ATOMIC WAVE FUNCTIONS FOR GOLD AND THALLIUM

By A. S. DOUGLAS, D. R. HARTREE and W. A. RUNCIMAN

Received 1 September 1954

1. *Introduction.* Before the war, self-consistent field calculations for the Au^+ ion had been carried out by W. Hartree but were left still unpublished at his death (see prefatory note in (5)). These results have been used by Brenner and Brown (1) in a relativistic calculation of the K-absorption edge for gold, and they were also used in obtaining initial estimates for the partial self-consistent field calculations for thallium of which results are given in §§3–5 of the present paper. In the meantime an independent calculation for Au^+ has been carried out by Henry (6), and his results agree closely with those of W. Hartree. However, it still seems desirable to publish the latter, since they give directly the radial wave function $P(nl; r)$ at exact values of r, whereas Henry used $\log r$ as independent variable, as had been done for similar calculations for Hg (4), and has tabulated $r^{\frac{1}{2}}P(nl; r)$ which is the natural dependent variable to use with $\log r$ as independent variable (2); in some applications it is more convenient to have the radial wave functions themselves.

The calculations for thallium were carried out in order to provide data for a refinement of the work of Williams (10) on the theory of luminescence of solids and its application to the luminescence of KCl activated by Tl. Williams used a Thomas-Fermi approximation to the field of the Tl^{+3} ion for calculating the radial wave functions for the valence electrons in the normal and first excited state of Tl^+, and obtained results in encouraging agreement with observation. Results of self-consistent field calculations for other atoms suggest that the Thomas–Fermi field may be rather inaccurate in the outer regions of an atom, and this may appreciably affect the wave functions for the valence electrons. It seemed worth while examining whether the quantitative agreement of Williams's theory with experiment would be improved by the use of wave functions for the Tl^+ ion derived from a self-consistent field calculation. It is hoped that the results for thallium may also be of value in other contexts.

Both for gold and for thallium the non-relativistic Schrödinger equation has been used. It is realized that relativistic effects are appreciable in atoms as heavy as these, but to include these would increase considerably the amount of calculation required; and in any case, if relativistic calculations were ever contemplated, it would probably be advisable to carry out a non-relativistic calculation first, to provide a good approximation to the field from which to start the relativistic calculation.

2. *Gold* (Au^+). In calculations for mercury (4), $\log r$ was used as independent variable and, correspondingly, $Pr^{-\frac{1}{2}}$ as dependent variable, partly because these variables had been used in earlier work (2) using a differential analyser for which they were convenient, and partly because this choice of independent variable reduces the number of changes of interval length required in the course of the integrations. It has

https://doi.org/10.1017/S0305004100030498 Published online by Cambridge University Press

also been used in some other work (8, 9). However, from the experience of the work for mercury, it was considered that for a hand calculation the advantage of a small number of changes of interval is more than offset by the disadvantage of not obtaining the radial wave functions $P(nl; r)$ directly, and by some minor inconveniences in the numerical work. So in the calculations for gold, a return was made to the use of r as independent variable.

The work was done for the Au^+ ion, with a configuration of complete groups up to and including $(5d)^{10}$. In the calculation of a self-consistent field without exchange, it is most convenient to start from estimates of 'contributions to Z' from the different (nl) groups; for a configuration of complete groups these are (see (3), § 5)

$$2(2l+1)[1-Z_0(nl, nl; r)] = 2(2l+1)\int_r^\infty P^2(nl; r)\,dr.$$

Initial estimates of these contributions to Z for Au^+ were made by a process of scaling from the corresponding results for mercury, and the process of successive approximation to the self-consistent field was continued until the greatest difference between estimated and calculated contributions to Z from any group was less than 0·02.

The radial wave functions $P(nl; r)$ are given in Table 1 and the contributions to Z in Table 2.

3. *Thallium* (Tl^{+3}). The results required for application in luminescence theory are for the normal and first excited states of Tl^+. It seemed likely that the contributions to Z from all groups up to and including $(5p)^6$ could be estimated closely enough from the corresponding results for gold and mercury, but unlikely that this could be done for $(5d)^{10}$. So calculations for Tl^{+3} were carried out first to obtain a good approximation to the contribution to Z from the $(5d)^{10}$ group, which would be a good first approximation to use in calculation for Tl^+. The results for mercury suggested that the perturbation of the $(5d)^{10}$ group by the electrons of the $(6s)^2$ group of Tl^+ would be small but not negligible.

The estimates of the contributions to Z were made by a modified scaling procedure as follows. Let R be some characteristic length defining the radial scale of the wave function $P(nl; r)$ (for example, the radius of the main maximum of $P(nl; r)$, or the radius for which $Z_0(nl, nl; r) = \frac{1}{2}$). If, for different atoms and given values of nl, the normalized radial wave functions $P(nl; r)$ can be derived from one another simply by a change of scale, then

$$R^{\frac{1}{2}}P(nl; r) \text{ is a function of } r/R \text{ only,} \tag{1}$$

independent of the atomic number N (the $R^{\frac{1}{2}}$ factor here arises from the condition that the functions $P(nl; r)$ are normalized). Let $P(N; nl; r)$ be written for the (nl) radial wave function for an atom of atomic number N, and similarly $Z_0(N; nl, nl; r)$ for the function $Z_0(nl, nl; r)$ for such an atom (for a particular atom or ion, N may be replaced by the chemical symbol for the element with, if necessary, an index indicating the degree of ionization). Then if the relation (1) holds, the wave functions and contributions for Z for two atoms of atomic number N_0 and N are related by

$$P(N; nl; r) = (R_0/R)^{\frac{1}{2}}P(N_0; nl; R_0 r/R) \tag{2}$$

and

$$Z_0(N; nl, nl; r) = Z_0(N_0; nl, nl; R_0 r/R). \tag{3}$$

https://doi.org/10.1017/S0305004100030498 Published online by Cambridge University Press

Further, if $R_{(H)}$ is the value of R for the (nl) wave function of the hydrogen atom, then in the Coulomb field of a point charge N'

$$R = R_{(H)}/N', \tag{4}$$

so that $N' = R_{(H)}/R$ can be considered as the 'effective nuclear charge' for R, and

$$\sigma = N - R_{(H)}/R$$

expresses the effect on the value of R, for the wave function considered, of the screening of the nucleus by the electrons in other occupied wave functions of the atom. It will of course depend on (nl), and will be written σ_{nl} when it is necessary to specify the values of (nl).

For each complete (nl) group this screening number σ_{nl} is likely to vary only slowly with the atomic number N, so that for atoms of neighbouring atomic numbers N_0 and N we have

$$R/R_0 = (N_0 - \sigma)/(N - \sigma),$$

so that (2) and (3) become

$$P(N; nl; r) = \left(\frac{N_0-\sigma}{N-\sigma}\right)^{\frac{1}{2}} P\left(N_0; nl; \frac{N_0-\sigma}{N-\sigma} r\right) \tag{5}$$

and

$$Z_0(N; nl, nl; r) = Z_0\left(N_0; nl, nl; \frac{N_0-\sigma}{N-\sigma} r\right). \tag{6}$$

For neighbouring values of N the scaling ratio $(N_0-\sigma)/(N-\sigma)$ is not sensitive to the value taken for σ.

For Tl^{+3} $(N = 81)$, formula (6) was used both with $N_0 = 79\,(Au^+)$ and with $N_0 = 80\,(Hg^{+2})$, with the following values of σ_{nl}:

(nl)	$1s$	$2s$	$2p$	$3s$	$3p$	$3d$	$4s$	$4p$	$4d$	$4f$	$5s$	$5p$
σ_{nl}	0·3	3·6	4·2	10·3	11·6	16·2	21	25	31	47	40	46

(7)

For the inner groups, up to $(4d)$, there were no systematic differences, to two decimals, between the values of $2(2l+1)\,[1 - Z_0(nl, nl; r)]$ for Tl^{+3} derived in this way from Au^+ and from Hg^{+2}, and the agreement between the values obtained from these two sources provided a valuable check. For the $(4f)^{14}$ to $(5p)^6$ groups there were systematic, though small, differences between the contributions to Z for Tl^{+3} estimated by this scaling procedure from Au^+ and Hg^{+2}; these differences indicate a departure from the similarity on which (6) is based, and enable estimates for Tl^{+3} to be made allowing for these departures from similarity. For the $(5d)^{10}$ group the difference between the results of applying formula (6) with $N_0 = 79$ and with $N_0 = 80$ were considerably larger than for the inner groups, and only rather rough estimates could be made of the contribution to Z from this group.

It is hoped that the estimates for the $(1s)^2$ to $(5p)^6$ groups, which are given in Table 3, are not in error by more than 0·03 for any (nl) group except perhaps for $(4f)^{14}$, and for this group the greatest uncertainty occurs in a range of r (0·3 to 0·6) where the total Z is large, and is not more than $\frac{1}{500}$ of the whole. These estimates were taken as given, and only the $(5d)$ wave function and the contribution of the $(5d)^{10}$ group to Z have been determined by further calculation.

As for Au^+ and Hg^{+2}, the $(5d)$ wave function is rather sensitive to the estimate of the field, and several steps of successive approximation were required in order to make

https://doi.org/10.1017/S0305004100030498 Published online by Cambridge University Press

it self-consistent. The greater part of the numerical work of this calculation was carried out on the EDSAC, the automatic digital calculating machine at the University Mathematical Laboratory, Cambridge. The final $(5d)$ wave function is given in Table 4, and contribution to Z from the $(5d)^{10}$ group is included in Table 3.

If further work on this ion is contemplated, attention should first be given to the $(4f)$ and $(5p)$ groups, for which the estimated contributions to Z in Table 3 are least certain (though the uncertainties are probably no greater than the exchange and relativistic effects which have been neglected).

Approximate wave functions $P(1s)$ to $P(5p)$ for Tl^+ were obtained by the scaling procedure expressed by formula (6), using the values (7) for the screening numbers σ_{nl}, and have been used to calculate the radial charge distribution (see §5); the normalized wave functions are tabulated in Table 5, as they may be useful in other applications also.

4. *Thallium* (Tl^+). For application to the theory of luminescence, wave functions are required for the $(6s)^2$ and $(6s)(6p)$ states of Tl^+. The EDSAC was used to obtain these, using the contributions to Z from the $(1s)^2$ to $(5d)^{10}$ groups for Tl^{+3} given in Table 3. From the results for Hg and Hg^{+2}, it is to be expected that for Tl^+ the $(5d)^{10}$ group will be slightly but appreciably perturbed by the addition of the valence electrons to the Tl^{+3} ion, but that the other groups of the Tl^{+3} core will not be appreciably affected. A further calculation was carried out to make the $(5d)^{10}$ and $(6s)^2$ groups of the normal state of Tl^+ self-consistent in the field of the $(1s)^2$ to $(5p)^6$ groups regarded as given; the contribution to Z from the $(5d)^{10}$ group obtained in this way was also used in a calculation for the $(6s)(6p)$ state. Radial wave functions are given in Table 4 and contributions to Z in Table 3. It will be seen that the perturbation of the $(5d)^{10}$ group by the $(6s)^2$ group is appreciable.

5. *Thallium. Charge distribution.* If $q(nl)$ is the number of electrons in the (nl) group, the radial charge distribution function $U(r)$ is

$$U(r) = \Sigma_{nl} q(nl)\, P^2(nl; r), \tag{8}$$

the radial wave functions $P(nl; r)$ being normalized. The radial charge distribution function $U(r)$ given by (8) was evaluated for Tl^{+3} and Tl^+ from these estimated wave functions for the inner groups given in Table 5 and from the $(5d)$, $(6d)$ and $(6p)$ wave functions given in Table 4. The results are given in Table 6.

The integral $\int_0^\infty r^2 U(r)\, dr$, which occurs both in the diamagnetic susceptibility and in Kirkwood's (7) approximate theory of the electrical polarizability, has the values (in atomic units):

	$\int_0^\infty r^2 U(r)\, dr$
Tl^{+3}	42·8
$Tl^+(6s)^2$	64·7
$(6s)(6p)$	69·6

The field of the core used in this work should be a considerable improvement on the Thomas–Fermi field, especially in the outer regions of the core which particularly

https://doi.org/10.1017/S0305004100030498 Published online by Cambridge University Press

affect the wave functions of the valence electrons. These wave functions, and hence the radial charge distributions, would be still further improved by the use of the relativistic equations, and by the inclusion of exchange and correlation effects at least among the outer electrons of the core and the wave functions of the valence electrons. Inclusion of exchange between the (6*s*) and the (6*p*) wave functions of the (6*s*) (6*p*) configuration would be interesting, as it would enable separate radial wave functions and charge distributions to be calculated for the ^3P and ^1P states, which are both of interest for the luminescence applications.

REFERENCES

(1) BRENNER, S. and BROWN, G. E. *Proc. roy. Soc.* A, 218 (1953), 422.
(2) HARTREE, D. R. *Phys. Rev.* (2), 46 (1934), 738.
(3) HARTREE, D. R. *Rep. Progr. Phys.* 11 (1948), 113.
(4) HARTREE, D. R. and HARTREE, W. *Proc. roy. Soc.* A, 149 (1935), 210.
(5) HARTREE, D. R. and HARTREE, W. *Proc. roy. Soc.* A, 193 (1948), 299.
(6) HENRY, W. G. *Proc. phys. Soc. Lond.* A, 67 (1954), 789.
(7) KIRKWOOD, J. G. *Phys. Z.* 33 (1932), 57.
(8) MANNING, M. F. and GOLDBERG, L. *Phys. Rev.* (2), 53 (1938), 662.
(9) MANNING, M. F. and MILLMAN, J. *Phys.* (2), 49 (1936), 848.
(10) WILLIAMS, F. E. *J. chem. Phys.* 19 (1951), 457.

UNIVERSITY MATHEMATICAL LABORATORY
CAMBRIDGE

CAVENDISH LABORATORY
CAMBRIDGE

G.E.C. RESEARCH LABORATORIES
WEMBLEY, MIDDLESEX†

† Present address: Atomic Energy Research Establishment, Harwell.

https://doi.org/10.1017/S0305004100030498 Published online by Cambridge University Press

Table 1. Au^+. *Radial wave functions* (*unnormalized*)

(nl)	$(1s)$	$(2s)$	$(2p)$	$(3s)$	$(3p)$	$(3d)$	$(4f)$
ϵ_{nl}	5405	898	865	209·8	193·6	164·3	7·69
$\int_0^\infty P^2 dr$	0·003296	0·03002	0·03919	0·1353	0·1576	0·1748	0·8287
r			Table of $P(nl;r)/r^{l+1}$				
0·000	80·00	80·00	2000	80·00	2000	10000	12000
0·001	73·92	73·87	1922	73·86	1922	9741	11765
0·002	68·31	68·10	1848	68·07	1848	9489	11536
0·003	63·13	62·69	1777	62·61	1776	9244	11312
0·004	58·34	57·58	1708	57·46	1707	9006	11094
0·005	53·91	52·79	1643	52·62	1641	8775	10881
r			Table of $P(nl;r)$				
0·000	0·000	0·000	0·000	0·000	0·000	0·000	—
0·001	0·074	0·074	0·002	0·074	0·002	0·000	—
0·002	0·137	0·136	0·007	0·136	0·007	0·000	—
0·003	0·189	0·188	0·016	0·188	0·016	0·000	—
0·004	0·233	0·230	0·027	0·230	0·027	0·000	—
0·005	0·270	0·264	0·041	0·263	0·041	0·001	—
0·006	0·299	0·290	0·057	0·288	0·057	0·002	—
0·007	0·322	0·308	0·074	0·306	0·074	0·003	—
0·008	0·341	0·321	0·094	0·318	0·093	0·004	—
0·009	0·354	0·328	0·114	0·323	0·113	0·006	—
0·010	0·364	0·329	0·135	0·324	0·134	0·008	—
0·015	0·368	0·277	0·251	0·264	0·247	0·023	—
0·020	0·332	0·163	0·368	0·141	0·357	0·048	—
0·025	0·280	0·023	0·475	−0·007	0·451	0·083	—
0·030	0·227	−0·120	0·565	−0·155	0·522	0·126	—
0·04	0·139	−0·369	0·689	−0·394	0·587	0·234	—
0·05	0·080	−0·537	0·741	−0·522	0·552	0·360	—
0·06	0·044	−0·624	0·736	−0·537	0·439	0·492	—
0·07	0·024	−0·647	0·692	−0·460	0·275	0·619	—
0·08	0·013	−0·625	0·627	−0·320	0·083	0·735	—
0·09	0·007	−0·575	0·551	−0·144	−0·115	0·834	—
0·10	0·004	−0·512	0·474	+0·045	−0·307	0·915	—
0·12	0·001	−0·376	0·332	0·404	−0·631	1·017	—
0·14	—	−0·258	0·222	0·679	−0·851	1·050	—
0·16	—	−0·169	0·143	0·850	−0·968	1·026	—
0·18	—	−0·108	0·090	0·926	−1·000	0·963	—
0·20	—	−0·067	0·056	0·929	−0·971	0·878	—
0·22	—	−0·041	0·034	0·881	−0·901	0·780	—
0·24	—	−0·024	0·020	0·802	−0·809	0·681	—
0·26	—	−0·014	0·012	0·708	−0·709	0·584	—
0·28	—	−0·008	0·007	0·611	−0·608	0·495	—
0·30	—	−0·005	0·004	0·517	−0·513	0·414	—
0·32	—	−0·003	0·002	0·431	−0·427	0·344	—
0·34	—	−0·002	0·001	0·354	−0·352	0·283	—
0·36	—	−0·001	0·001	0·288	−0·287	0·231	—
0·38	—	—	—	0·232	−0·232	0·188	—
0·40	—	—	—	0·185	−0·186	0·152	—
0·45	—	—	—	0·103	−0·105	0·088	—
0·50	—	—	—	0·056	−0·058	0·050	—
0·55	—	—	—	0·029	−0·031	0·028	—
0·60	—	—	—	0·015	−0·016	0·015	—
0·65	—	—	—	0·008	−0·009	0·008	—
0·70	—	—	—	0·004	−0·004	0·004	—
0·8	—	—	—	0·001	−0·001	0·001	—

https://doi.org/10.1017/S0305004100030498 Published online by Cambridge University Press

Table 1 (cont.). Au^+. *Radial wave functions (unnormalized)*

(nl)	$(4s)$	$(4p)$	$(4d)$	$(4f)$	$(5s)$	$(5p)$	$(5d)$
ϵ_{nl}	44·24	37·32	24·60	7·69	6·89	4·635	1·171
$\int_0^\infty P^2 dr$	0·5508	0·6561	0·6889	0·8287	2·825	3·925	8·65
r			Table of $P(nl;r)$				
0·000	0·000	0·000	0·000	0·000	0·000	0·000	0·000
0·005	0·263	0·041	0·001	0·000	0·263	0·041	0·001
0·010	0·323	0·134	0·008	0·000	0·322	0·134	0·008
0·015	0·261	0·245	0·023	0·000	0·260	0·245	0·023
0·020	0·136	0·354	0·048	0·001	0·134	0·353	0·048
0·025	−0·014	0·445	0·082	0·003	−0·016	0·444	0·082
0·030	−0·162	0·512	0·125	0·006	−0·165	0·510	0·125
0·04	−0·399	0·564	0·230	0·015	−0·401	0·559	0·230
0·05	−0·516	0·511	0·350	0·030	−0·516	0·504	0·348
0·06	−0·514	0·379	0·470	0·053	−0·510	0·368	0·467
0·07	−0·416	0·197	0·580	0·083	−0·405	0·183	0·575
0·08	−0·254	−0·008	0·672	0·120	−0·239	−0·024	0·663
0·09	−0·060	−0·212	0·740	0·165	−0·041	−0·229	0·727
0·10	0·142	−0·400	0·782	0·215	+0·162	−0·415	0·764
0·12	0·493	−0·681	0·785	0·329	0·509	−0·685	0·754
0·14	0·710	−0·809	0·692	0·456	0·711	−0·795	0·646
0·16	0·774	−0·792	0·526	0·587	0·750	−0·751	0·465
0·18	0·702	−0·658	0·312	0·716	0·647	−0·588	0·237
0·20	0·528	−0·442	0·073	0·838	0·441	−0·345	−0·011
0·22	0·292	−0·182	−0·171	0·948	0·177	−0·063	−0·259
0·24	0·026	+0·095	−0·406	1·045	−0·108	+0·226	−0·490
0·26	−0·242	0·365	−0·621	1·126	−0·383	0·497	−0·694
0·28	−0·495	0·614	−0·810	1·193	−0·627	0·732	−0·863
0·30	−0·719	0·831	−0·970	1·244	−0·826	0·920	−0·993
0·32	−0·907	1·012	−1·100	1·281	−0·972	1·058	−1·085
0·34	−1·057	1·155	−1·200	1·305	−1·063	1·143	−1·138
0·36	−1·169	1·262	−1·272	1·319	−1·102	1·179	−1·157
0·38	−1·247	1·336	−1·321	1·322	−1·092	1·169	−1·144
0·40	−1·293	1·380	−1·348	1·316	−1·040	1·119	−1·102
0·45	−1·300	1·386	−1·340	1·273	−0·764	0·856	−0·901
0·50	−1·204	1·291	−1·259	1·203	−0·358	0·464	−0·603
0·55	−1·055	1·145	−1·139	1·116	+0·096	0·017	−0·253
0·60	−0·891	0·981	−1·002	1·023	0·543	−0·434	+0·114
0·65	−0·731	0·819	−0·863	0·927	0·945	−0·853	0·476
0·70	−0·587	0·670	−0·732	0·834	1·283	−1·220	0·817
0·8	−0·361	0·429	−0·508	0·662	1·746	−1·767	1·400
0·9	−0·212	0·264	−0·340	0·515	1·951	−2·069	1·836
1·0	−0·121	0·157	−0·222	0·396	1·961	−2·174	2·132
1·1	−0·067	0·092	−0·143	0·301	1·847	−2·139	2·310
1·2	−0·037	0·053	−0·091	0·228	1·667	−2·015	2·398
1·3	−0·020	0·030	−0·057	0·172	1·459	−1·842	2·419
1·4	−0·011	0·017	−0·036	0·130	1·250	−1·648	2·392
1·5	−0·006	0·010	−0·022	0·098	1·053	−1·450	2·333
1·6	−0·003	0·006	−0·014	0·074	0·876	−1·262	2·252
1·8	−0·001	0·002	−0·005	0·042	0·589	−0·931	2·055
2·0	—	0·001	−0·002	0·024	0·386	−0·670	1·841
2·2	—	—	−0·001	0·014	0·249	−0·475	1·632
2·4	—	—	—	0·008	0·159	−0·333	1·435
2·6	—	—	—	0·005	0·101	−0·231	1·256
2·8	—	—	—	0·003	0·063	−0·160	1·096

https://doi.org/10.1017/S0305004100030498 Published online by Cambridge University Press

Table 1 (*cont.*). Au^+. *Radial wave functions* (*unnormalized*)

(nl)	$(4s)$	$(4p)$	$(4d)$	$(4f)$	$(5s)$	$(5p)$	$(5d)$
r			Table of $P(nl; r)$				
3·0	—	—	—	0·002	0·039	−0·110	0·951
3·2	—	—	—	0·001	0·025	−0·075	0·824
3·4	—	—	—	—	0·015	−0·051	0·713
3·6	—	—	—	—	0·009	−0·035	0·615
3·8	—	—	—	—	0·006	−0·024	0·529
4·0	—	—	—	—	0·004	−0·016	0·455
4·5	—	—	—	—	0·001	−0·006	0·309
5·0	—	—	—	—	—	−0·002	0·208
5·5	—	—	—	—	—	−0·001	0·138
6·0	—	—	—	—	—	—	0·091
6·5	—	—	—	—	—	—	0·060
7·0	—	—	—	—	—	—	0·039
8	—	—	—	—	—	—	0·016
9	—	—	—	—	—	—	0·007
10	—	—	—	—	—	—	0·003
11	—	—	—	—	—	—	0·001

Table 2. Au^+. *Contributions to Z. Table of* $2(2l+1)[1-Z_0(nl, nl; r)]$

r	$(1s)$	$(2s)$	$(2p)$	$(3s)$	$(3p)$	$(3d)$
0·000	2·00	2·00	6·00	2·00	6·00	10·00
0·002	1·99	2·00	6·00	2·00	6·00	10·00
0·004	1·95	1·99	6·00	2·00	6·00	10·00
0·006	1·86	1·98	6·00	2·00	6·00	10·00
0·008	1·73	1·97	6·00	1·99	6·00	10·00
0·010	1·58	1·96	5·99	1·99	6·00	10·00
0·015	1·16	1·93	5·96	1·98	5·99	10·00
0·020	0·79	1·91	5·89	1·98	5·97	10·00
0·025	0·50	1·90	5·75	1·98	5·94	10·00
0·030	0·30	1·90	5·54	1·98	5·89	9·99
0·04	0·10	1·86	4·93	1·97	5·77	9·98
0·05	0·03	1·71	4·13	1·93	5·65	9·93
0·06	0·01	1·48	3·29	1·89	5·55	9·82
0·07	—	1·21	2·50	1·85	5·51	9·64
0·08	—	0·94	1·83	1·83	5·49	9·38
0·09	—	0·70	1·30	1·82	5·49	9·03
0·10	—	0·50	0·90	1·82	5·47	8·59
0·12	—	0·24	0·40	1·80	5·29	7·50
0·14	—	0·10	0·17	1·71	4·86	6·27
0·16	—	0·04	0·07	1·54	4·22	5·03
0·18	—	0·02	0·03	1·30	3·47	3·89
0·20	—	0·01	0·01	1·04	2·73	2·92
0·22	—	—	—	0·80	2·06	2·13
0·24	—	—	—	0·59	1·50	1·52
0·26	—	—	—	0·42	1·06	1·06
0·28	—	—	—	0·29	0·73	0·73
0·30	—	—	—	0·19	0·49	0·49
0·32	—	—	—	0·13	0·33	0·33
0·34	—	—	—	0·09	0·22	0·22
0·36	—	—	—	0·05	0·14	0·14
0·38	—	—	—	0·03	0·09	0·09
0·40	—	—	—	0·02	0·06	0·06
0·45	—	—	—	—	0·02	0·02

https://doi.org/10.1017/S0305004100030498 Published online by Cambridge University Press

Table 2 (cont.). Au^+. *Contributions to Z.*

r	(4s)	(4p)	(4d)	(4f)	(5s)	(5p)	(5d)
0·00	2·00	6·00	10·00	14·00	2·00	6·00	10·00
0·02	2·00	5·99	10·00	14·00	2·00	6·00	10·00
0·04	1·99	5·95	9·99	14·00	2·00	5·99	10·00
0·06	1·97	5·90	9·96	14·00	2·00	5·99	10·00
0·08	1·96	5·89	9·86	14·00	1·99	5·98	9·99
0·10	1·96	5·88	9·70	13·99	1·99	5·98	9·98
0·12	1·95	5·83	9·52	13·96	1·99	5·97	9·96
0·14	1·92	5·72	9·36	13·91	1·99	5·96	9·95
0·16	1·88	5·60	9·25	13·82	1·98	5·94	9·94
0·18	1·84	5·50	9·20	13·67	1·97	5·92	9·94
0·20	1·81	5·44	9·18	13·47	1·97	5·92	9·94
0·22	1·80	5·42	9·18	13·20	1·96	5·91	9·94
0·24	1·80	5·42	9·16	12·86	1·96	5·91	9·94
0·26	1·80	5·41	9·08	12·46	1·96	5·91	9·93
0·28	1·79	5·37	8·93	12·01	1·96	5·90	9·91
0·30	1·76	5·27	8·70	11·51	1·95	5·88	9·89
0·32	1·71	5·11	8·38	10·97	1·94	5·85	9·87
0·34	1·64	4·90	8·00	10·40	1·93	5·81	9·84
0·36	1·55	4·63	7·55	9·82	1·91	5·76	9·81
0·38	1·44	4·32	7·06	9·23	1·89	5·72	9·78
0·40	1·33	3·98	6·54	8·64	1·88	5·68	9·75
0·45	1·01	3·09	5·22	7·22	1·85	5·61	9·69
0·50	0·73	2·27	3·98	5·92	1·83	5·57	9·66
0·55	0·49	1·58	2·93	4·78	1·83	5·56	9·65
0·60	0·32	1·06	2·10	3·81	1·83	5·56	9·65
0·65	0·20	0·69	1·46	3·01	1·81	5·53	9·64
0·70	0·12	0·44	1·00	2·35	1·76	5·45	9·61
0·8	0·05	0·17	0·45	1·41	1·59	5·09	9·47
0·9	0·02	0·06	0·19	0·83	1·35	4·52	9·16
1·0	0·01	0·02	0·08	0·48	1·08	3·82	8·70
1·1	—	—	0·03	0·27	0·82	3·10	8·12
1·2	—	—	0·01	0·15	0·60	2·44	7·48
1·3	—	—	—	0·09	0·42	1·87	6·80
1·4	—	—	—	0·05	0·29	1·41	6·13
1·5	—	—	—	0·03	0·20	1·04	5·49
1·6	—	—	—	0·02	0·13	0·75	4·88
1·8	—	—	—	—	0·06	0·39	3·80
2·0	—	—	—	—	0·02	0·20	2·92
2·2	—	—	—	—	0·01	0·10	2·23
2·4	—	—	—	—	—	0·04	1·68
2·6	—	—	—	—	—	0·02	1·26
2·8	—	—	—	—	—	0·01	0·94
3·0	—	—	—	—	—	—	0·70
3·2	—	—	—	—	—	—	0·52
3·4	—	—	—	—	—	—	0·38
3·6	—	—	—	—	—	—	0·28
3·8	—	—	—	—	—	—	0·21
4·0	—	—	—	—	—	—	0·15
4·5	—	—	—	—	—	—	0·07
5·0	—	—	—	—	—	—	0·03
5·5	—	—	—	—	—	—	0·01

https://doi.org/10.1017/S0305004100030498 Published online by Cambridge University Press

Table 3. *Contributions to Z for* Tl^{+3} *and* Tl^{+}

r	$1s$	$2s$	$2p$	$3s$	$3p$	$3d$
0·000	2·00	2·00	6·00	2·00	6·00	10·00
0·001	2·00	2·00	6·00	2·00	6·00	10·00
0·002	1·99	2·00	6·00	2·00	6·00	10·00
0·003	$1·97_5$	$1·99_5$	6·00	2·00	6·00	10·00
0·004	$1·94_5$	$1·99_5$	6·00	2·00	6·00	10·00
0·005	1·90	1·99	6·00	$1·99_5$	6·00	10·00
0·006	1·85	$1·98_5$	6·00	$1·99_5$	6·00	10·00
0·007	1·79	1·98	6·00	$1·99_5$	6·00	10·00
0·008	1·72	1·97	$5·99_5$	$1·99_5$	6·00	10·00
0·009	1·64	1·96	$5·99_5$	$1·99_5$	6·00	10·00
0·010	1·56	$1·95_5$	5·99	1·99	6·00	10·00
0·015	1·13	$1·92_5$	5·96	$1·98_5$	5·99	10·00
0·020	$0·75_5$	1·91	$5·87_5$	1·98	5·97	10·00
0·025	0·47	$1·90_5$	$5·72_5$	1·98	$5·93_5$	10·00
0·030	0·28	1·90	5·50	1·98	$5·88_5$	$9·99_5$
0·035	0·16	1·88	5·20	$1·97_5$	$5·82_5$	$9·98_5$
0·040	$0·09_5$	$1·84_5$	$4·84_5$	$1·96_5$	5·76	9·97
0·05	$0·02_5$	$1·68_5$	$4·01_5$	$1·92_5$	5·63	9·91
0·06	0·01	1·44	3·15	$1·88_5$	5·54	9·79
0·07	—	$1·15_5$	$2·36_5$	1·85	5·50	$9·58_5$
0·08	—	$0·88_5$	1·70	$1·82_5$	5·49	$9·29_5$
0·09	—	$0·64_5$	1·19	1·82	$5·48_5$	8·91
0·10	—	$0·45_5$	0·81	1·82	$5·45_5$	8·44
0·11	—	$0·30_5$	0·54	$1·81_5$	$5·37_5$	$7·88_5$
0·12	—	$0·19_5$	$0·35_5$	$1·79_5$	$5·23_5$	$7·27_5$
0·14	—	0·09	0·14	$1·68_5$	$4·73_5$	5·99
0·16	—	$0·03_5$	$0·05_5$	$1·48_5$	$4·04_5$	$4·72_5$
0·18	—	$0·01_5$	0·02	1·23	3·27	3·60
0·20	—	$0·00_5$	0·01	0·97	2·52	2·65
0·22	—	—	—	0·73	$1·86_5$	1·90
0·24	—	—	—	$0·52_5$	1·33	$1·32_5$
0·26	—	—	—	$0·36_5$	0·92	$0·91_5$
0·28	—	—	—	0·25	0·62	$0·61_5$
0·30	—	—	—	0·16	$0·41_5$	0·41
0·32	—	—	—	$0·10_5$	$0·27_5$	0·27
0·34	—	—	—	0·07	$0·17_5$	$0·17_5$
0·36	—	—	—	0·04	0·11	0·11
0·38	—	—	—	$0·02_5$	$0·07_5$	$0·07_5$
0·40	—	—	—	$0·01_5$	$0·04_5$	$0·04_5$
0·45	—	—	—	—	0·01	$0·01_5$
0·50	—	—	—	—	—	$0·00_5$

https://doi.org/10.1017/S0305004100030498 Published online by Cambridge University Press

Table 3 (cont.). *Contributions to Z for* Tl^{+3} *and* Tl^{+}

r	$4s$	$4p$	$4d$	$4f$	$5s$	$5p$
0·00	2·00	6·00	10·00	14·00	2·00	6·00
0·02	$1·99_5$	$5·99_5$	10·00	14·00	2·00	6·00
0·04	1·99	$5·94_5$	9·99	14·00	2·00	5·99
0·06	$1·97_5$	5·90	9·95	14·00	$1·99_5$	$5·98_5$
0·08	1·96	$5·89_5$	9·84	$13·99_5$	$1·99_5$	$5·98_5$
0·10	1·96	$5·87_5$	$9·66_5$	13·98	1·99	5·98
0·12	1·95	$5·80_5$	9·48	13·95	1·99	$5·96_5$
0·14	$1·91_5$	5·69	9·32	13·88	1·98	$5·94_5$
0·16	1·87	5·57	$9·22_5$	13·76	$1·97_5$	$5·92_5$
0·18	1·83	5·48	$9·18_5$	13·59	$1·96_5$	$5·91_5$
0·20	$1·80_5$	$5·43_5$	9·18	13·33	$1·96_5$	5·91
0·22	1·80	5·42	9·17	13·00	$1·96_5$	5·91
0·24	1·80	5·42	9·12	12·60	$1·96_5$	5·91
0·26	$1·79_5$	$5·39_5$	$9·00_5$	12·13	1·96	5·90
0·28	$1·77_5$	$5·32_5$	8·80	11·61	$1·95_5$	$5·87_5$
0·30	$1·73_5$	$5·19_5$	8·51	11·04	$1·94_5$	$5·84_5$
0·32	$1·67_5$	5·00	8·14	10·43	1·93	5·81
0·34	$1·59_5$	4·74	7·69	9·79	$1·91_5$	$5·76_5$
0·36	$1·49_5$	$4·43_5$	$7·19_5$	$9·16_5$	1·89	5·72
0·38	1·37	4·09	$6·66_5$	8·53	$1·87_5$	$5·67_5$
0·40	1·24	$3·72_5$	6·11	7·91	1·86	$5·63_5$
0·45	0·92	$2·81_5$	$4·74_5$	6·43	$1·83_5$	5·57
0·50	0·64	2·00	$3·52_5$	5·14	1·83	5·54
0·55	0·42	1·35	$2·52_5$	4·02	1·83	5·54
0·60	$0·26_5$	$0·88_5$	$1·75_5$	3·11	$1·81_5$	5·52
0·65	$0·16_5$	$0·56_5$	$1·19_5$	2·40	1·78	5·45
0·70	$0·09_5$	$0·34_5$	$0·79_5$	1·82	$1·71_5$	5·32
0·75	$0·05_5$	$0·20_5$	0·52	1·37	1·62	5·11
0·80	$0·03_5$	$0·12_5$	$0·33_5$	1·02	$1·50_5$	4·84
0·9	0·01	0·04	$0·13_5$	0·56	1·23	4·15
1·0	$0·00_5$	$0·01_5$	$0·05_5$	0·31	$0·93_5$	3·38
1·1	—	$0·00_5$	0·02	0·16	$0·68_5$	2·65
1·2	—	—	0·01	0·08	0·48	1·99
1·3	—	—	$0·00_5$	0·04	0·33	1·47
1·4	—	—	—	0·02	0·22	1·05
1·5	—	—	—	0·01	$0·14_5$	0·75
1·6	—	—	—	$0·00_5$	$0·09_5$	0·53
1·8	—	—	—	—	$0·03_5$	$0·26_5$
2·0	—	—	—	—	$0·01_5$	0·12
2·2	—	—	—	—	$0·00_5$	$0·05_5$
2·4	—	—	—	—	—	$0·02_5$
2·6	—	—	—	—	—	0·01
2·8	—	—	—	—	—	$0·00_5$

https://doi.org/10.1017/S0305004100030498 Published online by Cambridge University Press

Table 3 (cont.). *Contributions to Z for* Tl^{+3} *and* Tl^+

	Tl^{+3}	Tl^+	Tl^+ (ground state)	Tl^+ (excited state)	
r	$5d$	$5d$	$6s$	$6s$	$6p$
0·00	10·00	10·00	2·00	1·00	1·00
0·02	10·00	10·00	2·00	1·00	1·00
0·04	10·00	10·00	2·00	1·00	1·00
0·06	10·00	10·00	2·00	1·00	1·00
0·08	$9·98_5$	$9·98_5$	2·00	1·00	1·00
0·10	9·97	9·97	2·00	1·00	1·00
0·12	9·95	9·95	2·00	1·00	1·00
0·14	$9·93_5$	$9·93_5$	2·00	1·00	1·00
0·16	$9·92_5$	$9·92_5$	2·00	1·00	1·00
0·18	$9·92_5$	$9·92_5$	2·00	1·00	1·00
0·20	$9·92_5$	$9·92_5$	2·00	1·00	1·00
0·22	9·92	9·92	2·00	1·00	1·00
0·24	$9·91_5$	$9·91_5$	2·00	1·00	1·00
0·26	9·90	9·90	2·00	1·00	1·00
0·28	$9·87_5$	$9·87_5$	2·00	1·00	1·00
0·30	$9·84_5$	$9·84_5$	2·00	1·00	1·00
0·32	$9·80_5$	$9·80_5$	$1·99_5$	1·00	1·00
0·34	$9·76_5$	$9·76_5$	$1·99_5$	1·00	1·00
0·36	9·72	$9·72_5$	$1·99_5$	1·00	1·00
0·38	9·68	$9·68_5$	$1·99_5$	1·00	1·00
0·40	9·64	$9·64_5$	$1·99_5$	$0·99_5$	1·00
0·45	$9·57_5$	9·58	1·99	$0·99_5$	$0·99_5$
0·50	9·54	9·55	1·99	$0·99_5$	$0·99_5$
0·55	$9·53_5$	9·54	1·99	$0·99_5$	$0·99_5$
0·60	9·53	9·54	1·99	$0·99_5$	$0·99_5$
0·65	9·51	$9·51_5$	$1·98_5$	$0·99_5$	$0·99_5$
0·70	$9·44_5$	$9·45_5$	1·98	0·99	$0·99_5$
0·75	9·33	9·34	$1·97_5$	$0·98_5$	$0·99_5$
0·80	$9·15_5$	9·17	$1·96_5$	0·98	0·99
0·9	$8·63_5$	$8·66_5$	1·95	$0·97_5$	$0·98_5$
1·0	7·93	$7·97_5$	1·94	$0·96_5$	0·98
1·1	7·12	$7·18_5$	1·93	$0·96_5$	$0·97_5$
1·2	$6·26_5$	6·35	1·93	0·96	$0·97_5$
1·3	5·43	5·53	1·93	0·96	0·97
1·4	4·64	$4·75_5$	1·93	0·96	0·97
1·5	$3·92_5$	$4·04_5$	1·92	$0·95_5$	0·97
1·6	$3·28_5$	$3·41_5$	1·90	$0·94_5$	0·97
1·8	$2·25_5$	2·39	$1·83_5$	0·91	0·96
2·0	$1·50_5$	1·64	1·73	$0·85_5$	0·94
2·2	0·99	1·11	1·59	0·78	$0·90_5$
2·4	$0·63_5$	0·74	1·43	$0·69_5$	0·86
2·6	$0·40_5$	$0·49_5$	1·26	0·61	$0·80_5$
2·8	$0·25_5$	$0·32_5$	1·09	0·52	$0·74_5$
3·0	$0·15_5$	$0·21_5$	0·93	0·44	0·68
3·2	$0·09_5$	0·14	0·78	$0·36_5$	$0·61_5$
3·4	0·06	0·09	$0·64_5$	0·30	$0·54_5$
3·6	$0·03_5$	0·06	0·53	0·24	$0·48_5$
3·8	0·02	$0·03_5$	$0·42_5$	$0·19_5$	$0·42_5$
4·0	0·01	$0·02_5$	0·34	$0·15_5$	$0·36_5$
4·5	—	0·01	0·19	0·08	0·25
5·0	—	$0·00_5$	0·10	0·04	0·16
5·5	—	—	0·05	0·02	0·10
6·0	—	—	$0·02_5$	0·01	0·06
6·5	—	—	$0·01_5$	$0·00_5$	$0·03_5$
7·0	—	—	$0·00_5$	—	0·02
7·5	—	—	$0·00_5$	—	0·01
8·0	—	—	—	—	$0·00_5$
8·5	—	—	—	—	$0·00_5$

https://doi.org/10.1017/S0305004100030498 Published online by Cambridge University Press

Table 4. *Normalized radial wave functions* $P_N(nl; r)$ *for* Tl^{+3} *and* Tl^+

	Tl^{+3}	Tl^+	Tl^+ (ground state)	Tl^+ (excited state)	
r	$5d$	$5d$	$6s$	$6s$	$6p$
0·000	0·000	0·000	0·000	0·000	0·000
0·001	0·000	0·000	0·013	0·014	0·001
0·002	0·000	0·000	0·024	0·025	0·002
0·003	0·000	0·000	0·034	0·035	0·003
0·004	0·000	0·000	0·041	0·043	0·004
0·005	0·001	0·000	0·047	0·048	0·006
0·006	0·001	0·001	0·051	0·053	0·008
0·007	0·001	0·001	0·054	0·056	0·010
0·008	0·002	0·002	0·056	0·057	0·013
0·009	0·003	0·002	0·057	0·058	0·016
0·010	0·003	0·003	0·056	0·058	0·018
0·015	0·010	0·010	0·046	0·047	0·032
0·020	0·021	0·020	0·022	0·022	0·047
0·025	0·036	0·035	−0·005	−0·005	0·059
0·030	0·054	0·053	−0·032	−0·033	0·067
0·035	0·075	0·074	−0·054	−0·056	0·071
0·040	0·098	0·097	−0·072	−0·074	0·072
0·05	0·148	0·146	−0·090	−0·093	0·063
0·06	0·197	0·194	−0·087	−0·090	0·044
0·07	0·240	0·237	−0·066	−0·068	0·018
0·08	0·275	0·271	−0·034	−0·036	−0·010
0·09	0·298	0·295	0·001	0·001	−0·037
0·10	0·310	0·306	0·037	0·038	−0·060
0·11	0·309	0·306	0·069	0·071	−0·079
0·12	0·298	0·294	0·095	0·098	−0·093
0·14	0·245	0·242	0·126	0·130	−0·102
0·16	0·163	0·161	0·126	0·130	−0·092
0·18	0·064	0·064	0·102	0·106	−0·066
0·20	−0·041	−0·040	0·062	0·064	−0·032
0·22	−0·142	−0·140	0·013	0·014	0·007
0·24	−0·235	−0·231	−0·038	−0·040	0·045
0·26	−0·313	−0·309	−0·086	−0·088	0·079
0·28	−0·375	−0·371	−0·126	−0·130	0·107
0·30	−0·421	−0·416	−0·156	−0·161	0·129
0·32	−0·449	−0·444	−0·176	−0·182	0·143
0·34	−0·461	−0·456	−0·185	−0·190	0·149
0·36	−0·459	−0·454	−0·185	−0·191	0·149
0·38	−0·444	−0·439	−0·177	−0·182	0·142
0·40	−0·417	−0·413	−0·162	−0·166	0·131
0·45	−0·314	−0·311	−0·098	−0·101	0·085
0·50	−0·175	−0·174	−0·016	−0·017	0·026
0·55	−0·020	−0·021	0·068	0·070	−0·037
0·60	0·136	0·133	0·145	0·150	−0·096
0·65	0·285	0·280	0·208	0·215	−0·148
0·70	0·420	0·414	0·254	0·262	−0·188
0·75	0·538	0·531	0·282	0·290	−0·217
0·80	0·640	0·631	0·293	0·302	−0·236
0·9	0·790	0·780	0·274	0·282	−0·243
1·0	0·878	0·868	0·212	0·218	−0·218
1·1	0·918	0·908	0·126	0·129	−0·172
1·2	0·923	0·914	0·029	0·028	−0·112
1·3	0·904	0·896	−0·071	−0·075	−0·047
1·4	0·869	0·862	−0·167	−0·174	0·022
1·5	0·823	0·818	−0·256	−0·266	0·089
1·6	0·772	0·768	−0·335	−0·348	0·154

https://doi.org/10.1017/S0305004100030498 Published online by Cambridge University Press

Table 4 (cont.). *Normalized radial wave functions* $P_N(nl; r)$ *for* Tl^{+3} *and* Tl^+

			Tl^+	Tl^+ (excited state)	
	Tl^{+3}	Tl^+	(ground state)		
r	$5d$	$5d$	$6s$	$6s$	$6p$
1·8	0·663	0·663	−0·465	−0·482	0·274
2·0	0·558	0·561	−0·558	−0·575	0·371
2·2	0·461	0·469	−0·616	−0·631	0·446
2·4	0·377	0·388	−0·646	−0·660	0·501
2·6	0·305	0·319	−0·655	−0·664	0·539
2·8	0·245	0·261	−0·646	−0·652	0·563
3·0	0·195	0·213	−0·626	−0·628	0·575
3·2	0·154	0·173	−0·596	−0·594	0·577
3·4	0·121	0·140	−0·561	−0·555	0·570
3·6	0·095	0·113	−0·522	−0·512	0·557
3·8	0·074	0·091	−0·480	−0·469	0·539
4·0	0·057	0·073	−0·439	−0·425	0·517
4·5	0·030	0·042	−0·340	−0·325	0·452
5·0	0·015	0·024	−0·255	−0·240	0·381
5·5	0·008	0·014	−0·186	−0·173	0·313
6·0	0·004	0·008	−0·134	−0·122	0·251
6·5	0·002	0·004	−0·095	−0·086	0·198
7·0	0·001	0·002	−0·066	−0·060	0·154
7·5	—	0·001	−0·046	−0·041	0·118
8·0	—	0·001	−0·032	−0·028	0·089
8·5	—	—	−0·022	−0·019	0·067
9·0	—	—	−0·015	−0·012	0·050
9·5	—	—	−0·010	−0·008	0·037
10·0	—	—	−0·006	−0·005	0·027
11·0	—	—	−0·003	−0·002	0·014
12·0	—	—	−0·001	−0·001	0·007
13·0	—	—	−0·001	—	0·004
14·0	—	—	—	—	0·002
15·0	—	—	—	—	0·001
16·0	—	—	—	—	0·001
ϵ	3·181	1·799	1·054	1·100	0·749

https://doi.org/10.1017/S0305004100030498 Published online by Cambridge University Press

Table 5. *Normalized radial wave functions* $P_N(nl; r)$ *for* Tl^{+3} *and* Tl^{+}

r	$1s$	$2s$	$2p$	$3s$	$3p$	$3d$
0·000	0·000	0·000	0·000	0·000	0·000	0·000
0·001	1·341	0·444	0·010	0·210	0·005	0·000
0·002	2·470	0·813	0·036	0·383	0·020	0·000
0·003	3·388	1·118	0·087	0·530	0·043	0·000
0·004	4·182	1·370	0·143	0·645	0·074	0·001
0·005	4·835	1·569	0·220	0·736	0·110	0·002
0·006	5·347	1·715	0·307	0·803	0·153	0·005
0·007	5·735	1·820	0·399	0·852	0·199	0·007
0·008	6·070	1·885	0·502	0·883	0·250	0·010
0·009	6·282	1·919	0·609	0·894	0·304	0·015
0·010	6·459	1·919	0·722	0·891	0·359	0·022
0·015	6·459	1·580	1·331	0·703	0·656	0·061
0·020	5·771	0·872	1·925	0·345	0·942	0·126
0·025	4·817	0·035	2·498	−0·080	1·181	0·219
0·030	3·882	−0·831	2·958	−0·494	1·358	0·328
0·035	3·052	−1·606	3·317	−0·852	1·470	0·459
0·040	2·329	−2·288	3·574	−1·144	1·501	0·605
0·05	1·306	−3·236	3·804	−1·461	1·376	0·926
0·06	0·706	−3·699	3·743	−1·458	1·054	1·256
0·07	0·370	−3·781	3·487	−1·201	0·602	1·564
0·08	0·212	−3·605	3·134	−0·775	0·092	1·851
0·09	0·106	−3·283	2·723	−0·262	−0·428	2·087
0·10	0·071	−2·892	2·324	0·276	−0·919	2·274
0·11	0·040	−2·482	1·939	0·791	−1·355	2·409
0·12	0·018	−2·078	1·597	1·265	−1·730	2·497
0·14	—	−1·399	1·049	1·990	−2·254	2·548
0·16	—	−0·902	0·665	2·412	−2·509	2·461
0·18	—	−0·562	0·415	2·572	−2·544	2·286
0·20	—	−0·345	0·251	2·534	−2·432	2·060
0·22	—	−0·205	0·148	2·365	−2·228	1·810
0·24	—	−0·117	0·087	2·123	−1·975	1·562
0·26	—	−0·071	0·051	1·850	−1·710	1·326
0·28	—	−0·041	0·031	1·577	−1·450	1·113
0·30	—	−0·024	0·015	1·320	−1·210	0·923
0·32	—	−0·015	0·010	1·086	−0·996	0·758
0·34	—	−0·009	0·005	0·883	−0·812	0·617
0·36	—	−0·006	0·003	0·712	−0·653	0·498
0·38	—	—	—	0·565	−0·523	0·401
0·40	—	—	—	0·447	−0·416	0·323
0·45	—	—	—	0·243	−0·230	0·182
0·50	—	—	—	0·127	−0·123	0·102
0·55	—	—	—	0·061	−0·064	0·056
0·60	—	—	—	0·033	−0·033	0·029
0·65	—	—	—	0·017	−0·018	0·015
0·70	—	—	—	0·008	−0·008	0·007
0·75	—	—	—	0·004	−0·004	0·003
0·80	—	—	—	0·003	−0·003	0·002
0·90	—	—	—	—	—	0·001

https://doi.org/10.1017/S0305004100030498 Published online by Cambridge University Press

Table 5 (cont.). *Normalized radial wave functions* $P_N(nl; r)$ *for* Tl^{+3} *and* Tl^{+}

r	$4s$	$4p$	$4d$	$4f$	$5s$	$5p$
0·000	0·000	0·000	0·000	0·000	0·000	0·000
0·001	0·104	0·003	0·000	0·000	0·047	0·001
0·002	0·192	0·010	0·000	0·000	0·086	0·004
0·003	0·263	0·021	0·000	0·000	0·119	0·009
0·004	0·321	0·036	0·000	0·000	0·145	0·016
0·005	0·367	0·055	0·001	0·000	0·165	0·024
0·006	0·402	0·077	0·002	0·000	0·180	0·033
0·007	0·425	0·099	0·004	0·000	0·190	0·043
0·008	0·437	0·124	0·006	0·000	0·195	0·054
0·009	0·443	0·151	0·008	0·000	0·197	0·064
0·010	0·440	0·179	0·011	0·000	0·195	0·076
0·015	0·341	0·326	0·031	0·001	0·149	0·138
0·020	0·164	0·463	0·065	0·002	0·064	0·196
0·025	−0·055	0·577	0·111	0·005	−0·034	0·243
0·030	−0·262	0·652	0·168	0·008	−0·126	0·274
0·035	−0·438	0·697	0·234	0·013	−0·204	0·289
0·040	−0·578	0·707	0·306	0·020	−0·265	0·289
0·05	−0·718	0·619	0·461	0·041	−0·320	0·244
0·06	−0·687	0·430	0·614	0·071	−0·296	0·159
0·07	−0·522	0·182	0·749	0·111	−0·214	0·050
0·08	−0·277	−0·087	0·858	0·161	−0·098	−0·064
0·09	0·004	−0·350	0·933	0·217	0·032	−0·174
0·10	0·285	−0·581	0·973	0·282	0·159	−0·266
0·11	0·539	−0·768	0·976	0·352	0·269	−0·337
0·12	0·754	−0·908	0·947	0·426	0·358	−0·386
0·14	1·009	−1·028	0·799	0·581	0·453	−0·412
0·16	1·050	−0·958	0·564	0·738	0·441	−0·356
0·18	0·903	−0·744	0·275	0·890	0·343	−0·241
0·20	0·619	−0·440	−0·036	1·028	0·189	−0·092
0·22	0·265	−0·088	−0·346	1·152	0·010	0·007
0·24	−0·118	0·273	−0·636	1·254	−0·170	0·221
0·26	−0·491	0·614	−0·894	1·337	−0·336	0·356
0·28	−0·832	0·918	−1·115	1·403	−0·473	0·465
0·30	−1·125	1·177	−1·296	1·448	−0·574	0·543
0·32	−1·364	1·384	−1·439	1·479	−0·640	0·592
0·34	−1·545	1·541	−1·543	1·494	−0·670	0·612
0·36	−1·673	1·652	−1·612	1·496	−0·667	0·605
0·38	−1·754	1·722	−1·653	1·488	−0·634	0·575
0·40	−1·794	1·755	−1·666	1·471	−0·577	0·526
0·45	−1·751	1·712	−1·619	1·401	−0·420	0·339
0·50	−1·586	1·560	−1·492	1·302	−0·080	0·102
0·55	−1·362	1·357	−1·324	1·191	0·213	−0·148
0·60	−1·129	1·142	−1·147	1·077	0·487	−0·386
0·65	−0·910	0·937	−0·973	0·964	0·717	−0·595
0·70	−0·721	0·756	−0·814	0·856	0·902	−0·769
0·75	−0·561	0·600	−0·672	0·755	1·039	−0·905
0·80	−0·429	0·469	−0·548	0·662	1·132	−1·007

https://doi.org/10.1017/S0305004100030498 Published online by Cambridge University Press

Table 5 (cont.). *Normalized radial wave functions* $P_N(nl; r)$ *for* Tl^{+3} *and* Tl^{+}

r	$4s$	$4p$	$4d$	$4f$	$5s$	$5p$
0·9	−0·245	0·280	−0·358	0·504	1·204	−1·115
1·0	−0·136	0·162	−0·227	0·378	1·167	−1·125
1·1	−0·074	0·092	−0·143	0·282	1·067	−1·072
1·2	−0·040	0·052	−0·089	0·209	0·939	−0·983
1·3	−0·021	0·029	−0·055	0·155	0·804	−0·878
1·4	−0·012	0·015	−0·033	0·116	0·674	−0·768
1·5	−0·005	0·009	−0·021	0·085	0·557	−0·663
1·6	−0·003	0·005	−0·012	0·063	0·456	−0·568
1·8	−0·001	0·001	−0·005	0·035	0·296	−0·406
2·0	—	—	−0·002	0·018	0·188	−0·283
2·2	—	—	−0·001	0·011	0·118	−0·195
2·4	—	—	—	0·006	0·073	−0·133
2·6	—	—	—	0·003	0·045	−0·090
2·8	—	—	—	0·002	0·027	−0·061
3·0	—	—	—	0·001	0·016	−0·040
3·2	—	—	—	—	0·010	−0·027
3·4	—	—	—	—	0·006	−0·018
3·6	—	—	—	—	0·004	−0·012
3·8	—	—	—	—	0·002	−0·008
4·0	—	—	—	—	0·001	−0·005
4·5	—	—	—	—	—	−0·002
5·0	—	—	—	—	—	−0·001

https://doi.org/10.1017/S0305004100030498 Published online by Cambridge University Press

Table 6. *Radial charge density $U(r)$ for* Tl^{+3} *and* Tl^{+}

r	$U(r)$ (all states)	r	Tl^{+3}	Tl^{+} (ground state) $(6s)^2$	Tl^{+} (excited state) $(6s)(6p)$
0·000	0·0	0·45	80·19	80·19	80·19
0·001	4·1	0·50	66·20	66·19	66·19
0·002	13·9	0·55	52·40	52·41	52·41
0·003	26·2	0·60	41·31	41·37	41·36
0·004	40·0	0·65	33·37	33·43	33·41
0·005	53·5	0·70	28·29	28·37	28·34
0·006	65·5	0·75	25·26	25·35	25·32
0·007	75·6	0·80	23·58	23·63	23·61
0·008	84·8				
0·009	91·3	0·9	22·02	22·01	22·00
0·010	97·0	1·0	20·74	20·65	20·66
		1·1	18·99	18·83	18·85
0·015	103·7	1·2	16·81	16·64	16·65
0·020	97·7	1·3	14·48	14·35	14·35
0·025	95·2	1·4	12·19	12·13	12·10
0·030	100·2	1·5	10·13	10·18	10·13
0·035	110·8	1·6	8·371	8·531	8·452
0·040	123·1				
		1·8	5·579	6·007	5·882
0·05	141·6	2·0	3·663	4·324	4·170
0·06	145·7	2·2	2·386	3·216	3·054
0·07	138·5	2·4	1·540	2·457	2·309
0·08	129·2	2·6	0·985	1·929	1·803
0·09	122·0	2·8	0·623	1·539	1·446
0·10	120·3	3·0	0·392	1·249	1·190
0·11	122·4	3·2	0·242	1·013	0·989
0·12	127·1	3·4	0·149	0·827	0·831
		3·6	0·091	0·674	0·701
0·14	135·4	3·8	0·055	0·544	0·594
0·16	134·2	4·0	0·0326	0·4387	0·5012
0·18	123·4				
0·20	108·3	4·5	0·0088	0·2488	0·3275
0·22	94·1	5·0	0·0023	0·1359	0·2086
0·24	84·3	5·5	0·0006	0·0712	0·1299
0·26	79·7	6·0	0·0001	0·0365	0·0785
0·28	79·6	6·5	—	0·0183	0·0468
0·30	82·0	7·0	—	0·0087	0·0273
0·32	85·5	7·5	—	0·0042	0·0156
0·34	88·7	8·0	—	0·0020	0·0087
0·36	90·5	8·5	—	0·0010	0·0049
0·38	90·9	9·0	—	0·0005	0·0026
0·40	89·5	9·5	—	0·0002	0·0015
		10·0	—	0·0001	0·0007
		11·0	—	—	0·0002

https://doi.org/10.1017/S0305004100030498 Published online by Cambridge University Press