UCRL-10134

University of California

Ernest O. Lawrence Radiation Laboratory

TWO-WEEK LOAN COPY

This is a Library Circulating Copy which may be borrowed for two weeks. For a personal retention copy, call Tech. Info. Division, Ext. 5545

Berkeley, California

DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.

J. Chem. Phys.

UCRL-10134

UNIVERSITY OF CALIFORNIA

Lawrence Radiation Laboratory
Berkeley, California

Contract No. W-7405-eng-48

APPROXIMATE EXCITED EIGENFUNCTIONS FOR Pr^{+3} AND Tm^{+3}

Katheryn Rajnak

May 1962

APPROXIMATE EXCITED EIGENFUNCTIONS FOR Pr^{+3} and Tm^{+3} *

By Katheryn Rajnak

Department of Chemistry and Lawrence Radiation Laboratory
University of California, Berkeley, California

ABSTRACT

Approximate 5d, 6s, 6p and 5f radial wave functions, which are necessary for any investigation of the effect of configuration interaction in rare earth spectra, have been obtained for Pr^{+3} and Tm^{+3}. The calculations were based on the ground state eigenfunctions obtained by Ridley in an SCF calculation without exchange. $< r^2 >$, $< r^4 >$, R^k (4f4f, 4f6p) and R^k (4f4f, 4f5f) integrals have been calculated.

* This work was done under the auspices of the United States Atomic Energy Commission.

Analysis of the optical spectra of rare earth ions have so far been based on the assumption that the electronic configurations are pure. In order to investigate the effect of configuration interaction, eigenfunctions of excited states are required. The present work was undertaken to obtain the 5d, 6s, 6p and 5f functions for Pr^{+3} and Tm^{+3}, these two ions being chosen because of the availability of ground state eigenfunctions from Ridley's SCF calculations.[1]

Since it was necessary to compute the effect of promoting one of the 4f electrons of Pr^{+3} to an excited orbital, the contribution of one of the 4f electrons was removed from the effective potential tabulated by Ridley. The resulting potential was treated as that of a core in whose field the excited electron moves, i.e. the 4f and excited electron were assumed to move in the same central field. The inner 4f and outer 5d, 6s, etc. electrons actually do see different fields, but the present functions are a good first approximation. They are certainly better than the presently available hydrogenic functions.

CALCULATIONS

In addition to the wave functions, Ridley's results include a tabulation of a total effective charge $Z_p(r)$ for the ion and a contribution to Z from each shell of electrons. $Z_p(r)/r$ is the total potential at any point due to the nucleus and the average charge distribution of the electrons. For a single electron in a state of radial and angular momentum quantum numbers n and ℓ the radial wave function is denoted by $P(n\ell;r)$ where $\int_0^\infty P^2(n\ell;r)\,dr = 1$. The effective charge due to one electron and one nuclear charge, $Z_p(n'\ell';r)$, i.e. the contribution to the total Z_p from a single electron can be obtained from a differential equation given by Ridley.[2]

$Z(n\ell;r)$ is tabulated by Ridley and the integral is easily evaluated numerically from her tabulated $P(n\ell;r)$.

For the present calculation the potential was assumed to be the same for all the states of interest, i.e. Eq. (1) becomes

$$\left\{ \frac{d^2}{dr^2} + \frac{2}{r}\left[1 + i + \sum_{n'\ell'} q(n'\ell')\, Z_p(n'\ell';r) - Z_p(4f;r)\right] + 2E - \frac{\ell(\ell+1)}{r^2}\right\} P(n\ell;r) = 0 \quad (2)$$

where $n\ell$ = 4f, 5d, 6s, 6p, 5f. Equation (2) was solved on the IBM 7090 for both Pr^{+3} and Tm^{+3}. The resulting wave functions are shown in Figs. 1 and 2 and tabulated in Tables I and II. Since $\langle r^2 \rangle$, $\langle r^4 \rangle$ and the R^k integral defined by Condon and Shortley[4]

$$R^k(n\ell,\ n\ell,\ n\ell\ n'\ell') = \int_0^\infty\int_0^\infty \frac{r_<^k}{r_>^{k+1}}\ P^2(n\ell;r_1)\ P(n\ell;r_2)\ P(n'\ell';\ r_2)\ dr_1\ dr_2$$

are of interest in crystal field and configuration interaction calculations these integrals are tabulated in Table III along with the one electron energies.

DISCUSSION

Dieke et al[5] have determined experimentally the centers of various excited configurations of doubly and triply ionized rare earths. They found that for the doubly ionized atoms a plot of the center of the configuration, relative to the $4f^{n-1}6s$ taken as zero, vs. atomic number yields a straight line. Although experimental points are available only for Ce^{+3} and Yb^{+3} they also drew straight lines on a similar plot for the triply ionized atoms. In Fig. 3 the calculated one electron energies (relative to 6s) are plotted along with the experimental centers of configurations from Fig. 5 of Dieke et al. The results are remarkably good when one considers the approximations made. Since only the first ionization energy is available for Pr it is impossible to compare absolute energies, but it

is probable that in taking energy differences many of the errors have cancelled yielding a reasonably good fit to the experimental spectrum.

The 4f energies differ slightly from those of Ridley. This is probably due to a slight difference in the potentials used or the method of machine solution of the Schrödinger equation. However, the 4f functions differ only slightly from those of Ridley and the $F^k(4f,4f)$ integrals agree very well. (See Table III.)

The $\langle r^2 \rangle$ and $\langle r^4 \rangle$ integrals are not very sensitive to the grid size used in the numerical integration but this is not true for the R^k integrals. A grid size ~ .005 is necessary to obtain integrals which do not change appreciably with a change in grid size. It is felt that a further reduction of grid size would change the values given by less than $\pm 2 \times 10^{-4}$ a.u.

Wong[6] has used functions obtained in this manner to calculate Slater integrals connecting $4f^2$ and $5d^2$ configurations of Pr^{+3}. These have led to an appreciable improvement in the agreement between the calculated and observed spectra.

Since no other experimental data are available for comparison it is difficult to establish any further criteria for the accuracy of these functions. They are certainly a much better approximation than hydrogenic functions, however, and they should prove useful in the analysis of rare earth spectra. Such a simple approximation to excited state eigenfunctions may also be useful in other heavy atoms where SCF calculations are available for the ground configuration.

ACKNOWLEDGMENTS

I wish to thank Dr. B. R. Judd and Dr. K. S. Pitzer for several helpful discussions and Dr. E. M. Mortensen for assistance with computer programming.

This work was done under the auspices of the United States Atomic Energy Commission.

REFERENCES

1. E. C. Ridley, Proc. Cambridge Phil. Soc. 56, 41 (1960).
2. E. C. Ridley, Proc. Cambridge Phil. Soc. 51, 702 (1955).
3. E. C. Ridley, Proc. Cambridge Phil. Soc. 51, 693 (1955).
4. E. U. Condon and G. H. Shortley, The Theory of Atomic Spectra (Cambridge University Press, Cambridge, 1957), p. 175.
5. G. H. Dieke, H. M. Crosswhite, and B. Dunn, J. Opt. Soc. Am. 51, 820 (1961)
6. E. Y. Wong, submitted to J. Chem. Phys.

FIGURE CAPTIONS

Figure 1. Normalized radial eigenfunctions, $P(r)$, for Pr^{+3}.

Figure 2. Normalized radial eigenfunctions, $P(r)$, for Tm^{+3}.

Figure 3. Experimental centers of configurations of triply ionized rare earth ions from Dieke et al[5] and calculated one electron energies.

Table I. Radial Wave Functions, P(r), for Pr^{+3}

r (atomic units)	4f	5d	6s	6p	5f
.01	.0000	.0008	-.0611	.0141	.0000
.02	.0002	.0055	-.0554	.0412	.0000
.03	.0008	.0155	-.0190	.0677	-.0002
.04	.0022	.0305	.0247	.0867	-.0005
.05	.0047	.0496	.0630	.0960	-.0011
.06	.0086	.0715	.0900	.0953	-.0021
.07	.0141	.0948	.1040	.0860	-.0034
.08	.0214	.1183	.1055	.0698	-.0051
.09	.0304	.1408	.0964	.0487	-.0073
.10	.0414	.1616	.0788	.0245	-.0100
.11	.0541	.1798	.0553	-.0010	-.0130
.12	.0687	.1950	.0281	-.0266	-.0165
.13	.0849	.2070	-.0008	-.0509	-.0204
.14	.1027	.2154	-.0297	-.0755	-.0247
.15	.1220	.2202	-.0572	-.0929	-.0293
.16	.1426	.2216	-.0823	-.1094	-.0343
.17	.1643	.2196	-.1042	-.1225	-.0395
.18	.1871	.2144	-.1224	-.1322	-.0449
.19	.2108	.2062	-.1368	-.1384	-.0506
.20	.2352	.1954	-.1470	-.1412	-.0564
.21	.2602	.1821	-.1532	-.1409	-.0624
.22	.2857	.1666	-.1556	-.1376	-.0685
.23	.3116	.1493	-.1542	-.1317	-.0746
.24	.3376	.1304	-.1495	-.1233	-.0808
.25	.3639	.1102	-.1417	-.1129	-.0871
.26	.3901	.0890	-.1312	-.1006	-.0933
.27	.4163	.0669	-.1184	-.0868	-.0995
.28	.4423	.0442	-.1035	-.0718	-.1056
.29	.4680	.0212	-.0870	-.0558	-.1116

r (atomic units)	4f	5d	6s	6p	5f
.30	.4934	-.0020	-.0691	-.0391	-.1176
.31	.5184	-.0252	-.0503	-.0220	-.1235
.32	.5430	-.0482	-.0308	-.0046	-.1292
.33	.5670	-.0709	-.0109	.0129	-.1347
.34	.5903	-.0931	.0091	.0302	-.1402
.35	.6131	-.1147	.0290	.0473	-.1454
.36	.6352	-.1356	.0487	.0639	-.1504
.37	.6565	-.1558	.0677	.0799	-.1553
.38	.6772	-.1750	.0862	.0953	-.1600
.39	.6970	-.1934	.1038	.1098	-.1645
.40	.7161	-.2107	.1205	.1236	-.1687
.41	.7343	-.2271	.1361	.1364	-.1728
.42	.7518	-.2423	.1506	.1482	-.1766
.43	.7684	-.2565	.1639	.1590	-.1802
.44	.7842	-.2695	.1760	.1688	-.1836
.45	.7993	-.2815	.1867	.1775	-.1868
.46	.8135	-.2923	.1962	.1851	-.1898
.47	.8269	-.3019	.2044	.1917	-.1926
.48	.8395	-.3105	.2112	.1972	-.1951
.49	.8514	-.3180	.2167	.2017	-.1975
.50	.8625	-.3253	.2210	.2051	-.1996
.52	.8826	-.3359	.2257	.2089	-.2033
.54	.8998	-.3394	.2257	.2089	-.2063
.56	.9145	-.3410	.2212	.2054	-.2086
.58	.9268	-.3392	.2128	.1986	-.2101
.60	.9368	-.3340	.2007	.1890	-.2111
.62	.9448	-.3258	.1855	.1767	-.2115
.64	.9509	-.3148	.1675	.1622	-.2113
.66	.9552	-.3014	.1472	.1457	-.2107
.68	.9580	-.2858	.1250	.1277	-.2096
.70	.9593	-.2683	.1013	.1082	-.2080

r (atomic units)	4f	5d	6s	6p	5f
.72	.9593	-.2490	-.0764	.0877	-.2061
.74	.9580	-.2282	.0507	.0664	-.2037
.76	.9557	-.2061	.0245	.0445	-.2011
.78	.9523	-.1838	-.0019	.0222	-.1981
.80	.9481	-.1587	-.0284	-.0002	-.1948
.82	.9430	-.1338	-.0546	-.0227	-.1912
.84	.9371	-.1083	-.0803	-.0450	-.1874
.86	.9306	-.0824	-.1054	-.0670	-.1833
.88	.9234	-.0560	-.1298	-.0885	-.1790
.90	.9157	-.0295	-.1532	-.1096	-.1745
.92	.9074	-.0029	-.1756	-.1299	-.1698
.94	.8987	.0237	-.1969	-.1496	-.1649
.96	.8896	.0503	-.2170	-.1684	-.1599
.98	.8801	.0767	-.2358	-.1864	-.1547
1.00	.8703	.1029	-.2532	-.2035	-.1494
1.10	.8174	.2282	-.3197	-.2741	-.1209
1.20	.7608	.3406	-.3514	-.3187	-.0902
1.30	.7030	.4371	-.3514	-.3380	-.0581
1.40	.6461	.5171	-.3247	-.3349	-.0253
1.50	.5913	.5811	-.2771	-.3128	+.0078
1.60	.5395	.6304	-.2145	-.2758	.0408
1.70	.4911	.6665	-.1418	-.2272	.0736
1.80	.4464	.6912	-.0632	-.1705	.1058
1.90	.4055	.7060	-.0175	-.1083	.1375
2.00	.3676	.7125	.0978	-.0431	.1685
2.10	.3333	.7119	.1755	.0232	.1987
2.20	.3020	.7054	.2490	.0890	.2280
2.30	.2736	.6940	.3171	.1531	.2563
2.40	.2477	.6786	.3791	.2144	.2835
2.50	.2242	.6600	.4344	.2721	.3096
2.60	.2028	.6389	.4830	.3258	.3334
2.70	.1835	.6159	.5246	.3749	.3579

r (atomic units)	4f	5d	6s	6p	5f
2.80	.1659	.5914	.5595	.4192	.3799
2.90	.1499	.5659	.5878	.4587	.4005
3.00	.1354	.5397	.6098	.4931	.4195
3.10	.1223	.5132	.6260	.5226	.4369
3.20	.1103	.4866	.6367	.5474	.4527
3.30	.0995	.4603	.6424	.5675	.4669
3.40	.0897	.4343	.6436	.5832	.4794
3.50	.0808	.4088	.6407	.5946	.4903
3.60	.0728	.3840	.6342	.6022	.4996
3.70	.0655	.3599	.6245	.6062	.5072
3.80	.0589	.3367	.6121	.6068	.5133
3.90	.0529	.3145	.5974	.6044	.5178
4.00	.0476	.2932	.5807	.5992	.5209
4.25	.0363	.2442	.5328	.5764	.5226
4.50	.0276	.2016	.4796	.5427	.5166
4.75	.0209	.1651	.4249	.5018	.5038
5.00	.0158	.1341	.3712	.4570	.4857
5.25	.0119	.1083	.3204	.4107	.4632
5.50	.0089	.0868	.2737	.3648	.4376
5.75	.0066	.0693	.2316	.3207	.4099
6.00	.0050	.0550	.1943	.2794	.3809
6.25	.0037	.0434	.1618	.2415	.3514
6.50	.0027	.0341	.1338	.2071	.3220
6.75	.0020	.0267	.1100	.1765	.2933
7.00	.0015	.0209	.0900	.1494	.2656
7.25	.0011	.0162	.0732	.1259	.2392
7.50	.0008	.0126	.0592	.1054	.2145
7.75	.0006	.0097	.0477	.0879	.1914
8.00	.0004	.0075	.0383	.0730	.1700
8.25	.0003	.0057	.0306	.0604	.1505
8.50	.0002	.0044	.0244	.0497	.1326
8.75	.0002	.0034	.0194	.0408	.1165
9.00	.0001	.0026	.0153	.0334	.1020
9.25	.0001	.0020	.0121	.0272	.0890

r (atomic units)	4f	5d	6s	6p	5f
9.50	.0001	.0015	.0095	.0221	.0774
9.75	.0000	.0011	.0075	.0179	.0671
10.00	-	.0008	.0058	.0145	.0581
10.25	-	.0006	.0046	.0117	.0501
10.50	-	.0005	.0036	.0094	.0431
10.75	-	.0004	.0028	.0076	.0369
11.00	-	.0003	.0022	.0060	.0316
11.25	-	.0002	.0017	.0048	.0270
11.50	-	.0002	.0013	.0038	.0229
11.75	-	.0001	.0010	.0031	.0194
12.00	-	.0001	.0008	.0024	.0164
12.25	-	.0001	.0006	.0019	.0138
12.50	-	.0000	.0004	.0015	.0115
12.75	-	-	.0003	.0012	.0095
13.00	-	-	.0002	.0009	.0078
13.25	-	-	.0002	.0007	.0063
13.50	-	-	.0001	.0005	.0050

Table II. Radial Wave Functions, P(r), for Tm^{+3}

r (atomic units)	4f	5d	6s	6p	5f
.01	.0000	.0014	-.0639	.0183	.0000
.02	.0005	.0087	-.0459	.0505	-.0001
.03	.0024	.0235	-.0024	.0780	-.0003
.04	.0064	.0448	.0510	.0929	-.0009
.05	.0135	.0705	.0863	.0938	-.0019
.06	.0242	.0981	.1036	.0824	-.0033
.07	.0388	.1254	.1036	.0617	-.0054
.08	.0575	.1508	.0893	.0349	-.0079
.09	.0803	.1727	.0645	.0051	-.0111
.10	.1069	.1902	.0332	-.0252	-.0148
.11	.1372	.2027	-.0009	-.0538	-.0189
.12	.1707	.2099	-.0351	-.0793	-.0236
.13	.2070	.2119	-.0669	-.1006	-.0286
.14	.2456	.2087	-.0949	-.1171	-.0339
.15	.2863	.2008	-.1178	-.1286	-.0394
.16	.3284	.1886	-.1350	-.1351	-.0452
.17	.3716	.1726	-.1464	-.1367	-.0512
.18	.4155	.1533	-.1519	-.1338	-.0572
.19	.4597	.1313	-.1520	-.1269	-.0632
.20	.5039	.1070	-.1470	-.1164	-.0692
.21	.5478	.0811	-.1375	-.1030	-.0752
.22	.5910	.0540	-.1240	-.0870	-.0810
.23	.6334	.0261	-.1073	-.0692	-.0868
.24	.6748	-.0021	-.0880	-.0499	-.0924
.25	.7148	-.0303	-.0666	-.0296	-.0977
.26	.7533	-.0582	-.0439	-.0088	-.1029
.27	.7903	-.0854	-.0202	-.0122	-.1078
.28	.8256	-.1117	.0038	.0330	-.1125
.29	.8590	-.1369	.0278	.0532	-.1168

r (atomic units)	4f	5d	6s	6p	5f
.30	.8906	-.1609	.0513	.0728	-.1210
.31	.9203	-.1834	.0740	.0913	-.1248
.32	.9480	-.2043	.0957	.1087	-.1284
.33	.9738	-.2236	.1160	.1248	-.1316
.34	.9977	-.2413	.1348	.1395	-.1346
.35	1.020	-.2572	.1519	.1527	-.1372
.36	1.040	-.2713	.1672	.1644	-.1396
.37	1.058	-.2837	.1807	.1745	-.1418
.38	1.074	-.2943	.1923	.1830	-.1436
.39	1.089	-.3032	.2020	.1898	-.1452
.40	1.102	-.3104	.2097	.1952	-.1466
.41	1.113	-.3160	.2155	.1990	-.1477
.42	1.123	-.3200	.2195	.2013	-.1486
.43	1.132	-.3225	.2217	.2022	-.1492
.44	1.138	-.3234	.2221	.2017	-.1496
.45	1.144	-.3231	.2209	.2000	-.1499
.46	1.149	-.3213	.2181	.1970	-.1499
.47	1.152	-.3183	.2139	.1928	-.1498
.48	1.154	-.3141	.2082	.1876	-.1495
.49	1.156	-.3088	.2013	.1813	-.1490
.50	1.156	-.3025	.1932	.1742	-.1484
.52	1.154	-.2868	.1737	.1573	-.1468
.54	1.149	-.2678	.1507	.1377	-.1446
.56	1.141	-.2459	.1247	.1157	-.1420
.58	1.131	-.2215	.0965	.0920	-.1390
.60	1.119	-.1951	.0668	.0670	-.1356
.62	1.105	-.1670	.0360	.0411	-.1320
.64	1.090	-.1376	.0047	.0147	-.1281
.66	1.074	-.1072	-.0266	-.0119	-.1239
.68	1.057	-.0761	-.0577	-.0384	-.1196
.70	1.039	-.0445	-.0880	-.0644	-.1150

r (atomic units)	4f	5d	6s	6p	5f
.72	1.021	-.0127	-.1175	-.0899	-.1103
.74	1.002	.0192	-.1457	-.1146	-.1055
.76	.9829	.0511	-.1726	-.1384	-.1005
.78	.9634	.0826	-.1979	-.1611	-.0955
.80	.9437	.1139	-.2215	-.1826	-.0903
.82	.9238	.1446	-.2433	-.2028	-.0851
.84	.9010	.1748	-.2633	-.2218	-.0798
.86	.8841	.2043	-.2814	-.2394	-.0744
.88	.8644	.2331	-.2976	-.2555	-.0690
.90	.8447	.2611	-.3119	-.2703	-.0635
.92	.8252	.2884	-.3242	-.2836	-.0580
.94	.8059	.3147	-.3347	-.2954	-.0525
.96	.7868	.3402	-.3432	-.3059	-.0469
.98	.7679	.3648	-.3500	-.3150	-.0413
1.00	.7493	.3885	-.3549	-.3227	-.0357
1.10	.6607	.4932	-.3553	-.3417	-.0075
1.20	.5804	.5756	-.3213	-.3324	.0208
1.30	.5089	.6380	-.2620	-.3004	.0490
1.40	.4457	.6828	-.1855	-.2516	.0770
1.50	.3903	.7128	-.0989	-.1908	.1048
1.60	.3419	.7305	-.0076	-.1224	.1325
1.70	.2996	.7381	.0840	-.0497	.1600
1.80	.2628	.7373	.1729	.0246	.1872
1.90	.2306	.7298	.2567	.0983	.2140
2.00	.2025	.7168	.3339	.1696	.2404
2.10	.1779	.6994	.4034	.2375	.2663
2.20	.1564	.6787	.4648	.3008	.2915
2.30	.1375	.6552	.5176	.3590	.3159
2.40	.1210	.6298	.5620	.4117	.3394
2.50	.1064	.6029	.5982	.4584	.3619
2.60	.0936	.5750	.6266	.4993	.3832
2.70	.0824	.5466	.6476	.5342	.4032

r (atomic units)	4f	5d	6s	6p	5f
2.80	.0725	.5179	.6617	.5632	.4219
2.90	.0637	.4894	.6695	.5867	.4392
3.00	.0560	.4611	.6717	.6048	.4549
3.10	.0493	.4333	.6689	.6180	.4691
3.20	.0433	.4063	.6616	.6264	.4818
3.30	.0380	.3800	.6506	.6305	.4928
3.40	.0334	.3547	.6363	.6307	.5023
3.50	.0293	.3304	.6192	.6274	.5102
3.60	.0257	.3072	.6000	.6209	.5165
3.70	.0226	.2851	.5789	.6117	.5213
3.80	.0198	.2641	.5565	.6000	.5246
3.90	.0173	.2443	.5331	.5863	.5266
4.00	.0152	.2256	.5090	.5708	.5271
4.25	.0109	.1836	.4477	.5263	.5228
4.50	.0078	.1482	.3875	.4767	.5115
4.75	.0055	.1187	.3308	.4254	.4942
5.00	.0039	.0944	.2790	.3746	.4724
5.25	.0028	.0747	.2329	.3262	.4470
5.50	.0020	.0587	.1926	.2812	.4191
5.75	.0014	.0459	.1580	.2402	.3897
6.00	.0010	.0357	.1286	.2035	.3597
6.25	.0007	.0277	.1040	.1712	.3297
6.50	.0005	.0213	.0836	.1431	.3003
6.75	.0003	.0164	.0668	.1189	.2719
7.00	.0002	.0126	.0531	.0982	.2448
7.25	.0002	.0096	.0420	.0807	.2193
7.50	.0001	.0073	.0331	.0660	.1955
7.75	.0001	.0055	.0260	.0538	.1736
8.00	.0000	.0042	.0203	.0437	.1534
8.25	--	.0032	.0158	.0353	.1351
8.50	--	.0024	.0123	.0284	.1185
8.75	--	.0018	.0095	.0228	.1036

r (atomic units)	4f	5d	6s	6p	5f
9.00	--	.0013	.0074	.0183	.0903
9.25	--	.0010	.0057	.0146	.0784
9.50	--	.0007	.0044	.0116	.0679
9.75	--	.0006	.0033	.0092	.0586
10.00	--	.0004	.0026	.0073	.0505
10.25	--	.0003	.0019	.0058	.0434
10.50	--	.0002	.0015	.0046	.0371
10.75	--	.0002	.0011	.0036	.0317
11.00	--	.0001	.0008	.0028	.0270
11.25	--	.0001	.0006	.0022	.0230
11.50	--	.0001	.0005	.0017	.0194
11.75	--	.0000	.0004	.0013	.0164
12.00	--	--	.0003	.0010	.0138
12.25	--	--	.0002	.0008	.0116
12.50	--	--	.0002	.0006	.0096
12.75	--	--	.0001	.0005	.0079
13.00	--	--	.0001	.0004	.0065
13.25	--	--	.0001	.0003	.0052
13.50	--	--	.0000	.0002	.0041

TABLE III. ONE ELECTRON ENERGIES AND RADIAL INTEGRALS FOR EXCITED ORBITALS OF Pr^{+3} AND Tm^{+3}

(energies and integrals in atomic units)

	Pr^{+3}				$R^k(4f4f,4fn\ell)$			Tm^{+3}				$R^k(4f4f,4fn\ell)$		
	Energy	$\langle r^2 \rangle$	$\langle r^4 \rangle$	$\langle r^6 \rangle$	k=2	k=4	k=6	Energy	$\langle r^2 \rangle$	$\langle r^4 \rangle$	$\langle r^6 \rangle$	k=2	k=4	k=6
$4f^a$	-1.159	-	-	-	.406	.253	.181	-1.452	-	-	-	.573	.358	.257
4f	-1.174	1.44	5.17	37.4	.408	.255	.186	-1.483	.747	1.50	6.72	.576	.360	.259
5s	- .9822	6.65	70.2	-	-	-	-	-1.060	5.27	46.3	-	-	-	-
6s	- .8637	14.2	279.	-	-	-	-	- .9631	11.5	184.	-	-	-	-
6p	- .7352	17.6	429.	-	-.0258	-.0172	-	- .8104	14.4	289.	-	-.0140	-.0067	-
5f	- .4898	23.8	831.	39300	-.0592	-.0392	-.0224	- .5007	22.2	731.	33000	-.0547	-.0362	-.0263

[a] Entries in this row are those of Ridley.[1]

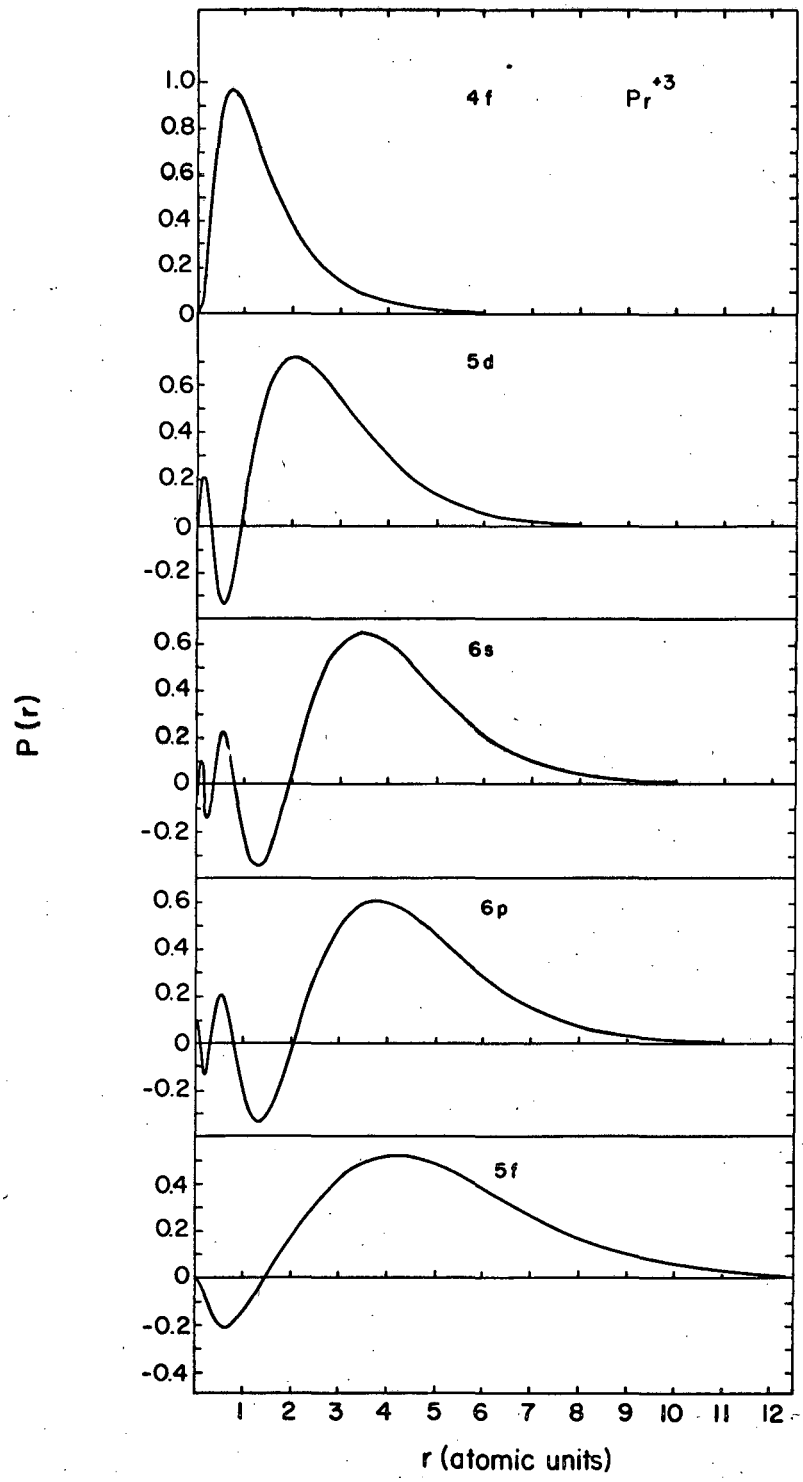

Fig. 1

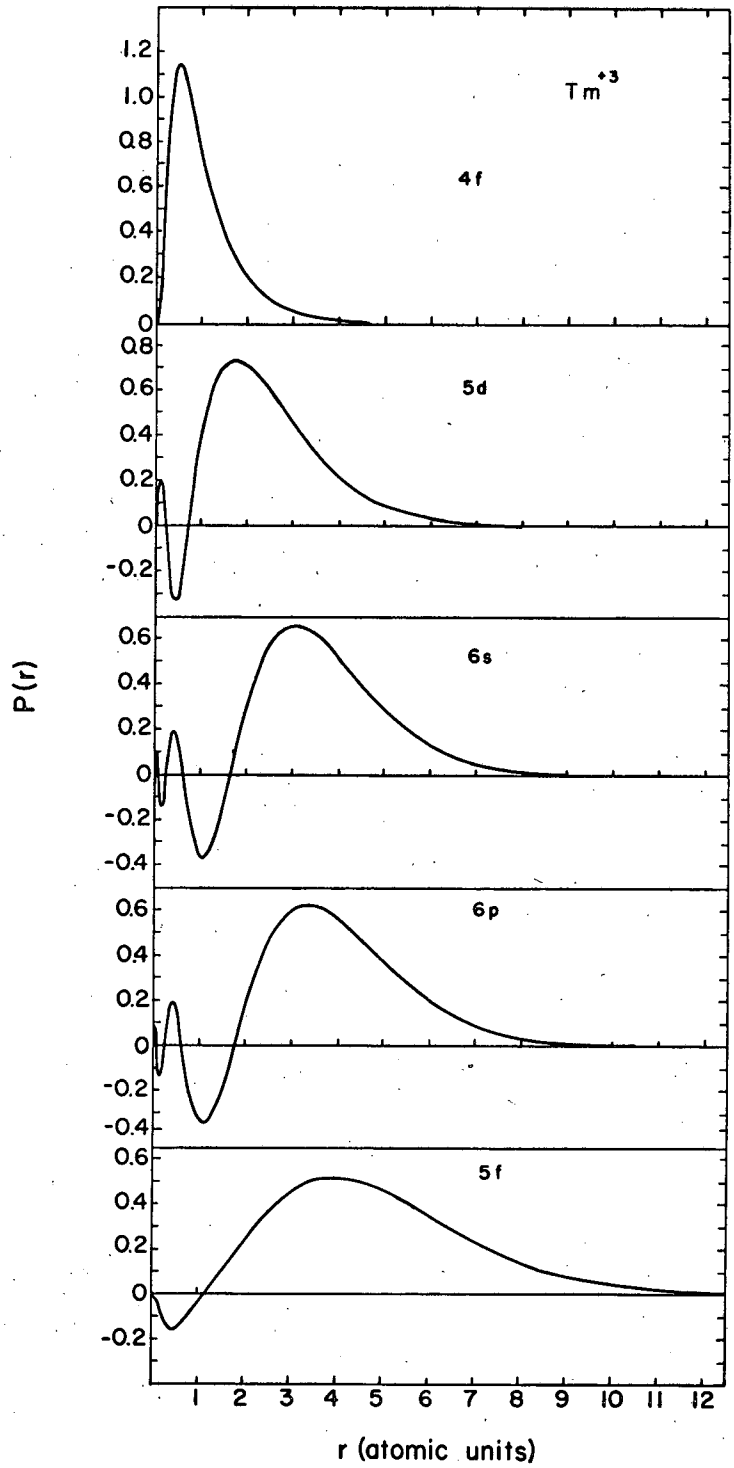

Fig. 2

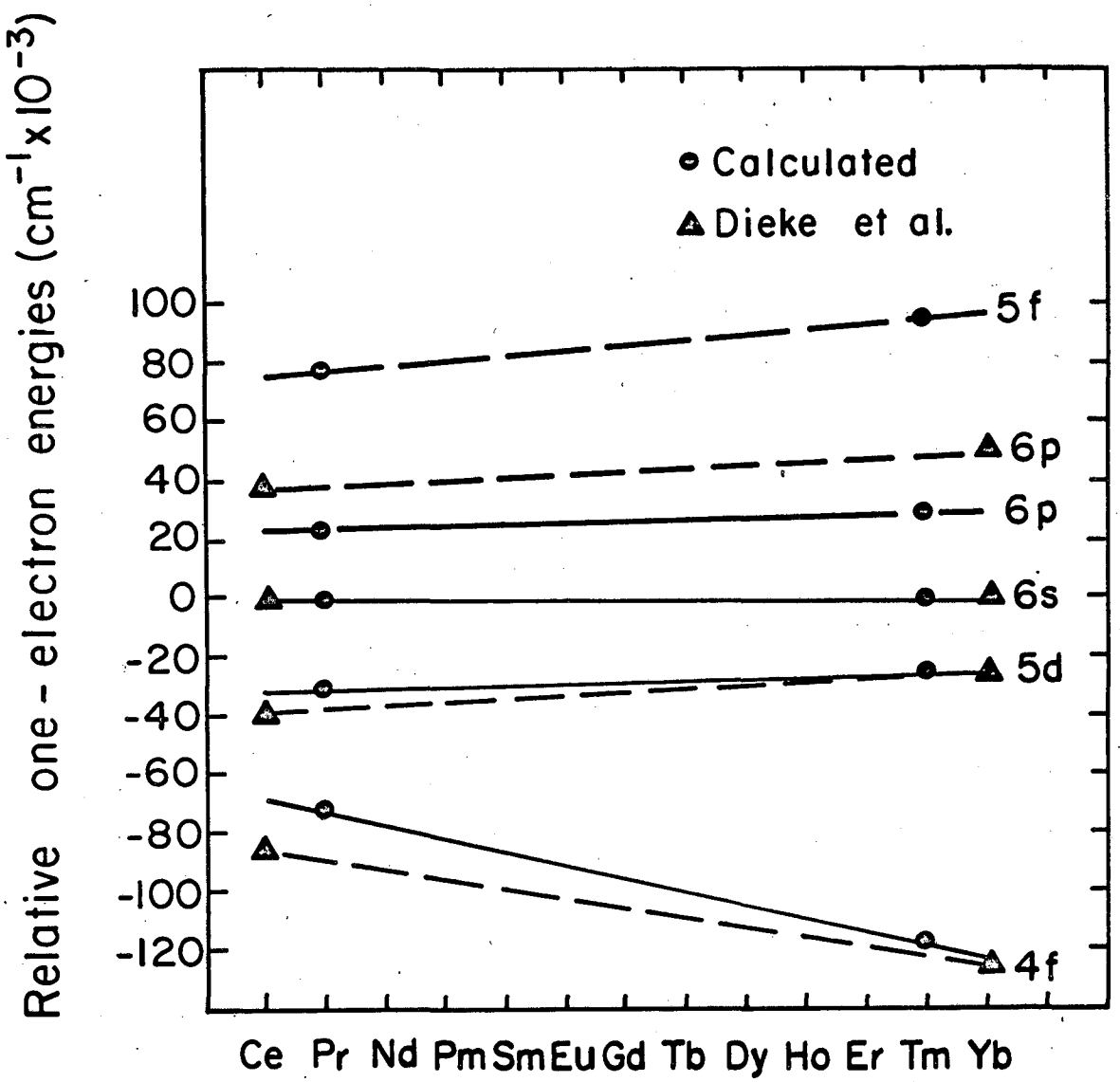

Fig. 3

MU-26544