SELF-CONSISTENT FIELDS WITHOUT EXCHANGE FOR Pr^{3+} AND Tm^{3+}

By E. CICELY RIDLEY

Communicated by N. F. Mott

Received 10 March 1959

ABSTRACT. Self-consistent fields without exchange have been calculated for the ground state of Pr^{3+} and Tm^{3+}. The spin-orbit coupling constant $\zeta(4f)$ is found to have the values 785 and 2742 cm^{-1} in Pr^{3+} and Tm^{3+}, respectively. The corresponding values of $\overline{(1/r^3)}$ are 29·4 and 77·5 $Å^{-3}$. Values of the Slater integrals $F^2(4f, 4f)$, $F^4(4f, 4f)$ and $F^6(4f, 4f)$ are also given for each structure.

1. *Introduction.* Self-consistent fields are now available for a large number of atomic structures scattered widely through the periodic table (Hartree (4); (6), p. 164). This means that when an unknown field is needed a good approximation to it can usually be obtained by interpolating with respect to atomic number ((5), (8)). There is, however, a serious dearth of results between Cs^+ (atomic number 55) and W(atomic number 74). This interval of 19 units of atomic number includes all the rare earths. These are of great interest spectroscopically and in connexion with measurements of paramagnetic resonance. In these contexts a knowledge of the form of the $(4f)$ wave function has long been needed.

Since the rare earths are characterized by a steady increase in the number of $4f$-electrons with increasing atomic number, it seems likely that two self-consistent fields calculated at either end of the range will form a good basis from which to interpolate for the intervening structures With this in mind, self-consistent fields without exchange were calculated for Pr^{3+} (atomic number 59), which has 2 $4f$-electrons, and for Tm^{3+} (atomic number 69), with 12 $4f$-electrons. These two structures are sufficiently widely separated to display clearly the way in which the shape of the $(4f)$ wave-function changes as the number of $4f$-electrons increases.

2. *The calculations.* Estimates of the electronic contributions to the total field, $Z(r)$, were obtained by a method of interpolation described in an earlier paper (8). In the case of Pr^{3+}, the approximations were derived from the known contributions for Cs^+ (3). Since Cs^+ contains no $4f$-electrons, the estimate of the contribution to $Z(r)$ from the 2 $4f$-electrons in Pr^{3+} was obtained from the self-consistent field for W (7). All the estimates of the contributions to $Z(r)$ in Tm^{3+} were obtained by adjusting the functions for W. Since so little data was available on the $(4f)$, $(5s)$ and $(5p)$ functions, estimates of these contributions were expected to be poor.

The calculation of the two self-consistent fields was carried out on the Ferranti Mark I* computer at the Atomic Weapons Research Establishment. The program used was one originally designed to calculate the self-consistent field of U^{6+} (Ridley (9)).

In Pr^{3+} with only 2 $4f$-electrons, the calculations converged reasonably rapidly. The self-consistent process was much more lengthy in the case of Tm^{3+}. This is due to the

https://doi.org/10.1017/S0305004100034277 Published online by Cambridge University Press

shape of $P(4f)$ and to the large number of electrons in the $(4f)$ group. Although the maximum of $P(4f)$ falls in the neighbourhood of those for other wave functions of principal quantum number 4, the function has appreciable charge density in the exponential tail and this overlaps with $P(5s)$ and $P(5p)$. The presence of 12 $4f$-electrons means that only a small change in $P(4f)$ will affect $P(4s)$, $P(4p)$, $P(4d)$, $P(5s)$ and $P(5p)$ considerably. It would probably have been an advantage to perform integrations simultaneously on all these functions and $P(4f)$ rather than working on one function at a time (9). This would mean calculating all these wave functions in the same estimated field. A new estimated field could then be calculated from the wave functions and the process repeated. The Aitken acceleration process could then be applied to the successive estimates of the contributions to the field as already described (9). Unfortunately, it was not possible to adopt this strategy as the storage capacity of the Mark I* was insufficient to hold the three sets of estimated contributions to the field needed for the acceleration process.

3. *Results and discussion.* In Tables 1 and 2 the results for Pr^{3+} are given. The results for Tm^{3+} appear in Tables 3 and 4. The maximum error, ΔZ, in the contribution to $Z(r)$ from any one group of electrons does not exceed 0·0005. Values of the screening constant σ and the slope constant α are included in Tables 2 and 4 as these may assist the determination of approximate fields for other rare earth atoms by interpolation (8).

The shape of the $(4f)$ wave functions displayed in the two structures is of particular interest. In Pr^{3+} $P(4f; r)$ is far from hydrogen-like in form, having a much greater concentration of charge in the exponential 'tail'. This is illustrated by the fact that at the position of the principal maximum of $P(5s; r)$, $P^2(4f; r)$ is reduced from its maximum value by a factor of only 0·40. The principal maximum of $P(4f; r)$ falls just outside that of $P(4d; r)$. In Tm^{3+}, the concentration of charge in the tail of the $(4f)$ function is much less and at the principal maximum of $P(5s; r)$, $P^2(4f; r)$ is only 0·25 of its maximum value. In addition, the principal maximum of $P(4f; r)$ now falls inside that of $P(4d; r)$ as for hydrogen-like functions. The importance of this contraction of the $(4f)$ charge density relative to $P(4d; r)$, $P(5s; r)$ and $P(5p; r)$ is well illustrated by the value of the screening constant $\sigma(4f)$ which is 40·60 in Pr^{3+} and 42·96 in Tm^{3+}. Tm^{3+} contains 10 more $4f$-electrons than does Pr^{3+} and these may be expected to contribute about 5 units to $\sigma(4f)$. In fact the screening constant for Tm^{3+} is greater than that of Pr^{3+} by less than half this amount and the relative movement of the functions must account for the discrepancy.

Values of the spin-orbit coupling constant $\zeta(4f)$ were calculated and found to be 785 cm^{-1} in Pr^{3+} and 2742 cm^{-1} in Tm^{3+}. These compare favourably with the experimental values of 790 and 2640 cm^{-1} quoted by Bleaney (1). $\overline{(1/r^3)}$ was also evaluated for the $(4f)$ wave function as this is needed in the interpretation of paramagnetic resonance experiments. The values obtained were 29·4 $Å^{-3}$ in Pr^{3+} and 77·5 $Å^{-3}$ in Tm^{3+}. These differ considerably from Bleaney's values of 37 and 92 $Å^{-3}$. However, since the latter are based on a formula which assumes a hydrogen-like relationship between ζ and $\overline{(1/r^3)}$, this is hardly surprising. The new values may be expected to give more reliable values of the nuclear magnetic moments.

https://doi.org/10.1017/S0305004100034277 Published online by Cambridge University Press

https://doi.org/10.1017/S0305004100034277 Published online by Cambridge University Press

Table 1. Pr^{3+}. *Radial wave functions. Table of P and total* Z_p

$\rho = \ln 1000r$	r	1s	2s	2p	3s	3p	3d	4s	4p	4d	4f	5s	5p	Total Z_p
0·0	0·001	1·250	0·625	0·010	0·313	0·010	0·000	0·314	0·005	0·000	0·000	0·156	0·002	58·65
0·2	0·001221	1·507	0·753	0·014	0·377	0·014	0·000	0·377	0·007	0·000	0·000	0·188	0·004	58·57
0·4	0·001492	1·811	0·905	0·021	0·453	0·021	0·000	0·453	0·011	0·000	0·000	0·226	0·005	58·47
0·6	0·001822	2·170	1·084	0·032	0·542	0·032	0·000	0·542	0·016	0·000	0·000	0·271	0·008	58·36
0·8	0·002226	2·588	1·292	0·047	0·646	0·047	0·000	0·646	0·023	0·000	0·000	0·323	0·012	58·21
1·0	0·002718	3·070	1·531	0·069	0·765	0·069	0·000	0·765	0·034	0·000	0·000	0·383	0·017	58·04
1·2	0·003320	3·620	1·802	0·101	0·900	0·101	0·001	0·900	0·050	0·001	0·000	0·450	0·025	57·83
1·4	0·004055	4·234	2·103	0·147	1·050	0·147	0·001	1·050	0·073	0·001	0·000	0·525	0·037	57·58
1·6	0·004953	4·905	2·427	0·213	1·212	0·213	0·002	1·211	0·107	0·002	0·000	0·606	0·053	57·27
1·8	0·006050	5·616	2·763	0·308	1·378	0·308	0·004	1·377	0·154	0·004	0·000	0·689	0·077	56·90
2·0	0·007389	6·339	3·091	0·442	1·540	0·441	0·007	1·539	0·221	0·007	0·000	0·769	0·110	56·46
2·2	0·009025	7·032	3·380	0·629	1·681	0·627	0·012	1·679	0·313	0·012	0·000	0·839	0·157	55·93
2·4	0·01102	7·637	3·588	0·886	1·778	0·882	0·021	1·775	0·440	0·021	0·000	0·887	0·220	55·31
2·6	0·01346	8·083	3·658	1·231	1·802	1·223	0·037	1·797	0·611	0·037	0·000	0·898	0·305	54·58
2·8	0·01644	8·288	3·519	1·685	1·717	1·669	0·063	1·708	0·833	0·063	0·001	0·853	0·416	53·73
3·0	0·02009	8·177	3·094	2·265	1·481	2·231	0·107	1·467	1·112	0·107	0·001	0·732	0·556	52·75
3·1	0·02220	7·986	2·751	2·605	1·295	2·556	0·139	1·278	1·273	0·139	0·002	0·637	0·636	52·20
3·2	0·02453	7·698	2·312	2·977	1·058	2·907	0·180	1·038	1·447	0·180	0·002	0·517	0·723	51·61
3·3	0·02711	7·316	1·772	3·379	0·769	3·281	0·232	0·745	1·631	0·231	0·003	0·370	0·815	50·98
3·4	0·02996	6·844	1·129	3·806	0·428	3·669	0·297	0·400	1·821	0·296	0·005	0·197	0·909	50·30
3·5	0·03312	6·293	0·388	4·253	0·039	4·062	0·378	0·007	2·012	0·376	0·007	0·000	1·004	49·57
3·6	0·03660	5·675	−0·442	4·710	−0·393	4·445	0·479	−0·428	2·196	0·476	0·010	−0·218	1·096	48·79
3·7	0·04045	5·011	−1·345	5·163	−0·856	4·799	0·604	−0·893	2·364	0·599	0·014	−0·450	1·179	47·95
3·8	0·04470	4·323	−2·298	5·599	−1·334	5·103	0·755	−1·370	2·503	0·748	0·020	−0·688	1·248	47·05
3·9	0·04940	3·634	−3·271	6·000	−1·805	5·329	0·937	−1·837	2·600	0·927	0·029	−0·921	1·294	46·10
4·0	0·05460	2·969	−4·226	6·344	−2·244	5·447	1·155	−2·266	2·638	1·139	0·040	−1·135	1·312	45·08
4·1	0·06034	2·351	−5·122	6·613	−2·620	5·423	1·410	−2·624	2·600	1·386	0·056	−1·312	1·290	44·00
4·2	0·06669	1·799	−5·912	6·784	−2·898	5·226	1·706	−2·876	2·469	1·670	0·077	−1·436	1·222	42·86
4·3	0·07370	1·324	−6·553	6·840	−3·045	4·824	2·042	−2·984	2·230	1·988	0·105	−1·486	1·100	41·67
4·4	0·08145	0·935	−7·003	6·766	−3·027	4·193	2·418	−2·915	1·871	2·338	0·143	−1·447	0·917	40·44
4·5	0·09002	0·630	−7·231	6·555	−2·818	3·318	2·828	−2·642	1·387	2·711	0·193	−1·304	0·671	39·15
4·6	0·09948	0·404	−7·221	6·207	−2·401	2·199	3·265	−2·149	0·780	3·094	0·259	−1·050	0·364	37·83
4·7	0·1099	0·244	−6·970	5·732	−1·774	0·855	3·716	−1·440	0·066	3·470	0·343	−0·688	0·004	36·46
4·8	0·1215	0·139	−6·498	5·150	−0·954	−0·676	4·164	−0·539	−0·727	3·815	0·451	−0·231	−0·394	35·05
4·9	0·1343	0·074	−5·841	4·490	0·023	−2·329	4·589	0·502	−1·554	4·100	0·587	0·295	−0·806	33·59
5·0	0·1484	0·036	−5·053	3·787	1·101	−4·020	4·967	1·606	−2·358	4·289	0·755	0·847	−1·203	32·08
5·1	0·1640	0·017	−4·196	3·081	2·206	−5·648	5·271	2·673	−3·067	4·348	0·960	1·374	−1·547	30·53

https://doi.org/10.1017/S0305004100034277 Published online by Cambridge University Press

Table 1. (*cont.*)

$\rho = \ln 1000r$	r	1s	2s	2p	3s	3p	3d	4s	4p	4d	4f	5s	5p	Total Z_p
5·2	0·1813	0·007	−3·335	2·409	3·254	−7·103	5·477	3·584	−3·606	4·237	1·207	1·813	−1·798	28·96
5·3	0·2003	0·003	−2·529	1·805	4·159	−8·281	5·564	4·221	−3·898	3·927	1·498	2·102	−1·918	27·37
5·4	0·2214	0·001	−1·823	1·289	4·845	−9·092	5·516	4·473	−3·878	3·391	1·837	2·183	−1·872	25·79
5·5	0·2447	0·000	−1·244	0·875	5·256	−9·476	5·328	4·259	−3·503	2·619	2·222	2·016	−1·639	24·24
5·6	0·2704	—	−0·799	0·561	5·366	−9·414	5·005	3·544	−2·758	1·618	2·650	1·587	−1·215	22·74
5·7	0·2989	—	−0·482	0·338	5·181	−8·927	4·561	2·347	−1·668	0·415	3·114	0·913	−0·619	21·29
5·8	0·3303	—	−0·270	0·191	4·740	−8·081	4·022	0·754	−0·299	−0·941	3·603	0·051	0·108	19·88
5·9	0·3650	—	−0·141	0·100	4·109	−6·975	3·422	−1·095	1·243	−2·376	4·100	−0·909	0·898	18·49
6·00	0·4034	—	−0·067	0·048	3·371	−5·728	2·800	−3·013	2·824	−3·800	4·585	−1·845	1·666	17·11
6·05	0·4241	—	−0·045	0·032	2·989	−5·090	2·493	−3·933	3·581	−4·476	4·815	−2·262	2·012	16·41
6·10	0·4459	—	−0·029	0·021	2·611	−4·463	2·195	−4·792	4·291	−5·112	5·033	−2·624	2·316	15·72
6·15	0·4687	—	−0·019	0·014	2·247	−3·858	1·911	−5·568	4·936	−5·694	5·236	−2·913	2·566	15·02
6·20	0·4927	—	−0·012	0·009	1·904	−3·288	1·643	−6·240	5·502	−6·212	5·422	−3·118	2·753	14·33
6·25	0·5180	—	−0·007	0·006	1·588	−2·761	1·396	−6·790	5·974	−6·657	5·588	−3·226	2·868	13·64
6·30	0·5446	—	−0·004	0·003	1·303	−2·283	1·170	−7·209	6·344	−7·020	5·732	−3·230	2·904	12·96
6·35	0·5725	—	−0·002	0·002	1·051	−1·858	0·967	−7·487	6·604	−7·297	5·853	−3·125	2·856	12·29
6·40	0·6018	—	−0·001	0·001	0·833	−1·488	0·789	−7·625	6·754	−7·483	5·949	−2·910	2·722	11·65
6·45	0·6327	—	−0·001	0·001	0·648	−1·171	0·634	−7·626	6·793	−7·578	6·021	−2·587	2·503	11·03
6·50	0·6651	—	−0·000	0·000	0·495	−0·906	0·502	−7·497	6·727	−7·583	6·066	−2·163	2·201	10·43
6·55	0·6992	—	—	—	0·371	−0·688	0·391	−7·252	6·564	−7·502	6·087	−1·649	1·822	9·87
6·60	0·7351	—	—	—	0·273	−0·513	0·299	−6·906	6·314	−7·340	6·082	−1·055	1·373	9·34
6·65	0·7728	—	—	—	0·196	−0·375	0·226	−6·477	5·989	−7·105	6·052	−0·399	0·864	8·84
6·70	0·8124	—	—	—	0·138	−0·269	0·167	−5·983	5·603	−6·804	5·998	0·303	0·305	8·37
6·75	0·8541	—	—	—	0·095	−0·189	0·121	−5·446	5·172	−6·448	5·920	1·032	−0·290	7·93
6·80	0·8978	—	—	—	0·064	−0·129	0·087	−4·883	4·710	−6·046	5·820	1·769	−0·908	7·52
6·85	0·9439	—	—	—	0·042	−0·087	0·061	−4·314	4·230	−5·610	5·697	2·494	−1·535	7·14
6·90	0·9923	—	—	—	0·027	−0·057	0·041	−3·753	3·748	−5·149	5·553	3·187	−2·157	6·77
6·95	1·043	—	—	—	0·017	−0·036	0·028	−3·216	3·274	−4·675	5·390	3·831	−2·759	6·43
7·00	1·097	—	—	—	0·010	−0·023	0·018	−2·712	2·820	−4·198	5·208	4·410	−3·327	6·10
7·05	1·153	—	—	—	0·006	−0·014	0·012	−2·251	2·393	−3·727	5·010	4·910	−3·849	5·79
7·10	1·212	—	—	—	0·003	−0·008	0·007	−1·837	2·001	−3·270	4·796	5·319	−4·315	5·50
7·15	1·274	—	—	—	0·002	−0·005	0·004	−1·475	1·648	−2·835	4·570	5·630	−4·713	5·21
7·20	1·339	—	—	—	0·001	−0·003	0·003	−1·163	1·335	−2·428	4·334	5·840	−5·038	4·95
7·25	1·408	—	—	—	0·001	−0·001	0·001	−0·901	1·065	−2·053	4·089	5·947	−5·285	4·70
7·30	1·480	—	—	—	0·000	−0·001	0·001	−0·685	0·835	−1·714	3·840	5·954	−5·451	4·46
7·35	1·556	—	—	—	—	−0·000	0·000	−0·511	0·643	−1·412	3·587	5·867	−5·536	4·25
7·40	1·636	—	—	—	—	—	—	−0·374	0·487	−1·147	3·334	5·695	−5·542	4·05

https://doi.org/10.1017/S0305004100034277 Published online by Cambridge University Press

Table 1. (*cont.*)

$\rho = \ln 1000r$	r	1s	2s	2p	3s	3p	3d	4s	4p	4d	4f	5s	5p	Total Z_p
7·45	1·720	—	—	—	—	—	—	−0·268	0·362	−0·919	3·084	5·449	−5·474	3·87
7·50	1·808	—	—	—	—	—	—	−0·188	0·264	−0·725	2·837	5·141	−5·338	3·72
7·55	1·901	—	—	—	—	—	—	−0·129	0·188	−0·564	2·597	4·784	−5·141	3·58
7·60	1·998	—	—	—	—	—	—	−0·086	0·132	−0·432	2·365	4·392	−4·891	3·46
7·65	2·101	—	—	—	—	—	—	−0·056	0·090	−0·325	2·142	3·977	−4·598	3·36
7·70	2·208	—	—	—	—	—	—	−0·036	0·060	−0·241	1·929	3·553	−4·272	3·28
7·75	2·322	—	—	—	—	—	—	−0·022	0·040	−0·175	1·727	3·131	−3·922	3·21
7·80	2·441	—	—	—	—	—	—	−0·014	0·025	−0·125	1·537	2·721	−3·557	3·15
7·85	2·566	—	—	—	—	—	—	−0·008	0·016	−0·088	1·358	2·331	−3·187	3·11
7·90	2·697	—	—	—	—	—	—	−0·005	0·010	−0·060	1·193	1·968	−2·819	3·08
7·95	2·836	—	—	—	—	—	—	−0·003	0·006	−0·040	1·039	1·636	−2·462	3·06
8·00	2·981	—	—	—	—	—	—	−0·001	0·003	−0·027	0·899	1·339	−2·121	3·04
8·05	3·134	—	—	—	—	—	—	−0·001	0·002	−0·017	0·770	1·079	−1·802	3·02
8·10	3·294	—	—	—	—	—	—	−0·000	0·001	−0·011	0·654	0·854	−1·508	3·02
8·15	3·463	—	—	—	—	—	—	—	0·001	−0·007	0·550	0·664	−1·244	3·01
8·20	3·641	—	—	—	—	—	—	—	0·000	−0·004	0·458	0·507	−1·009	3·01
8·25	3·828	—	—	—	—	—	—	—	—	−0·002	0·377	0·379	−0·805	3·00
8·30	4·024	—	—	—	—	—	—	—	—	−0·001	0·306	0·278	−0·631	3·00
8·35	4·230	—	—	—	—	—	—	—	—	−0·001	0·246	0·200	−0·486	3·00
8·40	4·447	—	—	—	—	—	—	—	—	−0·000	0·194	0·140	−0·367	3·00
8·45	4·675	—	—	—	—	—	—	—	—	—	0·151	0·096	−0·271	3·00
8·50	4·915	—	—	—	—	—	—	—	—	—	0·116	0·064	−0·197	3·00
8·55	5·167	—	—	—	—	—	—	—	—	—	0·088	0·042	−0·139	3·00
8·60	5·432	—	—	—	—	—	—	—	—	—	0·065	0·027	−0·096	3·00
8·65	5·710	—	—	—	—	—	—	—	—	—	0·047	0·016	−0·065	3·00
8·70	6·003	—	—	—	—	—	—	—	—	—	0·034	0·010	−0·043	3·00
8·75	6·311	—	—	—	—	—	—	—	—	—	0·023	0·006	−0·027	3·00
8·80	6·634	—	—	—	—	—	—	—	—	—	0·016	0·003	−0·017	3·00
8·85	6·974	—	—	—	—	—	—	—	—	—	0·011	0·002	−0·010	3·00
8·90	7·332	—	—	—	—	—	—	—	—	—	0·007	0·001	−0·006	3·00
8·95	7·708	—	—	—	—	—	—	—	—	—	0·004	0·000	−0·003	3·00
9·00	8·103	—	—	—	—	—	—	—	—	—	0·003	—	−0·002	3·00
9·05	8·519	—	—	—	—	—	—	—	—	—	0·002	—	−0·001	3·00
9·10	8·955	—	—	—	—	—	—	—	—	—	0·001	—	−0·000	3·00
9·15	9·414	—	—	—	—	—	—	—	—	—	0·001	—	—	3·00
9·20	9·897	—	—	—	—	—	—	—	—	—	0·000	—	—	3·00
$\int_0^\infty P^2 dr$		2·177	5·156	4·549	6·396	20·71	7·368	27·51	23·36	34·75	40·51	40·19	41·35	—
ϵ		2947	458·2	436·0	99·78	89·33	70·35	21·14	17·186	10·311	2·318	4·395	3·295	—

https://doi.org/10.1017/S0305004100034277 Published online by Cambridge University Press

Table 2. Pr^{3+}. *Contributions to Z*

ρ	$(1s)^2$	$(2s)^2$	$(2p)^6$	$(3s)^2$	$(3p)^6$	$(3d)^{10}$	ρ	$(4s)^2$	$(4p)^6$	$(4d)^{10}$	$(4f)^2$	$(5s)^2$	$(5p)^6$
0·0	2·000	2·000	6·000	2·000	6·000	10·000	0·0	2·000	6·000	10·000	2·000	2·000	6·000
0·2	1·999	2·000	6·000	2·000	6·000	10·000	2·0	1·999	6·000	10·000	2·000	2·000	6·000
0·4	1·998	2·000	6·000	2·000	6·000	10·000	3·0	1·997	5·998	10·000	2·000	1·999	6·000
0·6	1·997	2·000	6·000	2·000	6·000	10·000	3·2	1·996	5·997	10·000	2·000	1·999	6·000
0·8	1·995	1·999	6·000	2·000	6·000	10·000	3·4	1·996	5·993	10·000	2·000	1·999	5·999
1·0	1·991	1·999	6·000	2·000	6·000	10·000	3·6	1·996	5·986	10·000	2·000	1·999	5·998
1·2	1·985	1·998	6·000	2·000	6·000	10·000	3·8	1·995	5·974	9·999	2·000	1·999	5·996
1·4	1·975	1·997	6·000	1·999	6·000	10·000	4·0	1·993	5·957	9·996	2·000	1·999	5·994
1·6	1·958	1·996	6·000	1·999	6·000	10·000	4·2	1·987	5·936	9·989	2·000	1·998	5·991
1·8	1·929	1·993	6·000	1·999	6·000	10·000	4·4	1·978	5·918	9·972	2·000	1·996	5·989
2·0	1·885	1·988	6·000	1·998	6·000	10·000	4·6	1·969	5·909	9·933	2·000	1·995	5·987
2·2	1·818	1·982	5·999	1·996	6·000	10·000	4·8	1·965	5·908	9·856	2·000	1·994	5·987
2·4	1·718	1·972	5·997	1·994	5·999	10·000							
2·6	1·579	1·960	5·994	1·992	5·999	10·000	5·0	1·964	5·889	9·727	1·999	1·994	5·984
2·8	1·394	1·944	5·985	1·989	5·997	10·000	5·1	1·959	5·859	9·642	1·999	1·993	5·980
3·0	1·166	1·929	5·967	1·986	5·993	10·000	5·2	1·946	5·809	9·550	1·998	1·991	5·973
3·2	0·907	1·916	5·926	1·984	5·984	10·000	5·3	1·924	5·739	9·458	1·996	1·987	5·963
3·4	0·642	1·909	5·843	1·983	5·967	9·999	5·4	1·895	5·656	9·376	1·993	1·982	5·952
3·6	0·402	1·909	5·683	1·983	5·935	9·998	5·5	1·862	5·573	9·315	1·988	1·977	5·941
3·8	0·216	1·902	5·396	1·981	5·881	9·994	5·6	1·833	5·507	9·281	1·981	1·973	5·934
							5·7	1·815	5·470	9·271	1·969	1·970	5·930
4·0	0·095	1·859	4·925	1·970	5·800	9·982	5·8	1·808	5·461	9·269	1·952	1·970	5·930
4·1	0·058	1·810	4·606	1·959	5·750	9·969	5·9	1·808	5·457	9·239	1·926	1·969	5·928
4·2	0·033	1·734	4·229	1·944	5·698	9·948	6·0	1·795	5·414	9·131	1·890	1·966	5·918
4·3	0·018	1·628	3·799	1·925	5·646	9·914	6·1	1·746	5·272	8·884	1·842	1·955	5·894
4·4	0·009	1·489	3·324	1·902	5·600	9·862	6·2	1·640	4·977	8·446	1·778	1·935	5·849
4·5	0·004	1·319	2·822	1·879	5·565	9·782	6·3	1·467	4·503	7·785	1·698	1·908	5·787
4·6	0·002	1·126	2·312	1·858	5·544	9·662	6·4	1·234	3·864	6·910	1·601	1·881	5·720
4·7	0·001	0·921	1·819	1·844	5·536	9·488	6·5	0·968	3·117	5·868	1·488	1·860	5·663
4·8	0·000	0·717	1·366	1·837	5·535	9·244	6·6	0·702	2·347	4·740	1·360	1·850	5·630
4·9	—	0·527	0·974	1·836	5·526	8·910	6·7	0·468	1·638	3·621	1·221	1·849	5·621
5·0	—	0·365	0·655	1·834	5·484	8·471	6·8	0·284	1·052	2·602	1·073	1·844	5·618
5·1	—	0·235	0·413	1·820	5·376	7·914	6·9	0·156	0·618	1·748	0·922	1·814	5·583
5·2	—	0·140	0·242	1·779	5·170	7·235							
5·3	—	0·077	0·130	1·695	4·839	6·443	7·00	0·077	0·329	1·092	0·773	1·737	5·466
5·4	—	0·038	0·064	1·560	4·374	5·562	7·05	0·051	0·231	0·838	0·700	1·676	5·360
5·5	—	0·017	0·029	1·372	3·788	4·629	7·10	0·034	0·158	0·630	0·630	1·599	5·217

Table 2. (*cont.*)

ρ	$(1s)^2$	$(2s)^2$	$(2p)^6$	$(3s)^2$	$(3p)^6$	$(3d)^{10}$	ρ	$(4s)^2$	$(4p)^6$	$(4d)^{10}$	$(4f)^2$	$(5s)^2$	$(5p)^6$
5·6	—	0·007	0·012	1·143	3·118	3·694	7·15	0·021	0·105	0·464	0·563	1·506	5·032
5·7	—	0·002	0·004	0·893	2·420	2·808	7·20	0·013	0·068	0·334	0·499	1·398	4·806
5·8	—	0·001	0·001	0·650	1·759	2·021	7·25	0·008	0·042	0·235	0·439	1·279	4·540
5·9	—	0·000	0·000	0·436	1·186	1·367	7·30	0·004	0·026	0·161	0·383	1·152	4·237
							7·35	0·002	0·015	0·108	0·331	1·019	3·904
							7·40	0·001	0·008	0·070	0·284	0·886	3·548
							7·45	0·001	0·005	0·045	0·242	0·757	3·178
6·00	—	—	—	0·268	0·736	0·863	7·50	0·000	0·002	0·028	0·203	0·633	2·803
6·05	—	—	—	0·202	0·561	0·666	7·55	—	0·001	0·017	0·169	0·520	2·433
6·10	—	—	—	0·149	0·418	0·504	7·60	—	0·001	0·010	0·140	0·418	2·077
6·15	—	—	—	0·107	0·303	0·373	7·65	—	0·000	0·005	0·114	0·328	1·742
6·20	—	—	—	0·075	0·214	0·270	7·70	—	—	0·003	0·092	0·252	1·434
6·25	—	—	—	0·051	0·147	0·191	7·75	—	—	0·002	0·074	0·189	1·158
6·30	—	—	—	0·033	0·099	0·132	7·80	—	—	0·001	0·058	0·139	0·916
6·35	—	—	—	0·021	0·064	0·089	7·85	—	—	0·000	0·045	0·099	0·710
6·40	—	—	—	0·013	0·040	0·058	7·90	—	—	—	0·035	0·069	0·538
6·45	—	—	—	0·008	0·025	0·037	7·95	—	—	—	0·026	0·046	0·398
6·50	—	—	—	0·004	0·014	0·023							
6·55	—	—	—	0·002	0·008	0·014	8·00	—	—	—	0·019	0·030	0·287
6·60	—	—	—	0·001	0·005	0·008	8·05	—	—	—	0·014	0·019	0·202
6·65	—	—	—	0·001	0·002	0·005	8·10	—	—	—	0·010	0·012	0·138
6·70	—	—	—	0·000	0·001	0·002	8·15	—	—	—	0·007	0·007	0·092
6·75	—	—	—	—	0·001	0·001	8·20	—	—	—	0·005	0·004	0·059
6·80	—	—	—	—	0·000	0·001	8·25	—	—	—	0·003	0·002	0·037
6·85	—	—	—	—	—	0·000	8·30	—	—	—	0·002	0·001	0·022
6·90	—	—	—	—	—	—	8·35	—	—	—	0·001	0·001	0·013
6·95	—	—	—	—	—	—	8·40	—	—	—	0·001	0·000	0·007
							8·45	—	—	—	0·001	—	0·004
							8·50	—	—	—	0·000	—	0·002
							8·55	—	—	—	—	—	0·001
							8·60	—	—	—	—	—	0·000
σ	0·44	4·19	5·23	11·43	13·30	16·47	σ	21·12	23·65	28·94	40·60	33·67	37·04
α	1·00	1·03	1·03	1·08	1·08	1·10	α	1·17	1·18	1·22	1·55	1·33	1·38

https://doi.org/10.1017/S0305004100034277 Published online by Cambridge University Press

https://doi.org/10.1017/S0305004100034277 Published online by Cambridge University Press

Table 3. Tm^{3+}. *Radial wave functions. Table of P and total* Z_p

$\rho = \ln 1000r$	r	1s	2s	2p	3s	3p	3d	4s	4p	4d	4f	5s	5p	Total Z_p
0·0	0·001	1·250	0·625	0·020	0·625	0·010	0·000	0·313	0·010	0·000	0·000	0·156	0·005	68·56
0·2	0·001221	1·504	0·752	0·029	0·752	0·014	0·000	0·376	0·014	0·000	0·000	0·188	0·007	68·46
0·4	0·001492	1·803	0·901	0·043	0·901	0·021	0·000	0·450	0·021	0·000	0·000	0·225	0·011	68·34
0·6	0·001822	2·152	1·074	0·063	1·074	0·032	0·000	0·537	0·032	0·000	0·000	0·269	0·016	68·20
0·8	0·002226	2·556	1·275	0·093	1·275	0·046	0·000	0·637	0·046	0·000	0·000	0·319	0·023	68·02
1·0	0·002718	3·018	1·503	0·136	1·503	0·068	0·001	0·751	0·068	0·001	0·000	0·376	0·034	67·81
1·2	0·003320	3·537	1·758	0·199	1·756	0·099	0·001	0·878	0·099	0·001	0·000	0·439	0·050	67·55
1·4	0·004055	4·106	2·034	0·289	2·031	0·144	0·002	1·015	0·144	0·002	0·000	0·508	0·072	67·23
1·6	0·004953	4·715	2·323	0·418	2·318	0·209	0·004	1·158	0·209	0·004	0·000	0·579	0·104	66·85
1·8	0·006050	5·340	2·609	0·601	2·600	0·300	0·008	1·299	0·300	0·008	0·000	0·649	0·150	66·40
2·0	0·007389	5·948	2·869	0·857	2·853	0·427	0·013	1·425	0·427	0·013	0·000	0·712	0·213	65·86
2·2	0·009025	6·491	3·066	1·209	3·040	0·602	0·023	1·517	0·601	0·023	0·000	0·758	0·301	65·21
2·4	0·01102	6·911	3·156	1·685	3·113	0·837	0·041	1·551	0·836	0·041	0·000	0·775	0·418	64·45
2·6	0·01346	7·138	3·078	2·315	3·008	1·147	0·070	1·496	1·144	0·070	0·001	0·747	0·572	63·56
2·8	0·01644	7·105	2·767	3·124	2·658	1·539	0·120	1·317	1·534	0·120	0·002	0·657	0·767	62·53
3·0	0·02009	6·761	2·158	4·124	1·995	2·016	0·202	0·979	2·006	0·201	0·004	0·488	1·002	61·33
3·1	0·02220	6·466	1·727	4·694	1·532	2·282	0·260	0·744	2·268	0·259	0·006	0·370	1·133	60·66
3·2	0·02453	6·090	1·208	5·304	0·978	2·560	0·334	0·463	2·540	0·332	0·009	0·229	1·269	59·95
3·3	0·02711	5·642	0·602	5·945	0·336	2·844	0·426	0·139	2·817	0·424	0·013	0·067	1·406	59·17
3·4	0·02996	5·131	−0·086	6·606	−0·383	3·125	0·541	−0·224	3·087	0·537	0·019	−0·115	1·540	58·34
3·5	0·03312	4·572	−0·842	7·269	−1·165	3·389	0·682	−0·617	3·337	0·677	0·027	−0·312	1·664	57·44
3·6	0·03660	3·984	−1·650	7·915	−1·983	3·622	0·855	−1·026	3·552	0·847	0·038	−0·517	1·770	56·48
3·7	0·04045	3·386	−2·487	8·519	−2·805	3·805	1·064	−1·435	3·710	1·052	0·053	−0·720	1·847	55·46
3·8	0·04470	2·801	−3·321	9·051	−3·588	3·915	1·314	−1·819	3·789	1·295	0·074	−0·912	1·884	54·36
3·9	0·04940	2·247	−4·118	9·483	−4·281	3·929	1·609	−2·151	3·764	1·579	0·103	−1·077	1·868	53·19
4·0	0·05460	1·745	−4·838	9·782	−4·825	3·824	1·951	−2·402	3·611	1·905	0·142	−1·200	1·788	51·95
4·1	0·06034	1·305	−5·443	9·921	−5·161	3·575	2·341	−2·538	3·304	2·273	0·195	−1·265	1·630	50·65
4·2	0·06669	0·938	−5·894	9·877	−5·229	3·163	2·779	−2·528	2·826	2·678	0·265	−1·256	1·385	49·28
4·3	0·07370	0·645	−6·163	9·934	−4·978	2·575	3·258	−2·347	2·165	3·110	0·358	−1·160	1·049	47·86
4·4	0·08145	0·422	−6·228	9·189	−4·374	1·808	3·770	−1·977	1·323	3·555	0·479	−0·968	0·623	46·38
4·5	0·09002	0·261	−6·083	8·552	−3·402	0·870	4·300	−1·416	0·319	3·990	0·635	−0·681	0·116	44·84
4·6	0·09948	0·153	−5·739	7·747	−2·082	−0·211	4·828	−0·680	−0·810	4·388	0·834	−0·307	−0·451	43·24
4·7	0·1099	0·083	−5·221	6·813	−0·467	−1·393	5·330	0·192	−2·003	4·713	1·083	0·134	−1·047	41·58
4·8	0·1215	0·042	−4·573	5·801	1·354	−2·618	5·777	1·137	−3·175	4·922	1·391	0·608	−1·626	39·85
4·9	0·1343	0·020	−3·847	4·766	3·259	−3·811	6·136	2·070	−4·225	4·972	1·765	1·071	−2·136	38·07
5·00	0·1484	0·009	−3·098	3·766	5·101	−4·893	6·379	2·890	−5·038	4·817	2·211	1·468	−2·517	36·23
5·05	0·1560	0·005	−2·733	3·296	5·950	−5·366	6·448	3·224	−5·319	4·650	2·462	1·624	−2·640	35·29
5·10	0·1640	0·003	−2·382	2·852	6·728	−5·782	6·478	3·489	−5·499	4·418	2·732	1·743	−2·709	34·35
5·15	0·1724	0·002	−2·050	2·439	7·416	−6·133	6·467	3·673	−5·565	4·118	3·021	1·819	−2·717	33·41
5·20	0·1813	0·001	−1·742	2·061	7·999	−6·410	6·414	3·766	−5·508	3·748	3·328	1·845	−2·661	32·47

Table 3. (*cont.*)

$\rho = \ln \frac{1000r}{}$	r	$1s$	$2s$	$2p$	$3s$	$3p$	$3d$	$4s$	$4p$	$4d$	$4f$	$5s$	$5p$	Total Z_p
5·25	0·1906	0·001	−1·460	1·719	8·466	−6·610	6·319	3·758	−5·319	3·307	3·653	1·817	−2·535	31·52
5·30	0·2003	0·000	−1·206	1·415	8·807	−6·729	6·181	3·643	−4·994	2·795	3·994	1·733	−2·339	30·58
5·35	0·2106	—	−0·982	1·149	9·015	−6·764	6·002	3·418	−4·533	2·216	4·350	1·591	−2·071	29·65
5·40	0·2214	—	−0·787	0·919	9·090	−6·717	5·783	3·082	−3·936	1·574	4·718	1·391	−1·735	28·72
5·45	0·2328	—	−0·621	0·724	9·032	−6·590	5·529	2·639	−3·211	0·873	5·097	1·137	−1·335	27·80
5·50	0·2447	—	−0·482	0·561	8·849	−6·389	5·242	2·095	−2·369	0·122	5·482	0·832	−0·877	26·88
5·55	0·2572	—	−0·368	0·428	8·549	−6·120	4·927	1·461	−1·423	−0·669	5·870	0·484	−0·372	25·97
5·60	0·2704	—	−0·275	0·321	8·146	−5·791	4·589	0·751	−0·392	−1·489	6·257	0·103	0·171	25·06
5·65	0·2843	—	−0·202	0·236	7·654	−5·413	4·235	−0·018	0·702	−2·326	6·638	−0·302	0·736	24·15
5·70	0·2989	—	−0·146	0·170	7·093	−4·996	3·870	−0·826	1·834	−3·165	7·009	−0·717	1·308	23·24
5·75	0·3142	—	−0·103	0·120	6·480	−4·553	3·500	−1·651	2·977	−3·991	7·364	−1·129	1·871	22·32
5·80	0·3303	—	−0·071	0·083	5·836	−4·094	3·131	−2·469	4·102	−4·788	7·699	−1·522	2·406	21·40
5·85	0·3472	—	−0·048	0·056	5·179	−3·633	2·771	−3·259	5·182	−5·542	8·007	−1·882	2·895	20·47
5·90	0·3650	—	−0·031	0·037	4·527	−3·179	2·423	−3·997	6·188	−6·238	8·286	−2·194	3·321	19·55
5·95	0·3838	—	−0·020	0·024	3·897	−2·742	2·094	−4·662	7·095	−6·861	8·529	−2·444	3·667	18·62
6·00	0·4034	—	−0·013	0·015	3·302	−2·331	1·787	−5·237	7·882	−7·399	8·735	−2·622	3·919	17·69
6·05	0·4241	—	−0·008	0·009	2·753	−1·951	1·505	−5·708	8·531	−7·844	8·899	−2·717	4·065	16·78
6·10	0·4459	—	−0·005	0·006	2·257	−1·608	1·250	−6·064	9·028	−8·188	9·020	−2·722	4·096	15·88
6·15	0·4687	—	−0·003	0·003	1·819	−1·304	1·024	−6·300	9·366	−8·426	9·096	−2·634	4·005	15·00
6·20	0·4927	—	−0·001	0·002	1·441	−1·040	0·827	−6·415	9·543	−8·557	9·128	−2·453	3·792	14·15
6·25	0·5180	—	−0·001	0·001	1·120	−0·815	0·657	−6·412	9·562	−8·583	9·116	−2·180	3·458	13·33
6·30	0·5446	—	−0·000	0·001	0·855	−0·628	0·515	−6·300	9·433	−8·507	9·062	−1·822	3·007	12·54
6·35	0·5725	—	—	0·000	0·639	−0·475	0·396	−6·088	9·168	−8·337	8·967	−1·387	2·450	11·80
6·40	0·6018	—	—	—	0·469	−0·352	0·300	−5·791	8·783	−8·080	8·833	−0·885	1·796	11·10
6·45	0·6327	—	—	—	0·337	−0·256	0·223	−5·425	8·298	−7·747	8·663	−0·331	1·060	10·44
6·50	0·6651	—	—	—	0·237	−0·182	0·163	−5·006	7·732	−7·349	8·460	0·262	0·259	9·83
6·55	0·6992	—	—	—	0·163	−0·127	0·117	−4·551	7·109	−6·898	8·227	0·877	−0·590	9·25
6·60	0·7351	—	—	—	0·109	−0·087	0·082	−4·076	6·447	−6·408	7·967	1·499	−1·467	8·71
6·65	0·7728	—	—	—	0·072	−0·058	0·057	−3·597	5·769	−5·890	7·682	2·112	−2·355	8·21
6·70	0·8124	—	—	—	0·046	−0·038	0·038	−3·127	5·092	−5·356	7·377	2·700	−3·232	7·73
6·75	0·8541	—	—	—	0·028	−0·024	0·025	−2·677	4·433	−4·819	7·054	3·249	−4·080	7·29
6·80	0·8978	—	—	—	0·017	−0·015	0·016	−2·257	3·805	−4·288	6·716	3·744	−4·882	6·87
6·85	0·9439	—	—	—	0·010	−0·009	0·010	−1·873	3·219	−3·773	6·367	4·177	−5·620	6·48
6·90	0·9923	—	—	—	0·006	−0·005	0·006	−1·529	2·684	−3·282	6·009	4·537	−6·281	6·11
6·95	1·043	—	—	—	0·003	−0·003	0·004	−1·228	2·204	−2·822	5·646	4·818	−6·853	5·78
7·00	1·097	—	—	—	0·002	−0·002	0·002	−0·969	1·782	−2·397	5·282	5·017	−7·326	5·43
7·05	1·153	—	—	—	0·001	−0·001	0·001	−0·752	1·418	−2·011	4·918	5·133	−7·694	5·12
7·10	1·212	—	—	—	0·000	−0·000	0·001	−0·573	1·110	−1·666	4·559	5·166	−7·953	4·84
7·15	1·274	—	—	—	—	—	0·000	−0·428	0·855	−1·362	4·207	5·123	−8·105	4·58
7·20	1·339	—	—	—	—	—	—	−0·314	0·646	−1·099	3·864	5·008	−8·150	4·34

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Table 3. (*cont.*)

$\rho = \ln 1000r$	r	1s	2s	2p	3s	3p	3d	4s	4p	4d	4f	5s	5p	Total Z_p
7·25	1·408	—	—	—	—	—	—	−0·226	0·480	−0·874	3·533	4·829	−8·093	4·13
7·30	1·480	—	—	—	—	—	—	−0·159	0·350	−0·685	3·215	4·595	−7·942	3·93
7·35	1·556	—	—	—	—	—	—	−0·109	0·250	−0·529	2·912	4·317	−7·706	3·77
7·40	1·636	—	—	—	—	—	—	−0·074	0·175	−0·403	2·625	4·005	−7·395	3·62
7·45	1·720	—	—	—	—	—	—	−0·048	0·120	−0·301	2·355	3·669	−7·019	3·49
7·50	1·808	—	—	—	—	—	—	−0·031	0·081	−0·222	2·102	3·320	−6·592	3·39
7·55	1·901	—	—	—	—	—	—	−0·019	0·053	−0·160	1·867	2·966	−6·124	3·30
7·60	1·998	—	—	—	—	—	—	−0·012	0·034	−0·114	1·648	2·616	−5·628	3·23
7·65	2·101	—	—	—	—	—	—	−0·007	0·021	−0·079	1·447	2·277	−5·116	3·17
7·70	2·208	—	—	—	—	—	—	−0·004	0·013	−0·054	1·263	1·956	−4·598	3·12
7·75	2·322	—	—	—	—	—	—	−0·002	0·008	−0·036	1·095	1·657	−4·085	3·09
7·80	2·441	—	—	—	—	—	—	−0·001	0·004	−0·024	0·943	1·384	−3·587	3·06
7·85	2·566	—	—	—	—	—	—	−0·001	0·002	−0·015	0·806	1·139	−3·110	3·04
7·90	2·697	—	—	—	—	—	—	−0·000	0·001	−0·009	0·683	0·923	−2·662	3·03
7·95	2·836	—	—	—	—	—	—	—	0·001	−0·006	0·574	0·736	−2·248	3·02
8·00	2·981	—	—	—	—	—	—	—	0·000	−0·003	0·478	0·577	−1·872	3·01
8·05	3·134	—	—	—	—	—	—	—	—	−0·002	0·394	0·445	−1·536	3·01
8·10	3·294	—	—	—	—	—	—	—	—	−0·001	0·322	0·336	−1·241	3·00
8·15	3·463	—	—	—	—	—	—	—	—	−0·001	0·259	0·250	−0·987	3·00
8·20	3·641	—	—	—	—	—	—	—	—	−0·000	0·206	0·182	−0·771	3·00
8·25	3·828	—	—	—	—	—	—	—	—	—	0·162	0·129	−0·592	3·00
8·30	4·024	—	—	—	—	—	—	—	—	—	0·126	0·090	−0·446	3·00
8·35	4·230	—	—	—	—	—	—	—	—	—	0·096	0·061	−0·329	3·00
8·40	4·447	—	—	—	—	—	—	—	—	—	0·072	0·041	−0·238	3·00
8·45	4·675	—	—	—	—	—	—	—	—	—	0·053	0·026	−0·168	3·00
8·50	4·915	—	—	—	—	—	—	—	—	—	0·039	0·017	−0·117	3·00
8·55	5·167	—	—	—	—	—	—	—	—	—	0·027	0·010	−0·079	3·00
8·60	5·432	—	—	—	—	—	—	—	—	—	0·019	0·006	−0·052	3·00
8·65	5·710	—	—	—	—	—	—	—	—	—	0·013	0·003	−0·033	3·00
8·70	6·003	—	—	—	—	—	—	—	—	—	0·009	0·002	−0·021	3·00
8·75	6·311	—	—	—	—	—	—	—	—	—	0·006	0·001	−0·013	3·00
8·80	6·634	—	—	—	—	—	—	—	—	—	0·004	0·001	−0·007	3·00
8·85	6·974	—	—	—	—	—	—	—	—	—	0·002	0·000	−0·004	3·00
8·90	7·332	—	—	—	—	—	—	—	—	—	0·001	—	−0·002	3·00
8·95	7·708	—	—	—	—	—	—	—	—	—	0·001	—	−0·001	3·00
9·00	8·103	—	—	—	—	—	—	—	—	—	0·000	—	−0·001	3·00
9·05	8·519	—	—	—	—	—	—	—	—	—	—	—	−0·000	3·00
$\int_0^\infty P^2 dr$		1·3852	3·209	8·068	15·048	8·548	7·979	15·838	37·34	34·75	62·89	25·98	77·79	—
ϵ		4083	658·3	631·3	148·25	135·00	110·94	29·94	24·56	14·959	2·903	5·321	3·860	—

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Table 4. Tm^{3+}. *Contributions to Z*

ρ	$(1s)^2$	$(2s)^2$	$(2p)^6$	$(3s)^2$	$(3p)^6$	$(3d)^{10}$	ρ	$(4s)^2$	$(4p)^6$	$(4d)^{10}$	$(4f)^{12}$	$(5s)^2$	$(5p)^6$
0·0	1·999	2·000	6·000	2·000	6·000	10·000	0·0	2·000	6·000	10·000	12·000	2·000	6·000
0·2	1·999	2·000	6·000	2·000	6·000	10·000	2·0	1·999	6·000	10·000	12·000	2·000	6·000
0·4	1·998	2·000	6·000	2·000	6·000	10·000	3·0	1·996	5·997	10·000	12·000	1·999	6·000
0·6	1·996	2·000	6·000	2·000	6·000	10·000	3·2	1·996	5·993	10·000	12·000	1·999	5·999
0·8	1·992	1·999	6·000	2·000	6·000	10·000	3·4	1·996	5·986	10·000	12·000	1·999	5·998
1·0	1·987	1·999	6·000	2·000	6·000	10·000	3·6	1·995	5·974	9·999	12·000	1·999	5·997
1·2	1·978	1·998	6·000	1·999	6·000	10·000	3·8	1·993	5·956	9·996	12·000	1·999	5·995
1·4	1·962	1·996	6·000	1·999	6·000	10·000	4·0	1·987	5·934	9·989	12·000	1·998	5·992
1·6	1·937	1·993	6·000	1·999	6·000	10·000	4·2	1·978	5·913	9·970	12·000	1·997	5·990
1·8	1·896	1·989	6·000	1·998	6·000	10·000	4·4	1·968	5·902	9·928	11·999	1·995	5·988
2·0	1·834	1·983	5·999	1·996	6·000	10·000	4·6	1·963	5·901	9·845	11·998	1·994	5·988
2·2	1·742	1·974	5·998	1·994	5·999	10·000	4·8	1·962	5·884	9·705	11·993	1·994	5·986
2·4	1·612	1·962	5·995	1·992	5·999	10·000							
2·6	1·437	1·947	5·987	1·989	5·997	10·000	5·0	1·947	5·806	9·516	11·976	1·992	5·977
2·8	1·217	1·931	5·971	1·986	5·993	10·000	5·1	1·926	5·736	9·420	11·958	1·989	5·968
3·0	0·963	1·917	5·935	1·983	5·985	10·000	5·2	1·897	5·650	9·336	11·928	1·984	5·959
3·2	0·696	1·908	5·861	1·982	5·969	9·999	5·3	1·863	5·565	9·276	11·879	1·979	5·949
3·4	0·449	1·907	5·717	1·982	5·938	9·998	5·4	1·833	5·496	9·246	11·802	1·975	5·942
3·6	0·249	1·903	5·454	1·980	5·884	9·994	5·5	1·812	5·457	9·240	11·686	1·973	5·939
3·8	0·115	1·870	5·015	1·971	5·802	9·982	5·6	1·805	5·448	9·235	11·516	1·973	5·939
							5·7	1·804	5·443	9·188	11·277	1·972	5·937
4·0	0·042	1·763	4·354	1·947	5·696	9·949	5·8	1·792	5·396	9·042	10·951	1·969	5·928
4·1	0·023	1·668	3·938	1·928	5·640	9·916	5·9	1·745	5·244	8·733	10·526	1·959	5·906
4·2	0·012	1·540	3·475	1·905	5·589	9·863	6·0	1·639	4·932	8·212	9·993	1·942	5·866
4·3	0·005	1·380	2·977	1·880	5·548	9·783	6·1	1·465	4·437	7·462	9·352	1·918	5·812
4·4	0·002	1·194	2·465	1·857	5·522	9·663	6·2	1·231	3·779	6·507	8·613	1·893	5·755
4·5	0·001	0·990	1·962	1·840	5·510	9·487	6·3	0·964	3·022	5·413	7·793	1·875	5·708
4·6	0·000	0·783	1·493	1·830	5·509	9·239	6·4	0·697	2·252	4·272	6·916	1·866	5·681
4·7	—	0·587	1·080	1·828	5·503	8·900	6·5	0·463	1·555	3·183	6·011	1·865	5·675
4·8	—	0·413	0·738	1·827	5·469	8·451	6·6	0·280	0·988	2·228	5·109	1·860	5·672
4·9	—	0·272	0·473	1·817	5·375	7·880	6·7	0·153	0·574	1·457	4·240	1·833	5·637
5·0	—	0·166	0·282	1·783	5·184	7·184	6·8	0·076	0·303	0·886	3·430	1·763	5·525
5·1	—	0·093	0·155	1·709	4·868	6·372	6·9	0·033	0·144	0·497	2·700	1·636	5·294
5·2	—	0·048	0·078	1·583	4·413	5·470							
5·3	—	0·022	0·036	1·402	3·831	4·518	7·00	0·013	0·061	0·256	2·066	1·450	4·916

https://doi.org/10.1017/S0305004100034277 Published online by Cambridge University Press

https://doi.org/10.1017/S0305004100034277 Published online by Cambridge University Press

Table 4. (*cont.*)

ρ	$(1s)^2$	$(2s)^2$	$(2p)^6$	$(3s)^2$	$(3p)^6$	$(3d)^{10}$	ρ	$(4s)^2$	$(4p)^6$	$(4d)^{10}$	$(4f)^{12}$	$(5s)^2$	$(5p)^6$
5·4	—	0·009	0·015	1·176	3·157	3·570	7·05	0·008	0·038	0·178	1·787	1·338	4·671
5·5	—	0·003	0·005	0·924	2·450	2·680	7·10	0·004	0·023	0·121	1·534	1·217	4·391
5·6	—	0·001	0·002	0·676	1·776	1·899	7·15	0·002	0·014	0·080	1·306	1·090	4·081
5·7	—	0·000	0·000	0·455	1·193	1·261	7·20	0·001	0·008	0·051	1·103	0·961	3·748
5·8	—	—	—	0·280	0·736	0·778	7·25	0·001	0·004	0·032	0·924	0·833	3·398
5·9	—	—	—	0·156	0·414	0·443	7·30	0·000	0·002	0·020	0·767	0·709	3·039
							7·35	—	0·001	0·012	0·631	0·593	2·680
							7·40	—	0·001	0·007	0·515	0·486	2·329
							7·45	—	0·000	0·004	0·416	0·391	1·993
6·00	—	—	—	0·079	0·210	0·231	7·50	—	—	0·002	0·332	0·308	1·677
6·05	—	—	—	0·053	0·144	0·161	7·55	—	—	0·001	0·263	0·238	1·388
6·10	—	—	—	0·035	0·095	0·109	7·60	—	—	0·001	0·205	0·179	1·128
6·15	—	—	—	0·022	0·062	0·072	7·65	—	—	0·000	0·159	0·132	0·900
6·20	—	—	—	0·013	0·038	0·046	7·70	—	—	—	0·121	0·095	0·704
6·25	—	—	—	0·008	0·023	0·029	7·75	—	—	—	0·091	0·067	0·540
6·30	—	—	—	0·005	0·014	0·017	7·80	—	—	—	0·067	0·046	0·405
6·35	—	—	—	0·003	0·008	0·010	7·85	—	—	—	0·049	0·030	0·297
6·40	—	—	—	0·001	0·004	0·006	7·90	—	—	—	0·035	0·019	0·212
6·45	—	—	—	0·001	0·002	0·003	7·95	—	—	—	0·025	0·012	0·148
6·50	—	—	—	0·000	0·001	0·002							
6·55	—	—	—	—	0·001	0·001	8·00	—	—	—	0·017	0·007	0·100
6·60	—	—	—	—	0·000	0·000	8·05	—	—	—	0·012	0·004	0·066
6·65	—	—	—	—	—	—	8·10	—	—	—	0·008	0·002	0·042
6·70	—	—	—	—	—	—	8·15	—	—	—	0·005	0·001	0·026
6·75	—	—	—	—	—	—	8·20	—	—	—	0·003	0·001	0·016
6·80	—	—	—	—	—	—	8·25	—	—	—	0·002	0·000	0·009
6·85	—	—	—	—	—	—	8·30	—	—	—	0·001	—	0·005
6·90	—	—	—	—	—	—	8·35	—	—	—	0·001	—	0·003
6·95	—	—	—	—	—	—	8·40	—	—	—	0·000	—	0·001
							8·45	—	—	—	—	—	0·001
							8·50	—	—	—	—	—	0·000
σ	0·44	4·25	5·31	11·63	13·48	16·48	σ	22·67	25·29	30·75	42·96	38·92	43·02
α	1·00	1·02	1·03	1·07	1·07	1·08	α	1·17	1·18	1·22	1·55	1·37	1·43

In Table 5 the Slater integrals $F^2(4f, 4f)$, $F^4(4f, 4f)$ and $F^6(4f, 4f)$ are given for both Pr^{3+} and Tm^{3+}. According to the notation of Condon and Shortley ((2), p. 177),

$$F^k(4f, 4f) = \int_0^\infty \int_0^\infty \frac{r_<^k}{r_>^{k+1}} P^2(4f; r_1) P^2(4f; r_2)\, dr_1\, dr_2 \tag{1}$$

and

$$F_k = F^k/D_k. \tag{2}$$

Here $P(4f; r)$ is normalized and D_k is a constant tabulated by Condon and Shortley. From the values given in Table 5, it can be seen that F^k decreases monotonically with k, as is demanded by the definition (1). Again, $F^k(4f, 4f)$ is larger for Tm^{3+} than for Pr^{3+} because the $(4f)$ wave function is more localized in Tm^{3+}. The values of F_2, F_4 and F_6 as defined by (2) are also given. The ratios F_4/F_2 and F_6/F_2 are of particular interest

Table 5. *Values of Slater integrals in atomic units*

	Pr^{3+}	Tm^{3+}	H
$F^2(4f, 4f)$	0·4056	0·5730	—
$F^4(4f, 4f)$	0·2527	0·3578	—
$F^6(4f, 4f)$	0·1813	0·2568	—
$10^2F_2(4f, 4f)$	0·1803	0·2547	—
$10^3F_4(4f, 4f)$	0·2321	0·3285	—
$10^4F_6(4f, 4f)$	0·2462	0·3489	—
F_4/F_2	0·1287	0·1290	0·138
$10F_6/F_2$	0·1366	0·1370	0·151

spectroscopically and are included in the table. The hydrogenic values of these ratios are given for comparison and are seen to be some 10 % larger. A deviation in this direction would be expected since the $(4f)$ functions in the two structures are more diffuse than hydrogenic functions and F^k therefore decreases more rapidly with k than in the hydrogenic case. It is interesting to note that the ratios change by less than $\frac{1}{2}$ % as we pass from Pr^{3+} to Tm^{3+}, although the values for Tm^{3+} are slightly nearer hydrogenic. This near constancy of F_4/F_2 and F_6/F_2 is in accord with the constancy of the slope constant α $(4f)$ (see Tables 2 and 4) which is closely related to the width of the peak of $P(4f)$ (Ridley (8)). As it is likely that effects due to exchange and relativity will affect the screening of $P(4f)$ rather than its general shape, the ratios F_4/F_2 and F_6/F_2 are almost certainly more reliable than the absolute values of F_2, F_4 and F_6.

I am indebted to Mr W. A. Runciman for discussion on the values of the Slater integrals, spin-orbit coupling constants and $\overline{(1/r^3)}$. I also wish to thank Dr J. Corner and the staff of the Physics Division at A.W.R.E. for providing automatic computing facilities.

https://doi.org/10.1017/S0305004100034277 Published online by Cambridge University Press

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https://doi.org/10.1017/S0305004100034277 Published online by Cambridge University Press