	O-C (in cm^{-1})	$g_{obs.}$	$g_{calc.}$
^6H	2 ½	100 % ^6H	14 193	14 431	− 238	0.295	0.291
^6H	3 ½	97 % ^6H	14 668	14 772	− 104	0.84	0.832
^6H	4 ½	97 % ^6H	15 243	15 232	11	1.080	1.077
^6H	5 ½	96 % ^6H	15 897	15 828	69	1.21	1.208
^6H	6 ½	96 % ^6H	16 615	16 575	40	1.295	1.286
^6H	7 ½	98 % ^6H	17 392	17 484	− 92	1.34	1.337
^6G	1 ½	85 % ^6G	18 478	18 498	− 20	0.01	0.164
	2 ½	69 % ^6G + 25 % ^6F	19 035	19 060	− 25	—	1.012
	3 ½	56 % ^6G + 31 % ^6F	19 628	19 729	− 101	1.30	1.269
	4 ½	53 % ^6G + 34 % ^6F	20 179	20 386	− 207	1.35	1.359
	5 ½	72 % ^6G	20 648	20 853	− 205	1.35	1.371
	6 ½	96 % ^6G		21 150			1.383

TABLE V

Eigenvectors in L-S scheme for $4f^6(^7F)\,5d$ *of* Sm II

Level	J	^6P	^8P	^6D	^8D	^6F	^8F	^6G	^8G	^6H	^8H
7 272	1 ½	— .000 1		.000 4	— .000 1	— .004 1	.002 0	.042 6	— .036 5		.998 4
7 570	2 ½	— .000 2	0	.000 8	— .000 4	— .005 9	.004 3	— .040 0	— .057 1	— .010 6	.997 5
7 990	3 ½	— .000 2	0	.001 0	— .000 6	— .006 4	.006 7	— .036 1	— .073 4	— .014 9	.996 5
8 532	4 ½		0	.000 7	— .000 7	— .005 6	.008 4	.030 5	— .086 9	— .017 1	.995 7
9 200	5 ½				— .000 7	— .003 6	.008 8	.023 3	— .090 5	— .017 3	— .995 4
9 994	6 ½						.007 0	.014 3	— .087 8	— .015 3	.995 9
10 917	7 ½								— .072 1	— .011 0	.997 3
11 971	8 ½										1
9 043	1 ½	.361 1		— .031 0	.918 5	— .004 0	— .157 2	.000 9	— .016 8		.001 0
9 503	2 ½	— .185 9	.108 1	.014 7	— .941 2	.015 3	.256 6	— .004 0	— .040 8	.000 7	— .003 6
10 043	3 ½	— .060 5	.154 6	— .013 3	— .927 9	.033 4	.325 0	— .009 8	— .066 2	.002 5	— .007 0
10 747	4 ½		.139 7	— .028 8	— .908 6	.054 0	.376 6	— .018 0	— .093 9	.006 0	— .010 9
11 710	5 ½				— .894 6	.074 0	.419 3	— .027 9	— .131 6	.012 1	— .015 1
10 372	0 ½			.120 6		— .031 4	.948 8		— .290 4		
10 546	1 ½	— .072 8		— .096 7	— .130 3	.048 6	— .859 5	.001 9	— .476 3		.019 2
10 855	2 ½	— .008 5	— .091 4	.091 9	.226 6	— .057 3	.768 8	— .005 4	— .579 6	.008 2	— .036 5
11 305	3 ½	— .016 6	— .106 3	.076 7	.272 2	— .057 6	.701 5	— .012 5	— .640 2	.019 9	— .051 4
11 904	4 ½		— .084 9	.052 1	.320 7	— .053 1	.643 6	— .020 1	— .681 5	.036 7	— .062 4
13 500	5 ½				— .219 5	— .015 5	— .683 4	.038 8	— .690 2	.057 9	— .056 8
13 406	6 ½						.747 1	— .059 2	— .654 6	.078 3	— .061 0
10 790	0 ½			.032 9		.098 1	.290 2		.951 3		
11 083	1 ½	— .267 3		.085 8	.170 2	.074 9	.450 0	— .006 8	— .826 5		.029 9
11 533	2 ½	— .283 5	— .208 3	.006 9	— .090 9	— .072 9	— .564 4	.015 1	— .736 3	.010 0	— .040 7
12 083	3 ½	.055 1	.141 5	— .064 2	— .141 6	— .051 2	— .613 0	.020 4	— .755 4	.023 1	— .052 3
12 760	4 ½		.083 1	— .041 2	— .187 5	— .035 5	— .660 5	.029 2	— .716 4	.038 3	— .056 1
12 645	5 ½				— .380 8	.047 4	— .594 7	.031 1	.700 2	— .058 3	.067 1
14 202	6 ½						.660 3	— .048 0	.741 6	— .089 5	.060 0
14 765	7 ½								.948 9	— .158 8	.069 4
11 038	1 ½	— .881 5		.108 9	.330 2	— .043 8	— .145 8	.003 3	— .280 6		— .010 4
11 450	2 ½	.657 0	.644 0	— .151 9	— .078 0	— .006 6	— .124 8	.002 0	— .329 4	.004 9	— .018 1
14 069	3 ½	.791 5	— .561 0	— .189 0	— .138 5	.059 7	.002 3	— .012 0	— .011 2	.009 1	.000 3
12 641	2 ½	.642 8	— .722 4	— .135 5	— .213 2	.030 2	— .008 5	— .003 3	— .014 6	.001 0	— .000 3
12 623	3 ½	.549 7	.793 0	— .150 8	.146 4	.029 0	.144 8	— .007 8	.054 0	— .000 5	.003 9
14 240	4 ½		.974 2	— .119 7	.179 4	.011 5	.063 7	— .005 5	.013 3	.001 2	.001 1
17 080	0 ½			.353 1		.929 8	— .043 2		— .095 0		
17 444	1 ½	.059 7		.556 1	— .010 8	.739 6	— .064 4	— .361 2	— .071 6		.015 8
17 966	2 ½	— .110 0	— .008 1	— .647 5	.016 4	— .546 2	.069 0	.509 3	.049 4	.054 5	— .020 0
16 913	3 ½	.201 3	.016 3	.597 5	— .063 3	— .719 5	— .032 5	.265 1	.064 0	.071 5	— .008 8
17 613	4 ½		.092 0	.575 6	— .061 2	— .741 1	— .005 1	.310 1	.053 1	.089 9	— .008 1

TABLE V (contd.)

Level	J	^{6}P	^{8}P	^{6}D	^{8}D	^{6}F	^{8}F	^{6}G	^{8}G	^{6}H	^{8}H
19 100	5 ½				.071 6	.851 2	—.040 2	—.504 8	—.040 5	—.108 9	.009 8
16 063	0 ½			.927 2		—.353 5	—.117 3		.040 1		
16 155	1 ½	—.110 1		—.804 5	.035 6	.560 5	.092 0	—.114 1	—.061 4		.005 1
16 421	2 ½	.164 5	.003 1	.690 7	—.053 0	—.666 1	—.062 8	.198 2	.067 6	.039 0	—.007 9
18 598	3 ½	—.144 2	—.027 3	—.687 3	.015 4	—.389 2	.065 4	.584 3	.032 9	.084 4	—.019 7
19 241	4 ½		—.087 3	—.731 5	.001 3	—.321 7	.057 7	.583 3	.024 5	.096 6	—.015 9
14 222	2 ½	.003 4	—.000 5	.007 0	—.001 5	—.023 8	.000 7	.091 1	—.010 1	—.995 4	—.015 0
14 768	3 ½	.014 5	—.004 1	.009 4	—.004 3	—.040 0	.003 1	.131 2	—.024 7	—.989 8	—.021 7
15 233	4 ½		—.005 2	—.012 3	.004 1	.047 8	—.006 5	—.153 7	.047 0	.985 4	.026 0
15 836	5 ½				—.004 9	—.037 6	.009 3	.154 9	—.078 3	—.983 7	—.028 1
16 592	6 ½						—.009 1	—.127 7	.116 4	.984 5	.027 3
17 511	7 ½								.157 6	.987 2	.022 3
18 498	1 ½	—.010 8		—.118 5	.000 4	—.358 9	.008 1	—.924 5	.027 8		.039 0
19 063	2 ½	.032 6	.003 3	.231 4	.000 6	.497 6	—.011 5	.831 3	—.033 3	.066 7	—.031 7
19 739	3 ½	.053 2	.012 9	.319 2	.006 5	.563 8	—.007 1	.754 3	—.029 9	.082 2	—.024 9
20 403	4 ½		—.034 5	—.337 4	—.021 0	—.581 2	—.008 3	—.733 1	.020 9	—.092 1	.019 7
20 873	5 ½				—.038 2	—.515 8	—.041 1	—.847 0	.005 7	—.114 8	.016 8
21 184	6 ½						.075 6	.988 8	.013 1	.127 7	—.011 0

parameters makes position calculations a better criterion for the fitting of observed levels.

The small O-C values for both ^{8}F and ^{6}F indicates the weakness of configuration interaction with 4 f^6(^{7}F) 6 s.

In Table V we give the eigenvectors in L-S coupling for the 57 levels of f^6(^{7}F) 5 d of Sm II.

B. Gd II 4 f^8(^{7}F) 5 d. — From the available lists of even levels of Gd II established by Russell [9], Spector [1] and Blaise and Van Kleef [2] we picked 45 for the least squares calculations. From its first member, $^8G_{7\frac{1}{2}}$ at around 18 400 cm^{-1} up to approximately 25 000 cm^{-1} the 4 f^8(^{7}F) 5d group of levels is well isolated from other groups. In the region above 25 000 cm^{-1} where about half of its levels lie, it overlaps levels of 4 f^7(^{8}S) 5d 6p and 4 f^7(^{8}S) 6s 6p. Accurate predictions for both positions and g-factors are essential for the correct selection of experimental levels. In the case of ^{6}D, our predictions fit well, both in positions and g-factors, a certain ^{6}D given in ref. 2 the designation 4f^8 6s. Such designation seems, at present to need further corroboration. The theoretical prediction for the location of the center of gravity of the ^{5}D of 4 f^8 above the ^{7}F is given by Elliott [12] et al. as 51.8 F_2 where.

$$F_2 = 12.4\,(Z - 34)\ \mathrm{cm}^{-1}.$$

This puts ^{5}D about 19 300 cm^{-1} above ^{7}F. Also in ref. 12 Table 3 we get values for the splitting factors that enable us to estimate the total splitting of each multiplet. For ^{5}D we get an estimated spread of about 9 000 cm^{-1}. Since the ^{6,4}D of 4f^8(^{5}D) 6s are obtained by adding 6s electron to the ^{5}D, we expect the two terms to follow closely the structure of ^{5}D, as do the ^{8,6}F of 4f^8(^{7}F) 6s. Also the transitions made from a ^{6}D belonging to 4 f^8(^{5}D) 6 s to the ground configuration 4f^7(^{8}S) 5d 6s should be quite different from those made from a ^{6}D which belongs to 4 f^8(^{7}F) 5d that overlaps 4 f^7(^{8}S) 6s 6p. While the new ^{6}D indeed falls close to its predicted position its spread of about 2 300 cm^{-1} is far from what can be expected from the same prediction. On the other hand its structure agrees with the predictions of our calculation. Furthermore, this ^{6}D makes transitions to the ground configuration which are very similar in character to those made by the neighboring sextet belonging to 4 f^8(^{7}F) 5 d (see Table IX). We see, therefore, no reason to exclude it at this stage from the least squares calculation.

The final parameters obtained after the optimization process are given in Table VI. In Table VII we give our predictions for the positions and g-values of the levels of 4 f^8(^{7}F) 5d and compare these to the available observed levels. The agreement is quite satisfactory. Again there is no evident perturbation of either ^{6}F or ^{8}F by their analogues in 4 f^8(^{7}F) 6 s. The *rms* error is 239 cm^{-1} which is 1.76 % of the total width of this configuration.

Table VIII presents the eigenvectors in L-S coupling of the levels of this subconfiguration.

TABLE VI

Parameters for 4 f^8(^{7}F) 5 d *of* Gd II

Name	Diagonalization (in cm^{-1})	Least squares (in cm^{-1})
A	27 500	27 527 ± 87
F_2	147	144 ± 4
F_4	12	10 ± 1
G_1	144	129 ± 9
G_3	15	15 ± 2
G_5	2.5	2.5 ± 0.5
ζ_f	1 240	1 219 ± 39
ζ_d	550	607 ± 73
rms error		239
in % of total width		1.76 %

TABLE VII

Calculated positions, g factors and L-S percentages for the $4f^8(^7F)\,5d$ *levels of* Gd II

Observed designation	J	Percentage composition	Observed level (in cm^{-1})	Calculated level (in cm^{-1})	O-C (in cm^{-1})	$g_{obs.}$	$g_{calc.}$
^8G	$7\frac{1}{2}$	98 % ^8G	18 367	18 687	− 320	1.465	1.464
	$6\frac{1}{2}$	72 % ^8G	18 389	18 618	− 229	1.46	1.472
	$5\frac{1}{2}$	56 % ^8G + 30 % ^8F	18 690	18 852	− 162	1.515	1.494
	$4\frac{1}{2}$	56 % ^8G + 30 % ^8F	19 377	19 379	− 2	1.51	1.493
	$3\frac{1}{2}$	66 % ^8G + 25 % ^8F	20 098	20 010	88	1.440	1.456
	$2\frac{1}{2}$	79 % ^8G	20 631	20 596	39	1.325	1.354
	$1\frac{1}{2}$	90 % ^8G	21 006	21 060	− 54	1.01	1.034
	$0\frac{1}{2}$	98 % ^8G	21 227	21 356	− 129	− 1.21	− 1.198
^8D	$5\frac{1}{2}$	56 % ^8D + 30 % ^8G	20 093	20 381	− 288	1.555	1.559
	$4\frac{1}{2}$	50 % ^8D + 32 % ^8G	20 574	20 849	− 275	1.58	1.586
	$3\frac{1}{2}$	48 % ^8D + 25 % ^8G	21 365	21 500	− 135	1.675	1.644
	$2\frac{1}{2}$	40 % ^8F + 40 % ^8D	22 062	22 103	− 41	1.860	1.775
	$1\frac{1}{2}$	64 % ^8F + 26 % ^8D	22 677	22 597	80	2.32	2.111
^8F	$6\frac{1}{2}$	76 % ^8F	21 158	20 845	313	1.515	1.517
	$5\frac{1}{2}$	56 % ^8F + 32 % ^8D	22 533	22 389	144	1.555	1.565
	$4\frac{1}{2}$	55 % ^8F + 27 % ^8D	23 025	22 912	113	1.585	1.606
	$3\frac{1}{2}$	50 % ^8F + 40 % ^8D	23 473	23 485	− 12	1.66	1.688
	$2\frac{1}{2}$	53 % ^8D + 40 % ^8F	23 697	23 862	− 165	1.84	1.892
	$1\frac{1}{2}$	72 % ^8D + 25 % ^8F	23 732	24 067	− 335	2.385	2.575
	$0\frac{1}{2}$	98 % ^8F	23 255	22 926	329	3.93	3.861
^8H	$8\frac{1}{2}$	100 % ^8H	22 531	22 615	− 84	1.412	1.412
	$7\frac{1}{2}$	88 % ^8H	23 270	23 048	232	1.375	1.385
	$6\frac{1}{2}$	92 % ^8H	23 970	23 604	366	1.350	1.353
	$5\frac{1}{2}$	90 % ^8H	24 528	24 107	421	1.355	1.303
	$4\frac{1}{2}$	90 % ^8H	24 852	24 524	328	1.215	1.218
	$3\frac{1}{2}$	94 % ^8H		24 862			1.055
	$2\frac{1}{2}$	98 % ^8H		25 119			0.693
	$1\frac{1}{2}$	98 % ^8H		25 300			− 0.390
^6F	$5\frac{1}{2}$	90 % ^6F	24 412	24 580	− 168	1.470	1.449
	$4\frac{1}{2}$	85 % ^6F	25 438	25 521	− 83	1.415	1.440
	$3\frac{1}{2}$	86 % ^6F	26 373	26 373	0	1.385	1.394
	$2\frac{1}{2}$	90 % ^6F	27 130	27 109	21	1.305	1.308
	$1\frac{1}{2}$	94 % ^6F	27 662	27 677	− 15	1.05	1.059
	$0\frac{1}{2}$	100 % ^6F	27 990	28 033	− 48	− 0.61	− 0.639
^8P	$4\frac{1}{2}$	83 % ^8P	25 608	25 443	165	1.750	1.754
	$3\frac{1}{2}$	90 % ^8P	27 418	27 293	125	1.905	1.924
	$2\frac{1}{2}$	96 % ^8P	28 629	28 623	6	2.315	2.277
^6D	$4\frac{1}{2}$	85 % ^6D	28 443	27 993	450	1.515	1.528
	$3\frac{1}{2}$	73 % ^6D	28 562	28 805	− 243	1.560	1.561
	$2\frac{1}{2}$	85 % ^6D	29 716	29 639	77	1.700	1.638
	$1\frac{1}{2}$	94 % ^6D	30 403	30 259	144	1.89	1.859
	$0\frac{1}{2}$	100 % ^6D	30 758	30 636	122	3.33	3.309

TABLE VII (contd.)

Observed designation	J	Percentage composition	Observed level (in cm^{-1})	Calculated level (in cm^{-1})	O-C (in cm^{-1})	$g_{obs.}$	$g_{calc.}$
^{6}G	6 ½	94 % ^{6}G		25 075			1.380
	5 ½	84 % ^{6}G	26 640	26 343	297	1.320	1.338
	4 ½	77 % ^{6}G		27 346			1.287
	3 ½	79 % ^{6}G	28 220	28 151	69	1.205	1.164
	2 ½	88 % ^{6}G		28 770			0.868
	1 ½	96 % ^{6}G		29 196			0.034
^{6}H	7 ½	90 % ^{6}H		25 545			1.339
	6 ½	86 % ^{6}H		26 921			1.293
	5 ½	84 % ^{6}H		28 030			1.221
	4 ½	86 % ^{6}H		28 916			1.098
	3 ½	88 % ^{6}H		29 605			0.362
	2 ½	94 % ^{6}H	30 118	29 820	− 298	0.345	0.325
^{6}P	3 ½	86 % ^{6}P	30 145	30 252	− 107	1.655	1.698
	2 ½	92 % ^{6}P	31 238	31 510	− 272	1.835	1.870
	1 ½	98 % ^{6}P	31 915	32 368	− 453	2.32	2.386

TABLE VIII

Eigenvectors components in L-S scheme for $4f^8(^7F)\,5d$ *of* Gd II

Calc. Level (in cm^{-1})	J	^{6}P	^{8}P	^{6}D	^{8}D	^{6}F	^{8}F	^{6}G	^{8}G	^{6}H	^{8}H
18 687	7 ½								.986 6	— .053 5	.154 1
18 618	6 ½						.478 4	— .101 0	.859 8	— .040 4	.141 5
18 852	5 ½				.329 9	— .052 3	.556 9	— .089 2	.745 6	— .027 3	.117 5
19 379	4 ½		.071 2	— .004 0	.333 3	— .038 4	.550 4	— .076 7	.749 1	— .020 1	.109 6
20 010	3 ½	.005 9	.045 3	.005 8	.256 5	— .013 8	.505 7	— .065 2	.812 7	— .014 4	.106 0
20 596	2 ½	.005 4	.018 7	.012 3	.160 6	.012 0	.422 3	— .050 9	.885 3	— .008 1	.093 8
21 060	1 ½	— .002 9		— .012 8	— .071 7	— .034 1	— .303 3	.032 7	— .946 6		— .066 8
21 356	0 ½			.008 0		.048 9	.158 2		.986 2		
20 381	5 ½				.746 9	— .100 9	.325 6	.043 3	— .555 6	.027 2	— .120 9
20 849	4 ½		.200 7	— .032 1	.706 2	— .088 7	.340 5	.042 2	— .566 5	.020 5	— .114 5
21 500	3 ½	— .016 6	— .153 9	.016 6	— .689 6	.086 3	— .474 3	— .030 1	.507 8	— .012 6	.094 5
22 103	2 ½	— .022 2	— .092 4	— .004 7	— .639 2	— .078 3	— .634 2	— .017 2	.411 6	— .005 6	.065 1
22 597	1 ½	.021 2		.028 5	.510 2	— .061 8	.805 0	.007 1	— .292 3		— .032 7
20 845	6 ½						— .874 9	— .001 2	.461 5	— .037 7	.141 9
22 389	5 ½				— .573 9	— .065 9	.750 1	— .001 4	— .288 0	.031 0	— .140 3
22 912	4 ½		— .292 8	.059 4	— .518 3	— .088 2	.738 3	.002 0	— .268 4	.023 1	— .129 5
23 485	3 ½	.016 6	.217 7	— .059 9	.620 8	.077 7	— .706 2	— .001 8	.219 6	— .013 5	.100 4
23 862	2 ½	.026 9	.144 6	— .056 6	.730 5	.056 8	— .639 1	— .001 5	.162 7	— .005 1	.058 6
24 067	1 ½	— .038 6		.045 1	— .855 6	— .031 3	.504 1	.000 8	— .094 6		— .020 5
22 926	0 ½			.052 2		— .036 1	.985 6		— .156 8		
22 615	8 ½										1
23 048	7 ½								— .163 0	— .303 8	.938 7
23 604	6 ½						.061 0	.051 4	— .195 2	— .273 8	.938 4
24 107	5 ½				.031 2	.031 0	— .083 2	— .064 0	.199 6	.230 9	— .945 5
24 524	4 ½		.042 1	— .005 6	.017 1	.023 1	— .075 4	— .072 0	.182 8	.186 2	— .958 3
24 862	3 ½	.000 8	.014 8	— .004 0	.024 5	.016 1	— .064 3	— .074 0	.155 1	.140 5	— .972 5
25 119	2 ½	.000 6	.004 7	— .002 7	.016 5	.009 4	— .040 1	— .073 1	.117 0	.090 7	— .985 3
25 300	1 ½	.000 2		— .001 1	.005 7	.004 4	— .016 7	— .071 3	.072 5		— .994 6
24 580	5 ½				— .052 2	— .959 8	— .119 2	— .246 0	.015 9	— .030 1	— .010 0
25 521	4 ½		.161 4	.213 1	— .021 2	.917 1	.130 4	.261 1	— .025 8	.033 7	— .000 6
26 373	3 ½	— .037 9	.021 1	— .244 3	— .029 7	— .928 7	— .090 5	— .255 1	.028 3	— .030 6	.010 6
27 109	2 ½	— .027 4	.004 5	— .210 0	— .013 5	— .947 3	— .069 8	— .225 4	.037 0	— .020 4	.013 4

TABLE VIII (contd.)

Calc. Level (in cm^{-1})	J	^6P	^8P	^6D	^8D	^6F	^8F	^6G	^8G	^6H	^8H
27 677	1 ½	.012 9		.154 1	.005 2	.972 1	.046 9	.162 9	— .046 1		— .011 7
28 038	0 ½			.082 2		.994 9	.023 6		— .053 8		
25 443	4 ½		.911 0	— .123 4	— .347 2	— .144 7	.105 1	— .036 2	— .024 2	— .008 7	.019 2
27 293	3 ½	— .002 7	— .959 1	.058 1	.265 7	— .034 0	— .067 9	— .016 4	.009 8	— .002 1	— .001 7
28 623	2 ½	— .002 6	— .983 7	.039 5	.172 1	— .010 3	— .029 6	— .013 4	.002 5	— .002 3	.000 3
27 993	4 ½		.100 0	.919 5	.013 8	— .286 8	— .049 1	.208 5	.033 7	.122 1	.010 7
28 805	3 ½	.348 8	.065 6	.857 1	.013 3	— .289 2	— .056 9	.194 0	.031 1	.118 4	.004 3
29 639	2 ½	.264 2	.042 0	.923 8	.016 7	— .232 9	— .058 7	.099 8	.019 3	.082 4	.000 8
30 259	1 ½	.164 0		.970 4	.015 2	— .160 5	— .057 1	.045 8	.011 1		— .003 2
30 636	0 ½			.995 2		— .080 7	— .054 9		.004 8		
25 075	6 ½						.043 8	.966 7	.094 8	.231 6	.031 5
26 343	5 ½				— .015 1	— .242 2	.001 5	.916 1	.105 3	.298 6	.024 6
27 346	4 ½		.033 5	.297 0	.013 1	.184 9	— .002 2	— .881 3	— .094 0	— .301 2	— .005 6
28 151	3 ½	.081 0	.027 0	.269 8	.008 1	.179 0	— .001 2	— .894 5	— .081 8	— .284 1	.016 6
28 770	2 ½	.034 3	.018 0	.160 2	.003 5	.189 2	.002 7	— .937 4	— .067 7	— .227 9	.042 0
29 196	1 ½	.008 9		.070 9	.001 8	.151 8	.002 4	— .982 4	— .046 1		.067 7
25 545	7 ½								.003 4	.951 2	.308 5
26 921	6 ½						.007 6	.229 5	.025 0	— .931 9	— .279 7
28 030	5 ½				— .002 4	— .042 9	.0019	.292 0	.035 4	— .924 2	— .239 7
28 916	4 ½		.003 3	.033 3	— .001 0	— .061 9	— .003 2	.312 2	.035 5	— .925 8	— .197 9
29 605	3 ½	.024 5	.001 9	.032 7	— .000 4	— .059 6	— .004 5	.293 4	.028 4	— .940 2	— .154 4
29 820	2 ½	.015 5	.001 6	.045 2	.000 5	— .044 4	— .004 4	.228 2	.017 2	— .965 7	— .104 1
30 252	3 ½	.932 5	— .035 8	— .352 8	— .031 0	.056 5	.018 6	— .012 9	— .004 2	.003 9	.001 4
31 510	2 ½	.962 7	— .021 0	— .264 4	— .040 7	.031 1	.014 9	— .004 2	— .002 1	.000 5	.000 3
32 368	1 ½	.985 4		— .161 3	— .045 8	.012 6	.009 5	— .000 9	— .000 8		.000 1

TABLE IX

Classified lines of Gd II

λ	Intensity in arc	σ (in cm^{-1})	Odd level (in cm^{-1})	J	Even level (in cm^{-1})	J
8 598.760	50	11 626.39	19 223	3 ½	30 849	4 ½
7 963.250	500	12 554.23	19 750	5 ½	32 304	4 ½
7 535.290	6	13 267.23	19 223	3 ½	32 490	3 ½
7 220.390	5	13 845.85	19 750	5 ½	33 596	4 ½
7 201.410	150	13 882.34	9 142	3 ½	23 025	4 ½
7 069.930	80	14 140.51	8 884	4 ½	23 025	4 ½
6 909.900	15	14 474.28	8 551	5 ½	23 025	4 ½
5 982.420	60	16 711.01	19 750	5 ½	36 461	5 ½
5 901.670	10	16 939.66	12 776	2 ½	29 715	2 ½
5 524.600	150	18 095.83	19 750	5 ½	37 846	4 ½
5 469.050	100	18 279.63	19 750	5 ½	33 029	4 ½
5 460.660	15	18 307.72	19 750	5 ½	33 057	4 ½
5 412.642	200	18 470.13	10 091	4 ½	28 561	3 ½
5 368.284	10	18 622.75	19 223	3 ½	37 846	4 ½
5 316.801	100	18 803.07	19 750	5 ½	38 553	5 ½
5 315.794	20	18 806.63	19 223	3 ½	38 029	4 ½
5 285.830	8	18 913.24	10 802	1 ½	29 715	2 ½
5 173.455	30	19 324.06	10 391	3 ½	29 715	2 ½
5 123.652	60	19 511.89	10 633	2 ½	30 145	3 ½
5 121.930	3	19 518.45	18 955	2 ½	38 473	2 ½
5 061.063	100	19 753.19	10 391	3 ½	30 145	3 ½
5 052.416	60	19 786.94	19 750	5 ½	39 537	4 ½
5 048.785	50	19 801.22	19 223	3 ½	39 024	2 ½
4 985.300	100	20 053.37	10 091	4 ½	30 145	3 ½

TABLE IX (contd.)

λ	Intensity in arc	σ (in cm^{-1})	Odd level (in cm^{-1})	J	Even level (in cm^{-1})	J
4 933.452	20	20 264.12	9 451	1 ½	29 715	2 ½
4 919.210	15	20 322.79	18 150	3 ½	28 473	2 ½
4 859.400	30	20 572.92	9 142	3 ½	29 715	2 ½
4 851.862	25	20 604.88	10 633	2 ½	31 238	2 ½
4 760.020	2	21 002.13	9 142	3 ½	30 145	3 ½
4 752.650	4	21 035.01	19 750	5 ½	40 785	5 ½
4 702.311	8	21 260.19	8 884	4 ½	30 145	3 ½
4 606.641	8	21 701.71	19 223	3 ½	40 924	4 ½
4 588.763	10	21 786.26	9 451	1 ½	31 238	2 ½
4 570.360	1	21 873.94	19 223	3 ½	41 097	3 ½
4 563.030	4	21 909.12	9 328	2 ½	31 238	2 ½
4 536.560	5	22 036.95	19 223	3 ½	41 260	2 ½
4 429.500	2	22 569.57	18 319	4 ½	40 888	5 ½
4 152.025	10	24 077.84	4 483	3 ½	28 561	3 ½
4 105.792	15	24 348.96	4 212	2 ½	28 561	3 ½
4 065.610	15	24 589.61	3 972	4 ½	28 561	3 ½
3 962.105	30	25 231.97	4 483	3 ½	29 715	2 ½
3 952.600	1	25 292.65	4 852	4 ½	30 145	3 ½
3 923.569	4	25 479.78	3 082	2 ½	28 561	3 ½
3 919.99	6	25 503.05	4 212	2 ½	29 715	2 ½
3 891.680	4	25 688.56	4 027	1 ½	29 715	2 ½
3 802.850	40	26 288.60	3 427	3 ½	29 715	2 ½
3 753.560	10	26 633.81	3 082	2 ½	29 715	2 ½
3 741.770	4	26 717.72	3 427	3 ½	30 145	3 ½
3 694.030	80	27 063.00	3 082	2 ½	30 145	3 ½
3 612.880	15	27 670.86	10 802	1 ½	38 473	2 ½
3 596.903	1	27 793.76	3 444	3 ½	31 238	3 ½
3 594.709	6	27 810.73	3 427	3 ½	31 238	3 ½
3 586.576	10	27 973.79	10 599	3 ½	38 473	2 ½
3 550.630	8	28 155.97	3 082	2 ½	31 238	3 ½
3 522.446	50	28 381.25	2 856	1 ½	31 238	2 ½
3 500.182	30	28 561.77	0	2 ½	28 561	3 ½
3 444.705	3	29 021.75	9 451	1 ½	38 473	2 ½
3 411.570	50	29 303.61	19 750	5 ½	49 053	4 ½
3 394.151	40	29 453.99	261	3 ½	29 715	2 ½
3 387.511	4	29 511.73	633	4 ½	30 145	3 ½
3 364.241	500	29 715.85	0	2 ½	29 715	2 ½
3 352.512	40	29 819.81	0	2 ½	29 819	2 ½
3 352.271	3	29 821.85	11 066	4 ½	40 888	5 ½
3 345.412	100	29 883.09	261	3 ½	30 145	3 ½
3 324.860	4	30 067.80	19 223	3 ½	49 291	3 ½
3 320.317	20	30 108.94	19 223	3 ½	49 332	3 ½
3 316.342	100	30 145.03	0	2 ½	30 145	3 ½
3 296.782	6	30 323.87	19 223	3 ½	49 547	2 ½
3 288.165	20	30 403.34	0	2 ½	30 403	1 ½
3 246.099	25	30 797.32	10 091	4 ½	40 888	5 ½
3 227.361	6	30 976.12	261	3 ½	31 238	2 ½
3 200.312	50	31 237.93	0	2 ½	31 238	2 ½
3 132.340	15	31 915.76	0	2 ½	31 915	1 ½
3 123.694	100	32 004.10	8 884	4 ½	40 888	5 ½
2 902.220	2	34 446.29	4 027	1 ½	38 473	2 ½
2 853.914	150	35 029.31	3 444	3 ½	38 473	2 ½
2 824.702	6	35 391.55	3 082	2 ½	38 473	2 ½

C. Tb I 4 $f^8(^7F)$ 5 d 6 s^2. — The 4 $f^8(^7F)$ 5 d 6 s^2 subconfiguration of neutral terbium has been the subject of several theoretical calculations. If it turns out to be the ground configuration of neutral terbium it will provide a glaring exception to both Hund's rule and Landé interval rule. Its lowest term is not of highest L value, as required by Hund's rule. Its lowest level is not of highest J in this term as required by Lande's rule. This situation is quite well known in configurations where a 5 d electron coexists with a 4 f^N core. Our theoretical calculations accurately reproduce this situation.

Even if it is not the ground configuration it is low enough as to be a significant contributor to states appearing in atomic beam experiments. Such experiments determine magnetic dipole and electric quadrupole moments, and a set of good eigenvectors is essential for their determinations. The first published attempt to predict levels of this subconfiguration was made 5 years ago by Arnoult and Gerstenkorn [13]. They selected initial radial parameters for the electrostatic and spin orbit parameters and diagonalized its energy matrix. Their predictions fitted will the then available observed levels, established by Klinkenberg. But difficulties arose when attempts were made to establish further levels of 4 $f^8(^7F)$ 5 d 6 s^2 of Tb I. Several newly found ones did not retain the good agreement to their predicted positions as did the first levels. A calculation of the magnetic and quadrupole moment of Tb I by Childs and Goodman [14] using the eigenvectors of ref. 11 did not produce satisfactory results.

Ref. 11 did not mention a possibility for improving the initial values of the radial parameters by optimizing the theoretical prediction using the available observed levels. It also did not give a value for ζ_f. But it was clear that any attempt at performing a least squares calculation based on the levels used in ref. 13 would give reliable values to the F_2 and F_4, but not to G_1, G_3, G_5. We followed the gradual unravelling of the 4 $f^8(^7F)$ 5 d 6 S^2 of Tb I in a series of articles by Klinkenberg et al. Each time we inserted more levels to the least squares calculations. But it was clear that before some sextet levels are found, not all G_k' s would be usable in such calculations. At a certain point, a value was given to a $^6H_{6\frac{1}{2}}$ [15]. Its inclusion in an optimization process resulted in negative values to most of the electrostatic parameters and extremely large *rms* errors for the two spin orbit parameters. It was later concluded in ref. 10 that this level belonged to another configuration : the 4 $f^8(^7F)$ 5 d^2 6 s.

When the final list of observed 4 $f^8(^7F)$ 5 d 6 s^2 levels was published [10] we attempted another least squares calculation. This time very reasonable values for all parameters were obtained when G_5 was made equal to 2 cm^{-1} in the diagonalization and then held fixed during the least squares process. The results of this calculations are given in Tables X and XI. The

TABLE X

Parameters for 4 $f^8(^7F)$ 5 d 6 s^2 *of* Tb I

Name	Diagonalization (in cm^{-1})	Least squares (in cm^{-1})
—	—	—
A	10 000	10 334 ± 376
F_2	144	147 ± 5
F_4	12	16 ± 1
G_1	140	124 ± 19
G_3	15	26 ± 9
G_5	2	fixed
ζ_f	1 620	1 618 ± 31
ζ_d	750	793 ± 53
rms error		152
in % of total width		1.76 %

TABLE XI

Calculated positions, g-factors and L-S coupling percentages for the 4 $f^8(^7F)$ 5 d 6 s^2 *levels of* Tb I

Observed designation	J	Percentage composition	Observed level (cm^{-1})	Calculated level (cm^{-1})	O-C (cm^{-1})	$g_{obs.}$	$g_{calc.}$
—	—	—	—	—	—	—	—
^8G	$6\frac{1}{2}$	66 % ^8G + 28 % ^8F	0	193	− 193	1.464	1.475
^8G	$7\frac{1}{2}$	95 % ^8G	176	277	− 101	1.455	1.462
^8G	$5\frac{1}{2}$	41 % ^8G + 36 % ^8F	224	366	− 142	1.517	1.514
^8D	$4\frac{1}{2}$	40 % ^8G + 36 % ^8F	1 085	1 056	29	1.537	1.531
^8G	$3\frac{1}{2}$	52 % ^8G + 33 % ^8F	2 133	1 976	157	1.48	1.504
^8G	$2\frac{1}{2}$	66 % ^8G + 25 % ^8F	2 889	2 825	64	1.35	1.412
^8G	$1\frac{1}{2}$	83 % ^8G	3 420	3 477	− 57	1.015	1.099
^8G	$0\frac{1}{2}$	96 % ^8G	3 732	3 879	− 147	− 1.22	− 1.111

TABLE XI (contd.)

Observed designation	J	Percentage composition	Observed level (cm^{-1})	Calculated level (cm^{-1})	O-C (cm^{-1})	$g_{obs.}$	$g_{calc.}$
^8D	5 ½	52 % ^8D + 40 % ^8G	2 024	1 921	103	1.535	1.541
^8G	4 ½	42 % ^8D + 42 % ^8G	2 554	2 550	4	1.57	1.562
^8D	3 ½	46 % ^8D + 36 % ^8G	3 535	3 462	73	1.610	1.612
^8D	2 ½	43 % ^8D + 28 % ^8F	4 410	4 361	49	1.80	1.740
^8D	1 ½	67 % ^8D + 30 % ^8F	6 564	6 668	− 104	2.335	2.519
^8F	6 ½	71 % ^8F + 25 % ^8G	3 434	3 182	252	1.515	1.508
^8F	5 ½	53 % ^8F + 29 % ^8D	5 067	4 861	206	1.54	1.549
^8F	4 ½	50 % ^8F	5 544	5 484	60	1.58	1.595
^8F	3 ½	51 % ^8F + 29 % ^8D	6 202	6 203	− 1	1.63	1.661
^8F	2 ½	45 % ^8F + 46 % ^8D	6 515	6 592	− 77	1.80	1.855
^8F	1 ½	55 % ^8F + 30 % ^8D	5 198	5 213	− 15	2.305	2.090
^8F	0 ½	96 % ^8F	5 973	6 003	− 30	3.85	3.771
^8H	8 ½	100 % ^8H	4 361	4 485	− 124	1.412	1.412
^8H	7 ½	72 % ^8H	5 139	5 076	63	1.37	1.330
^8H	6 ½	77 % ^8H	6 066	5 831	235	1.35	1.353
^8H	5 ½	56 % ^8H	6 389	6 689	− 300		1.353
^8H	4 ½	85 % ^8H	7 155	7 065	90	1.24	1.231
^8H	3 ½	90 % ^8H	7 554	7 512	42	1.04	1.067
^8H	2 ½	94 % ^8H		7 840			0.705
^8H	1 ½	98 % ^8H		8 074			− 0.381
	5 ½	67 % ^6F		6 950			1.407
	4 ½	71 % ^6F		8 180			1.474
	3 ½	79 % ^6F		9 401			1.403
	2 ½	85 % ^6F		10 414			1.316
	1 ½	90 % ^6F		11 244			1.066
	0 ½	98 % ^6F		11 766			− 0.615
^8P	4 ½	61 % ^8P	7 812	8 004	− 192	1.75	1.699
	3 ½	85 % ^8P		10 287			1.911
	2 ½	90 % ^8P		12 010			2.189
	4 ½	46 % ^6D + 29 % ^6G		10 613			1.437
	3 ½	37 % ^6D + 46 % ^6G		11 092			1.360
	2 ½	66 % ^6D		12 808			1.549
	1 ½	88 % ^6D		13 654			1.822
	0 ½	98 % ^6D		14 149			3.289
	6 ½	92 % ^6G		6 808			1.381
^6F	5 ½	81 % ^6G	8 647	8 589	78	1.47	1.341
	4 ½	60 % ^6G		10 018			1.387
	3 ½	34 % ^6G + 29 % ^6D		11 594			1.376
	2 ½	72 % ^6G		11 796			1.045
	1 ½	94 % ^6G		12 255			0.073
	7 ½	76 % ^6H		7 863			1.346
	6 ½	79 % ^6H		9 668			1.299
	5 ½	81 % ^6H		11 114			1.226
	4 ½	83 % ^6H		12 270			1.104
	3 ½	86 % ^6H		13 176			0.073
	2 ½	92 % ^6H		13 861			0.329
	3 ½	76 % ^6P		13 379			1.678
	2 ½	88 % ^6P		15 015			1.860
	1 ½	96 % ^6P		16 131			2.379

TABLE XII

Eigenvectors components in L-S scheme for $4f^8(^7F)\,5d\,6s^2$ *of* Tb I

Calc. Level (in cm⁻¹)	J	^{6}P	^{8}P	^{6}D	^{8}D	^{6}F	^{8}F	^{6}G	^{8}G	^{6}H	^{8}H
512	6 ½						.534 1	−.142 6	.814 7	−.059 6	.165 0
653	7 ½								.975 4	−.088 5	.201 8
721	5 ½				.428 6	−.088 8	.604 0	−.111 5	.644 7	−.034 8	.119 2
1 421	4 ½		.128 6	−.013 3	.447 0	−.067 6	.599 0	−.090 8	.632 0	−.024 8	.108 6
2 342	3 ½	.011 9	.080 8	.005 8	.358 1	−.032 3	.575 5	−.078 5	.716 7	−.018 9	.112 2
3 203	2 ½	.011 3	.034 5	.019 4	.236 5	.006 6	.504 9	−.062 8	.819 7	−.011 4	.107 4
3 884	1 ½	−.006 3		−.022 4	−.110 8	−.042 5	−.377 8	.041 2	−.913 3		−.082 1
4 318	0 ½			.014 6		.067 8	.202 1		.976 9		
2 440	5 ½				.711 7	−.128 5	.192 7	.075 9	−.628 7	.048 0	−.167 3
3 038	4 ½		.268 2	−.054 4	.658 0	−.102 3	.165 8	.071 8	−.650 4	.035 6	−.157 5
3 944	3 ½	.024 0	.197 2	−.031 1	.676 0	−.108 0	.328 4	.050 9	−.601 2	.022 8	−.136 2
4 789	2 ½	−.033 0	−.119 4	.000 3	−.658 8	.104 7	−.525 3	−.020 9	.503 0	−.010 5	.098 8
5 519	1 ½	.032 9		.035 7	.554 1	−.086 9	.739 6	.011 9	−.365 0		−.052 2
3 292	6 ½						−.836 6	−.011 7	.496 8	−.077 1	.217 2
5 081	5 ½				−.542 2	−.142 4	.731 2	−.013 3	−.298 5	.070 2	−.238 7
5 617	4 ½		−.429 6	.091 2	−.372 0	−.153 4	.713 0	−.001 5	−.302 6	.047 8	−.207 2
6 429	3 ½	−.022 8	−.282 6	.085 3	−.539 1	−.130 3	.713 6	−.003 9	−.249 4	.031 0	−.179 8
6 918	2 ½	.036 8	.179 7	−.081 8	.676 1	.093 2	−.665 9	.001 7	.193 4	−.012 4	.113 0
7 129	1 ½	−.050 9		.067 2	−.822 0	−.051 7	.546 0	.000 2	−.121 3		−.041 1
6 086	0 ½			.074 5		−.053 2	.975 7		.199 3		
4 672	8 ½										1
5 130	7 ½								−.219 3	−.477 0	.851 1
5 969	6 ½						.108 0	.104 5	−.257 6	−.379 7	.875 7
6 736	5 ½				−.032 3	.457 0	.236 1	.249 5	−.244 3	−.231 9	.747 4
7 289	4 ½		.142 6	−.015 6	−.018 7	.065 6	−.093 1	−.108 7	.230 7	.239 3	−.918 6
7 770	3 ½	.002 6	.041 2	−.010 1	.045 7	.043 2	−.114 3	−.111 2	.206 9	.178 3	−.945 6
8 122	2 ½	.002 2	.013 5	−.007 6	.037 7	.022 5	−.075 8	−.107 5	.155 8	.114 6	−.971 1
8 369	1 ½	.000 9		−.003 1	.014 1	.009 3	−.030 7	−.102 3	.095 0		−.989 6
6 645	5 ½				.075 9	.817 8	.087 0	.175 8	.111 5	.198 0	−.485 1
7 772	4 ½		−.280 4	.323 1	.207 5	.835 4	.064 2	.263 3	−.010 9	−.042 9	−.022 8
8 916	3 ½	−.070 2	.028 2	−.328 3	−.037 8	−.888 0	−.123 5	−.278 8	.045 1	−.036 7	.012 8
9 916	2 ½	−.048 2	.006 9	−.281 7	−.016 0	−.917 4	−.092 0	−.253 0	.053 2	−.026 2	.020 9
10 706	1 ½	.022 6		.208 8	.006 1	.954 7	.060 1	.190 4	−.065 0		−.019 3
11 221	0 ½			.113 3		.990 2	.029 7		−.076 6		
8 038	4 ½		.779 3	.016 9	−.430 3	.300 3	.291 8	.128 4	−.094 0	−.006 0	.081 0
10 285	3 ½	.010 6	−.924 3	.090 5	.344 4	−.046 0	−.118 7	−.046 2	.019 8	−.007 9	−.004 0
11 963	2 ½	.019 5	.945 4	.016 5	−.208 3	.062 8	.046 1	−.226 3	−.029 6	−.061 0	.016 0
10 340	4 ½		.099 9	.681 1	.006 9	−.405 2	−.078 5	.535 9	.105 2	.239 6	.008 2
10 945	3 ½	.307 3	.104 1	.612 7	.000 1	−.022 2	−.040 2	−.683 3	−.075 1	−.209 5	.027 1
12 357	2 ½	.315 0	.091 0	.810 1	.006 7	−.341 4	−.087 0	.307 2	.054 4	.120 3	−.016 3
13 125	1 ½	.201 9		.941 0	.018 9	−.227 2	−.085 4	.117 2	.025 4		−.011 6
13 604	0 ½			.990 7		−.110 2	−.079 7		.009 4		
7 090	6 ½						.056 2	.959 6	.143 7	.234 0	.022 3
8 765	5 ½				−.020 5	−.274 8	−.012 4	.897 7	.156 0	.305 7	.017 2
9 907	4 ½		.103 6	.647 4	.016 9	.017 3	−.033 3	−.709 1	−.098 4	−.236 5	.006 9
11 359	3 ½	.363 8	.058 0	.535 0	.001 5	−.402 5	−.077 7	.584 0	.098 8	.242 9	−.012 4
11 890	2 ½	−.116 4	.220 8	−.383 0	−.065 3	−.112 9	.029 2	.847 2	.078 5	.214 4	−.057 5
12 517	1 ½	.026 8		.155 2	.004 0	.156 3	−.002 2	−.968 4	−.063 1		.095 2
7 429	7 ½								−.021 0	.874 4	.484 7
9 213	6 ½						.005 4	.218 4	.050 2	−.889 7	−.397 8
10 646	5 ½				−.002 6	−.045 8	−.002 1	.287 5	.058 9	−.897 3	−.326 6
11 783	4 ½		.003 0	.025 2	−.000 9	−.067 0	−.007 8	.314 5	.055 6	−.907 4	−.263 5
12 649	3 ½	.090 7	−.004 3	−.018 9	−.004 2	−.055 1	−.004 2	.296 5	.041 9	−.926 1	−.202 3
13 278	2 ½	.016 0	.000 6	.021 7	−.000 1	−.046 6	−.005 4	.237 1	.025 6	.960 0	.136 2
12 892	3 ½	.871 0	−.061 1	−.462 2	−.045 2	.110 6	.040 7	−.055 7	−.016 2	.065 9	.018 1
14 547	2 ½	.939 0	−.034 1	−.331 5	−.059 4	.052 8	.028 9	−.010 4	−.005 9	.002 5	.001 4
15 676	1 ½	.976 9		−.201 4	−.066 4	.020 6	.017 5	−.002 1	−.002 1		.000 2

APPENDIX 1

Spin orbit matrices for the f *and* d *electrons of* $f^6(^7F)\,d$

ζ_d $J=0\frac{1}{2}$	^6D	^6F	^8F	^8G
	0	$\frac{\sqrt{6}}{14}$	$-\frac{6\sqrt{2}}{7}$	0
		$\frac{5}{14}$	$\frac{\sqrt{3}}{14}$	$-\frac{15}{14}$
			$-\frac{27}{56}$	$-\frac{5\sqrt{3}}{56}$
				$-\frac{7}{8}$

ζ_f $J=6\frac{1}{2}$	^8F	^6G	^8G	^6H	^8H
	$\frac{9}{8}$	$\frac{5\sqrt{7}}{84}$	$\frac{5\sqrt{35}}{56}$	0	0
		$\frac{26}{21}$	$-\frac{13\sqrt{5}}{140}$	$\frac{2\sqrt{2}}{7}$	$-\frac{2\sqrt{5}}{105}$
			$\frac{169}{280}$	$\frac{\sqrt{10}}{35}$	$\frac{16}{35}$
				$\frac{4}{7}$	$-\frac{3\sqrt{10}}{35}$
					$\frac{9}{70}$

ζ_f $J=0\frac{1}{2}$	^8D	^6F	^8F	^6G
	$-\frac{4}{3}$	$\frac{2\sqrt{6}}{21}$	$-\frac{\sqrt{2}}{7}$	0
		$-\frac{10}{7}$	$-\frac{\sqrt{3}}{28}$	$-\frac{5}{28}$
			$-\frac{81}{56}$	$\frac{5\sqrt{3}}{56}$
				$-\frac{13}{8}$

ζ_f $J=2\frac{1}{2}$	^6P	^8P	^6D	^8D	^6F	^8F	^6G	^8G	^6H	^8H
	$-\frac{8}{21}$	$-\frac{2\sqrt{5}}{21}$	$\frac{32\sqrt{5}}{105}$	$-\frac{\sqrt{30}}{35}$	0	0	0	0	0	0
		$-\frac{9}{7}$	$\frac{1}{21}$	$\frac{3\sqrt{6}}{14}$	0	0	0	0	0	0
			$-\frac{4}{7}$	$-\frac{\sqrt{6}}{14}$	$\frac{18\sqrt{70}}{49\cdot 5}$	$-\frac{3\sqrt{7}}{49}$	0	0	0	0
				$-\frac{13}{14}$	$\frac{\sqrt{105}}{49\cdot 5}$	$\frac{4\sqrt{42}}{49}$	0	0	0	0
					$-\frac{6}{7}$	$-\frac{3\sqrt{10}}{56}$	$\frac{20\sqrt{105}}{441}$	$-\frac{25\sqrt{462}}{49\cdot 72}$	0	0
						$-\frac{57}{56}$	$\frac{5\sqrt{42}}{49\cdot 24}$	$\frac{5\sqrt{1155}}{49\cdot 8}$	0	0
							$-\frac{26}{21}$	$-\frac{13\sqrt{110}}{840}$	$\frac{2\sqrt{66}}{63}$	$-\frac{\sqrt{165}}{105}$
								$-\frac{351}{280}$	$\frac{\sqrt{15}}{315}$	$\frac{4\sqrt{6}}{35}$
									$-\frac{12}{7}$	$-\frac{3\sqrt{10}}{70}$
										$-\frac{111}{70}$

ζ_f $J=1\frac{1}{2}$	^6P	^6D	^8D	^6F	^8F	^6G	^8G	^8H
	$-\frac{4}{3}$	$\frac{2\sqrt{70}}{35}$	$-\frac{2\sqrt{105}}{105}$	0	0	0	0	0
		$-\frac{22}{21}$	$-\frac{\sqrt{6}}{21}$	$\frac{32\sqrt{105}}{49\cdot 15}$	$-\frac{2\sqrt{21}}{49}$	0	0	0
			$-\frac{9}{7}$	$\frac{\sqrt{70}}{490}$	$\frac{9\sqrt{14}}{98}$	0	0	0
				$-\frac{17}{14}$	$-\frac{3\sqrt{5}}{56}$	$\frac{5\sqrt{35}}{98}$	$-\frac{25\sqrt{7}}{8\cdot 49}$	0
					$-\frac{9}{7}$	$\frac{5\sqrt{7}}{24\cdot 49}$	$\frac{5\sqrt{35}}{98}$	0
						$-\frac{65}{42}$	$-\frac{13\sqrt{5}}{280}$	$-\frac{\sqrt{770}}{210}$
							$-\frac{52}{35}$	$\frac{\sqrt{154}}{70}$
								$-\frac{9}{5}$

ζ_d $J=6\frac{1}{2}$	^8F	^6G	^8G	^6H	^8H
	$\frac{3}{8}$	$\frac{5\sqrt{7}}{14}$	$-\frac{5\sqrt{35}}{56}$	0	
		$-\frac{1}{2}$	$\frac{3\sqrt{5}}{10}$	$\frac{3\sqrt{2}}{14}$	$-\frac{4\sqrt{5}}{35}$
			$\frac{13}{40}$	$\frac{6\sqrt{10}}{35}$	$-\frac{16}{35}$
				$-\frac{2}{7}$	$\frac{12\sqrt{10}}{35}$
					$\frac{3}{35}$

ζ_d $J=2\frac{1}{2}$	^6P	^8P	^6D	^8D	^6F	^8F	^6G	^8G	^6H	^8H
	$-\frac{1}{7}$	$-\frac{2\sqrt{5}}{7}$	$\frac{8\sqrt{5}}{35}$	$-\frac{6\sqrt{30}}{35}$	0	0	0	0	0	0
		$\frac{9}{14}$	$\frac{2}{7}$	$-\frac{3\sqrt{6}}{14}$	0	0	0	0	0	0
			0	0	$\frac{27\sqrt{70}}{490}$	$-\frac{18\sqrt{7}}{49}$	0	0	0	0
				0	$\frac{6\sqrt{105}}{49\cdot 5}$	$-\frac{4\sqrt{42}}{49}$	0	0	0	0
					$\frac{3}{14}$	$\frac{3\sqrt{10}}{28}$	$\frac{5\sqrt{105}}{49\cdot 3}$	$-\frac{25\sqrt{462}}{49\cdot 12}$	0	0
						$-\frac{19}{56}$	$\frac{5\sqrt{42}}{49\cdot 4}$	$-\frac{5\sqrt{1155}}{49\cdot 8}$	0	0
							$\frac{1}{2}$	$\frac{\sqrt{110}}{20}$	$\frac{\sqrt{66}}{42}$	$-\frac{2\sqrt{165}}{35}$
								$-\frac{27}{40}$	$\frac{2\sqrt{15}}{105}$	$-\frac{4\sqrt{6}}{35}$
									$\frac{6}{7}$	$\frac{6\sqrt{10}}{35}$
										$-\frac{37}{35}$

ζ_d $J=1\frac{1}{2}$	^6P	^6D	^8D	^6F	^8F	^6G	^8G	^8H
	$-\frac{1}{2}$	$\frac{3\sqrt{70}}{70}$	$-\frac{4\sqrt{105}}{35}$	0	0	0	0	0
		0	0	$\frac{8\sqrt{105}}{49\cdot 5}$	$-\frac{12\sqrt{21}}{49}$	0	0	0
			0	$\frac{3\sqrt{70}}{49\cdot 5}$	$-\frac{9\sqrt{14}}{98}$	0	0	0
				$\frac{17}{56}$	$\frac{3\sqrt{5}}{28}$	$\frac{15\sqrt{35}}{49\cdot 8}$	$-\frac{75\sqrt{7}}{49\cdot 4}$	0
					$-\frac{3}{7}$	$\frac{5\sqrt{7}}{49\cdot 4}$	$-\frac{5\sqrt{35}}{98}$	0
						$\frac{5}{8}$	$\frac{3\sqrt{5}}{20}$	$-\frac{\sqrt{770}}{35}$
							$-\frac{4}{5}$	$-\frac{\sqrt{154}}{70}$
								$-\frac{6}{5}$

ζ_f

$J=3\frac{1}{2}$	^6P	^8P	^6D	^8D	^6F	^8F	^6G	^8G	^6H	^8H
	$\frac{20}{21}$	$-\frac{\sqrt{3}}{7}$	$\frac{2\sqrt{6}}{7}$	$-\frac{\sqrt{2}}{14}$	0	0	0	0	0	0
		$-\frac{2}{7}$	$\frac{\sqrt{2}}{14}$	$\frac{2\sqrt{6}}{7}$	0	0	0	0	0	0
			$\frac{2}{21}$	$-\frac{5\sqrt{3}}{42}$	$\frac{16\sqrt{42}}{49\cdot 3}$	$-\frac{\sqrt{154}}{98}$	0	0	0	0
				$-\frac{3}{7}$	$\frac{\sqrt{14}}{49}$	$\frac{3\sqrt{462}}{98}$	0	0	0	0
					$-\frac{5}{14}$	$-\frac{\sqrt{33}}{28}$	$\frac{5\sqrt{1155}}{49\cdot 6}$	$-\frac{5\sqrt{231}}{49\cdot 12}$	0	0
						$-\frac{9}{14}$	$\frac{5\sqrt{35}}{49\cdot 12}$	$\frac{10\sqrt{7}}{49}$	0	0
							$-\frac{169}{210}$	$-\frac{13\sqrt{5}}{140}$	$\frac{16\sqrt{6}}{105}$	$-\frac{\sqrt{130}}{105}$
								$-\frac{13}{14}$	$\frac{\sqrt{30}}{210}$	$\frac{\sqrt{26}}{14}$
									$-\frac{46}{35}$	$-\frac{\sqrt{195}}{70}$
										$-\frac{9}{7}$

ζ_d

$J=4\frac{1}{2}$	^8P	^6D	^8D	^6F	^8F	^6G	^8G	^6H	^8H
	$-\frac{1}{2}$	$\frac{6\sqrt{35}}{35}$	$-\frac{\sqrt{2310}}{70}$	0	0	0	0	0	0
		0	0	$\frac{\sqrt{2310}}{98}$	$-\frac{6\sqrt{385}}{49\cdot 5}$	0	0	0	0
			0	$\frac{6\sqrt{35}}{98}$	$-\frac{10\sqrt{210}}{49\cdot 5}$	0	0	0	0
				$-\frac{1}{14}$	$\frac{5\sqrt{6}}{28}$	$\frac{5\sqrt{21}}{49}$	$-\frac{5\sqrt{546}}{49\cdot 4}$	0	0
					$-\frac{3}{56}$	$\frac{25\sqrt{14}}{49\cdot 4}$	$-\frac{25\sqrt{91}}{49\cdot 8}$	0	0
						$\frac{1}{10}$	$\frac{3\sqrt{26}}{20}$	$\frac{\sqrt{546}}{70}$	$-\frac{2\sqrt{91}}{35}$
							$-\frac{11}{40}$	$\frac{2\sqrt{21}}{35}$	$-\frac{4\sqrt{14}}{35}$
								$\frac{2}{5}$	$\frac{2\sqrt{6}}{5}$
									$-\frac{3}{5}$

ζ_d

$J=8\frac{1}{2}$	^8H
	1

ζ_f

$J=5\frac{1}{2}$	^8D	^6F	^8F	^6G	^8G	^6H	^8H
	1	$\frac{\sqrt{6}}{14}$	$\frac{\sqrt{78}}{14}$	0	0	0	0
		$\frac{15}{14}$	$-\frac{3\sqrt{13}}{56}$	$\frac{5\sqrt{195}}{126}$	$-\frac{5\sqrt{39}}{504}$	0	0
			$\frac{3}{7}$	$\frac{5\sqrt{15}}{168}$	$\frac{5\sqrt{3}}{14}$	0	0
				$\frac{13}{30}$	$-\frac{13\sqrt{5}}{120}$	$\frac{32\sqrt{21}}{315}$	$-\frac{\sqrt{210}}{210}$
					0	$\frac{2\sqrt{105}}{315}$	$\frac{\sqrt{42}}{14}$
						$-\frac{6}{35}$	$-\frac{3\sqrt{10}}{35}$
							$-\frac{3}{7}$

ζ_d

$J=3\frac{1}{2}$	^6P	^8P	^6D	^8D	^6F	^8F	^6G	^8G	^6H	^8H
	$\frac{5}{14}$	$-\frac{3\sqrt{3}}{7}$	$\frac{3\sqrt{6}}{14}$	$-\frac{3\sqrt{2}}{7}$	0	0	0	0	0	0
		$\frac{1}{7}$	$\frac{3\sqrt{2}}{7}$	$-\frac{2\sqrt{6}}{7}$	0	0	0	0	0	0
			0	0	$\frac{4\sqrt{42}}{49}$	$-\frac{3\sqrt{154}}{49}$	0	0	0	0
				0	$\frac{6\sqrt{14}}{49}$	$-\frac{3\sqrt{462}}{98}$	0	0	0	0
					$\frac{5}{56}$	$\frac{\sqrt{33}}{14}$	$\frac{5\sqrt{1155}}{49\cdot 8}$	$-\frac{5\sqrt{231}}{49\cdot 2}$	0	0
						$-\frac{3}{14}$	$\frac{5\sqrt{35}}{98}$	$-\frac{10\sqrt{7}}{49}$	0	0
							$\frac{13}{40}$	$\frac{3\sqrt{5}}{10}$	$\frac{4\sqrt{6}}{35}$	$-\frac{2\sqrt{130}}{35}$
								$-\frac{1}{2}$	$\frac{\sqrt{30}}{35}$	$-\frac{\sqrt{26}}{14}$
									$\frac{23}{35}$	$\frac{2\sqrt{195}}{35}$
										$-\frac{6}{7}$

ζ_f

$J=7\frac{1}{2}$	^8G	^6H	^8H
	$\frac{13}{10}$	$\frac{\sqrt{70}}{70}$	$\frac{\sqrt{714}}{70}$
		$\frac{10}{7}$	$-\frac{\sqrt{255}}{70}$
			$\frac{27}{35}$

ζ_d

$J=5\frac{1}{2}$	^8D	^6F	^8F	^6G	^8G	^6H	^8H
	0	$\frac{3\sqrt{6}}{7}$	$-\frac{\sqrt{78}}{14}$	0	0	0	0
		$-\frac{15}{56}$	$\frac{3\sqrt{13}}{28}$	$\frac{5\sqrt{195}}{168}$	$-\frac{5\sqrt{39}}{84}$	0	0
			$\frac{1}{7}$	$\frac{5\sqrt{15}}{28}$	$-\frac{5\sqrt{3}}{14}$	0	0
				$-\frac{7}{40}$	$\frac{7\sqrt{5}}{20}$	$\frac{8\sqrt{21}}{105}$	$-\frac{\sqrt{210}}{35}$
					0	$\frac{4\sqrt{105}}{105}$	$-\frac{\sqrt{42}}{14}$
						$\frac{3}{35}$	$\frac{12\sqrt{10}}{35}$
							$-\frac{2}{7}$

ζ_f

$J=4\frac{1}{2}$	^8P	^6D	^8D	^6F	^8F	^6G	^8G	^6H	^8H
	1	$\frac{\sqrt{35}}{35}$	$\frac{\sqrt{2310}}{70}$	0	0	0	0	0	0
		$\frac{20}{21}$	$-\frac{\sqrt{66}}{42}$	$\frac{2\sqrt{2310}}{3\cdot 49}$	$-\frac{\sqrt{385}}{49\cdot 5}$	0	0	0	0
			$\frac{3}{14}$	$\frac{\sqrt{35}}{49}$	$\frac{12\sqrt{210}}{49\cdot 5}$	0	0	0	0
				$\frac{2}{7}$	$-\frac{5\sqrt{6}}{56}$	$\frac{20\sqrt{21}}{3\cdot 49}$	$-\frac{5\sqrt{546}}{24\cdot 49}$	0	0
					$-\frac{9}{56}$	$\frac{25\sqrt{14}}{24\cdot 49}$	$\frac{25\sqrt{91}}{8\cdot 49}$	0	0
						$-\frac{26}{105}$	$-\frac{13\sqrt{26}}{280}$	$\frac{2\sqrt{546}}{105}$	$-\frac{\sqrt{91}}{105}$
							$-\frac{143}{280}$	$\frac{\sqrt{21}}{105}$	$\frac{4\sqrt{14}}{35}$
								$-\frac{4}{5}$	$-\frac{\sqrt{6}}{10}$
									$-\frac{9}{10}$

ζ_f

$J=8\frac{1}{2}$	^8H
	$\frac{3}{2}$

ζ_d

$J=7\frac{1}{2}$	^8G	^6H	^8H
	$\frac{7}{10}$	$\frac{3\sqrt{70}}{35}$	$-\frac{\sqrt{714}}{70}$
		$-\frac{5}{7}$	$\frac{2\sqrt{255}}{35}$
			$\frac{18}{35}$

former gives the adjusted values for the radial parameters resulting in an *rms* error of 152 cm^{-1}, which is 1.76 % of the total width. The latter gives the predictions for level position and g-values as well as a comparison between them and the available experimental values. L-S designations can be used throughout the Table, despite some heavy admixtures. Marked differences between our designation and the ones used in ref. 10 and 13 are noticed for $^8D_{4\frac{1}{2}}$ and $^8G_{4\frac{1}{2}}$. Also the level at 8 647 cm^{-1} whose observed designation is $^6F_{5\frac{1}{2}}$ fits well to our $^6G_{5\frac{1}{2}}$. When made to correspond to the predicted value of $^6F_{5\frac{1}{2}}$ (1 700 cm^{-1} below) unreasonable values for the radial parameters are obtained in the least squares. The most noticeable variation from ref. 13 is provided by our Table XII where eigenvectors for this low subconfiguration are given in L-S coupling (as was done in ref. 13). Differences in magnitude of various components and, in particular, prominent changes of phases are noteworthy.

With the scanty experimental material yet established there is a remarkable sensitivity of the optimized parameters to the presence or absence of even a single level or parameter. To demonstrate this sensitivity we give, in Tables XIII, the results of four least squares on the same diagonalization parameters. In l. s. 1 G_5 was free for adjustment and the level 8 647 cm^{-1} with $J = 5\frac{1}{2}$ was included. All G_k's have unreasonable values. The situation does not improve upon eliminating this level, nor yet upon fixing G_5 while the level is still out. Only when G_5 is held fixed and the level is restored to its place do we get acceptable values for all the parameters. It is seen that exactly then the *rms* error becomes the biggest. But it is also evident that the other *rms* errors, though smaller, are totally meaningless.

Contrary to the previous two sections the results reported in the present one for TbI should be considered merely as preliminary. Only when the sextets of this subconfiguration are established could we hope to have a more significant optimization for the parameters. Meanwhile the calculated positions for the missing levels given in Table XI should serve as guidelines for searching the latter.

TABLE XIII

Various least squares in Tb I

Name	Diagonalization	G_5 free, 8 647 in	G_5 free, 8 647 out	G_5 fixed, 8 647 in	G_5 fixed, 8 647 out
A	10 000	6 505 ± 1 373	8 089 ± 1 758	10 333 ± 376	9 234 ± 463
F_2	144	147 ± 4	147 ± 4	147 ± 5	148 ± 4
F_4	12	16 ± 1	16 ± 1	16 ± 1	17 ± 1
G_1	140	− 46 ± 62	− 30 ± 62	124 ± 19	0 ± 42
G_3	15	− 145 ± 60	− 26 ± 104	26 ± 9	44 ± 9
G_5	2	33 ± 10	14 ± 17	fixed	fixed
ζ_f	1 620	1 654 ± 30	1 632 ± 33	1 618 ± 31	1 619 ± 27
ζ_d	750	830 ± 47	800 ± 51	793 ± 53	783 ± 43
rms error		131	128	152	126

V. **Conclusion.** — New values for the 4 f-5 d interaction parameters around the half-filled 4 f shell have been obtained. The theoretical prediction are capable of reproducing quite accurately recent observational data in the 4 $f^6(^7F)$ 5 d and 4 $f^8(^7F)$ 5 d subconfiguration. The reliability of the parameters is manifest by their regular behaviour from Sm to Tb, by the accuracy of their reproducing observed level position and g-values, and by their being determined by 126 low levels observed in these atoms.

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