APPROXIMATE SELF-CONSISTENT FIELDS FOR In^{3+} AND Sb^{3+}

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ABSTRACT. Preliminary self-consistent field calculations without exchange have been performed for the ground states of the structures In^{3+} and Sb^{3+}. The results are presented.

1. *Introduction.* An important application of atomic self-consistent fields is as a starting point in the study of molecules and solids. Although the wave functions for the outer electrons of an atom are radically altered by association with other atoms, it is found that, to a good approximation, the core of inner wave functions is unchanged. Structures containing indium and antimony have recently become of interest in solid-state theory, and it was with this in mind that self-consistent fields were calculated for In^{3+} and Sb^{3+}. Since the solid-state problem is complex, any numerical approach to it is at present necessarily crude. For this reason, only rough self-consistent fields were needed. These approximate fields are given here since they would certainly give a good estimated field for more refined self-consistent field calculations and may be of use in their present form.

2. *The calculations.* Estimates of the electronic contributions to the total field, $Z(r)$, were obtained by a method described in an earlier paper (2). The approximations were derived from the known contributions for Cs^+ (Hartree (1)). As only $1\frac{1}{2}$–2 decimal accuracy in the contributions to the field from each group of electrons was required, the estimates of $Z(nl; r)$ for (nl) up to $(3p)$ were taken to be sufficiently accurate, and only the outer wave functions were evaluated by solution of the appropriate differential equations and made self-consistent.

The calculations were carried out on the automatic calculating machine at the University Mathematical Laboratory, Cambridge. A programme designed to calculate the self-consistent field of Mo^+ (Ridley (3)) was used in a slightly modified form.

The results for In^{3+} are given in Tables 1 and 2. Those for Sb^{3+} appear in Tables 3 and 4. Estimates of the maximum error, ΔZ, in the contributions to $Z(r)$ from each group of electrons are given. In each structure the contribution from the $(3p)$ electrons is least accurate, having a maximum error of about 0·02.

These results also provide further data for interpolation of contributions from the outer (nl) groups to the atomic field in this region of the periodic table. The values of the 'screening constant', σ, and 'slope constant', α, for the method of interpolation given in a previous paper (2) are included in Tables 1 and 3.

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Table 1. *Wave functions for outer electrons of* In^{3+}

r	$4s$	$4p$	$4d$	r	$4s$	$4p$	$4d$
0·000	0·00	0·00	0·00	0·60	−3·48	3·02	−3·21
0·002	0·30	0·01	0·00	0·65	−4·15	3·62	−3·83
0·004	0·55	0·03	0·00	0·70	−4·61	4·05	−4·34
0·006	0·74	0·07	0·00	0·8	−4·97	4·47	−5·01
0·008	0·89	0·11	0·00	0·9	−4·81	4·47	−5·32
0·010	0·99	0·16	0·01	1·0	−4·37	4·20	−5·37
0·015	1·11	0·33	0·02	1·1	−3·81	3·79	−5·25
0·020	1·05	0·51	0·04	1·2	−3·22	3·33	−5·02
0·025	0·88	0·71	0·07	1·3	−2·66	2·87	−4·72
0·030	0·63	0·90	0·11	1·4	−2·17	2·43	−4·40
0·035	0·34	1·08	0·16	1·6	−1·39	1·70	−3·73
0·040	0·03	1·24	0·22	1·8	−0·87	1·15	−3·09
0·05	−0·59	1·48	0·36	2·0	−0·53	0·77	−2·53
0·06	−1·12	1·62	0·54	2·2	−0·32	0·50	−2·04
0·07	−1·51	1·65	0·74	2·4	−0·19	0·33	−1·63
0·08	−1·76	1·58	0·96	2·6	−0·11	0·21	−1·29
0·09	−1·85	1·42	1·18	2·8	−0·06	0·13	−1·01
0·10	−1·81	1·20	1·41	3·0	−0·04	0·08	−0·79
0·12	−1·41	0·61	1·84	3·2	−0·02	0·05	−0·61
0·14	−0·74	−0·07	2·21	3·4	−0·01	0·03	−0·47
0·16	0·06	−0·74	2·50	3·6	−0·01	0·02	−0·36
0·18	0·85	−1·34	2·70	3·8	—	0·01	−0·28
0·20	1·55	−1·83	2·81	4·0	—	0·01	−0·21
0·225	2·23	−2·26	2·82	4·5	—	—	−0·11
0·250	2·66	−2·48	2·69	5·0	—	—	−0·05
0·275	2·83	−2·51	2·46	5·5	—	—	−0·02
0·300	2·77	−2·38	2·14	6·0	—	—	−0·01
0·35	2·12	−1·73	1·31	6·5	—	—	−0·01
0·40	1·02	−0·77	0·35	7·0	—	—	—
0·45	−0·25	0·29	−0·64	8·0	—	—	—
0·50	−1·49	1·33	−1·59	9·0	—	—	—
0·55	−2·59	2·25	−2·46	10·0	—	—	—
				11·0	—	—	—

	$3d$	$4s$	$4p$	$4d$
ϵ	34·72	10·11	7·593	3·422
$\int_0^\infty P^2 dr$	—	16·07	14·84	31·35
σ	16·41	20·59	23·32	30·28
α	1·14	1·21	1·26	1·43

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Table 2. In^{3+} *contributions to Z and total* Z_p

r	$(1s)^2$	$(2s)^2$	$(2p)^6$	$(3s)^2$	$(3p)^6$	$(3d)^{10}$	$(4s)^2$	$(4p)^6$	$(4d)^{10}$	Total Zp
0·000	2·00	2·00	6·00	2·00	6·00	10·00	2·00	6·00	10·00	49·00
0·002	2·00	2·00	6·00	2·00	6·00	10·00	2·00	6·00	10·00	48·45
0·004	$1·98_5$	2·00	6·00	2·00	6·00	10·00	2·00	6·00	10·00	47·90
0·006	$1·95_5$	$1·99_5$	6·00	2·00	6·00	10·00	2·00	6·00	10·00	47·37
0·008	1·91	1·99	6·00	2·00	6·00	10·00	2·00	6·00	10·00	46·85
0·010	$1·84_5$	$1·98_5$	6·00	$1·99_5$	6·00	10·00	2·00	6·00	10·00	46·34
0·015	1·63	$1·96_5$	$5·99_5$	$1·99_5$	6·00	10·00	2·00	6·00	10·00	45·15
0·020	$1·37_5$	$1·94_5$	$5·98_5$	1·99	$5·99_5$	10·00	2·00	6·00	10·00	44·05
0·025	$1·11_5$	1·93	$5·96_5$	$1·98_5$	5·99	10·00	$1·99_5$	6·00	10·00	43·02
0·030	$0·87_5$	$1·91_5$	$5·92_5$	$1·98_5$	$5·98_5$	10·00	$1·99_5$	$5·99_5$	10·00	42·06
0·035	0·67	1·91	$5·86_5$	$1·98_5$	$5·97_5$	10·00	$1·99_5$	$5·99_5$	10·00	41·15
0·040	0·50	1·91	$5·78_5$	$1·98_5$	$5·95_5$	10·00	$1·99_5$	$5·99_5$	10·00	40·27
0·05	0·27	1·91	$5·54_5$	1·98	5·91	$9·99_5$	$1·99_5$	$5·98_5$	10·00	38·62
0·06	$0·13_5$	1·89	$5·20_5$	$1·97_5$	5·85	9·99	$1·99_5$	$5·97_5$	10·00	37·08
0·07	0·07	$1·83_5$	$4·78_5$	$1·96_5$	$5·78_5$	9·98	$1·99_5$	$5·96_5$	10·00	35·64
0·08	0·03	1·75	4·31	1·95	5·72	9·96	1·99	$5·95_5$	$9·99_5$	34·29
0·09	$0·01_5$	$1·62_5$	3·81	$1·92_5$	5·66	9·93	$1·98_5$	$5·94_5$	9·99	33·04
0·10	$0·00_5$	1·48	$3·31_5$	$1·90_5$	$5·61_5$	$9·88_5$	1·98	$5·93_5$	$9·98_5$	31·88
0·12	0·00	1·15	$2·39_5$	$1·86_5$	5·56	9·74	$1·97_5$	5·93	9·97	29·78
0·14	—	$0·83_5$	1·64	$1·84_5$	5·55	$9·50_5$	1·97	5·93	$9·94_5$	27·93
0·16	—	0·57	1·08	1·84	$5·54_5$	9·17	1·97	5·93	$9·90_5$	26·25
0·18	—	$0·37_5$	$0·68_5$	1·84	$5·51_5$	8·75	1·97	5·92	$9·86_5$	24·73
0·20	—	$0·23_5$	$0·42_5$	1·83	$5·42_5$	$8·24_5$	$1·96_5$	5·90	$9·81_5$	23·32
0·225	—	$0·12_5$	$0·22_5$	$1·78_5$	5·21	$7·53_5$	$1·95_5$	$5·85_5$	9·75	21·71
0·250	—	$0·06_5$	$0·11_5$	1·70	$4·88_5$	$6·76_5$	$1·93_5$	$5·79_5$	9·69	20·26
0·275	—	$0·03_5$	0·06	$1·57_5$	4·47	5·98	1·91	5·73	$9·63_5$	18·97
0·300	—	$0·01_5$	0·03	1·42	$3·99_5$	5·21	$1·88_5$	5·67	$9·59_5$	17·82
0·35	—	$0·00_5$	$0·00_5$	$1·07_5$	3·00	3·81	$1·84_5$	5·58	$9·54_5$	15·89
0·40	—	0·00	0·00	$0·74_5$	$2·09_5$	2·67	1·83	5·55	9·53	14·35
0·45	—	—	—	$0·48_5$	1·39	$1·80_5$	$1·82_5$	$5·54_5$	9·53	13·09
0·50	—	—	—	0·30	0·88	$1·18_5$	1·82	5·53	9·51	12·00
0·55	—	—	—	0·18	$0·53_5$	0·76	$1·79_5$	$5·46_5$	$9·44_5$	11·03
0·60	—	—	—	0·10	0·32	0·48	$1·73_5$	5·32	$9·31_5$	10·14
0·65	—	—	—	$0·05_5$	$0·18_5$	$0·29_5$	$1·64_5$	$5·09_5$	$9·11_5$	9·34
0·70	—	—	—	0·03	$0·10_5$	0·18	$1·52_5$	4·80	$8·84_5$	8·60
0·8	—	—	—	0·01	0·03	$0·06_5$	$1·23_5$	4·05	8·14	7·31
0·9	—	—	—	0·00	0·01	0·02	0·93	$3·23_5$	7·28	6·29
1·0	—	—	—	—	$0·00_5$	0·01	$0·66_5$	2·47	$6·36_5$	5·48
1·1	—	—	—	—	0·00	$0·00_5$	0·46	1·82	5·46	4·87
1·2	—	—	—	—	—	0·00	$0·30_5$	$1·30_5$	4·62	4·40
1·3	—	—	—	—	—	—	$0·19_5$	0·92	3·86	4·05
1·4	—	—	—	—	—	—	$0·12_5$	$0·63_5$	$3·19_5$	3·79
1·6	—	—	—	—	—	—	0·05	0·29	2·14	3·45
1·8	—	—	—	—	—	—	0·02	0·13	$1·39_5$	3·25
2·0	—	—	—	—	—	—	$0·00_5$	$0·05_5$	$0·89_5$	3·14
2·2	—	—	—	—	—	—	0·00	$0·02_5$	0·56	3·08
2·4	—	—	—	—	—	—	—	0·01	0·35	3·05
2·6	—	—	—	—	—	—	—	$0·00_5$	$0·21_5$	3·03
2·8	—	—	—	—	—	—	—	0·00	0·13	3·01
3·0	—	—	—	—	—	—	—	—	$0·07_5$	3·01
3·2	—	—	—	—	—	—	—	—	$0·04_5$	3·00
3·4	—	—	—	—	—	—	—	—	$0·02_5$	3·00
3·6	—	—	—	—	—	—	—	—	$0·01_5$	3·00
3·8	—	—	—	—	—	—	—	—	0·01	3·00
4·0	—	—	—	—	—	—	—	—	$0·00_5$	3·00
4·5	—	—	—	—	—	—	—	—	0·00	3·00
ΔZ	0·005	0·005	0·006	0·01	0·02	0·01	0·005	0·01	0·01	

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Table 3. *Wave functions for outer electrons of* Sb^{3+}

r	$4s$	$4p$	$4d$	$5s$	r	$4s$	$4p$	$4d$	$5s$
0·000	0·00	0·00	0·00	0·00	0·65	−4·32	3·62	−3·70	−2·73
0·002	0·30	0·01	0·00	0·20	0·70	−4·62	3·90	−4·04	−2·71
0·004	0·55	0·03	0·00	0·36	0·8	−4·72	4·08	−4·42	−2·23
0·006	0·74	0·07	0·00	0·49	0·9	−4·38	3·91	−4·49	−1·37
0·008	0·88	0·11	0·00	0·59	1·0	−3·83	3·53	−4·36	−0·32
0·010	0·98	0·16	0·01	0·65	1·1	−3·22	3·08	−4·11	0·76
0·015	1·07	0·32	0·02	0·71	1·2	−2·64	2·62	−3·80	1·78
0·020	1·00	0·50	0·04	0·66	1·3	−2·12	2·19	−3·46	2·71
0·025	0·81	0·69	0·07	0·54	1·4	−1·67	1·80	−3·12	3·50
0·030	0·55	0·87	0·10	0·36	1·6	−1·01	1·18	−2·46	4·66
0·035	0·24	1·04	0·15	0·16	1·8	−0·59	0·75	−1·90	5·30
0·040	−0·08	1·19	0·21	−0·05	2·0	−0·34	0·47	−1·44	5·52
0·05	−0·69	1·40	0·35	−0·46	2·2	−0·19	0·29	−1·08	5·43
0·06	−1·19	1·50	0·52	−0·80	2·4	−0·11	0·18	−0·80	5·12
0·07	−1·55	1·50	0·71	−1·03	2·6	−0·06	0·11	−0·59	4·68
0·08	−1·75	1·40	0·91	−1·16	2·8	−0·03	0·06	−0·43	4·18
0·09	−1·79	1·22	1·11	−1·19	3·0	−0·02	0·04	−0·31	3·66
0·10	−1·70	0·98	1·32	−1·12	3·2	−0·01	0·02	−0·23	3·16
0·12	−1·21	0·38	1·70	−0·79	3·4	−0·01	0·01	−0·16	2·68
0·14	−0·47	−0·28	2·01	−0·30	3·6	—	0·01	−0·12	2·25
0·16	0·34	−0·91	2·24	0·25	3·8	—	—	−0·08	1·87
0·18	1·12	−1·44	2·38	0·77	4·0	—	—	−0·06	1·55
0·20	1·77	−1·86	2·43	1·20	4·5	—	—	−0·02	0·92
0·225	2·36	−2·19	2·37	1·58	5·0	—	—	−0·01	0·53
0·250	2·67	−2·30	2·19	1·76	5·5	—	—	—	0·30
0·275	2·72	−2·24	1·91	1·77	6·0	—	—	—	0·16
0·300	2·54	−2·01	1·57	1·61	6·5	—	—	—	0·09
0·35	1·68	−1·25	0·73	0·98	7·0	—	—	—	0·05
0·40	0·46	−0·25	−0·19	0·11	8·0	—	—	—	0·01
0·45	−0·84	0·78	−1·10	−0·79	9·0	—	—	—	—
0·50	−2·04	1·74	−1·93	−1·57	10·0	—	—	—	—
0·55	−3·04	2·54	−2·64	−2·17	11·0	—	—	—	—
0·60	−3·80	3·17	−3·23	−2·56					

	$3d$	$4s$	$4p$	$4d$	$5s$
ϵ	40·84	11·97	9·209	4·512	2·778
$\int_0^\infty P^2 dr$	—	13·66	11·18	18·53	50·18
σ	16·43	20·74	23·37	29·71	33·03
α	1·13	1·20	1·23	1·35	1·36

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Table 4. Sb^{3+} *contributions to Z and total* Z_p

r	$(1s)^2$	$(2s)^2$	$(2p)^6$	$(3s)^2$	$(3p)^6$	$(3d)^{10}$	$(4s)^2$	$(4p)^6$	$(4d)^{10}$	$(5s)^2$	Total Zp
0·000	2·00	2·00	6·00	2·00	6·00	10·00	2·00	6·00	10·00	2·00	51·00
0·002	2·00	2·00	6·00	2·00	6·00	10·00	2·00	6·00	10·00	2·00	50·42
0·004	$1·98_5$	2·00	6·00	2·00	6·00	10·00	2·00	6·00	10·00	2·00	49·85
0·006	1·95	$1·99_5$	6·00	2·00	6·00	10·00	2·00	6·00	10·00	2·00	49·28
0·008	$1·90_5$	1·99	6·00	2·00	6·00	10·00	2·00	6·00	10·00	2·00	48·74
0·010	$1·83_5$	$1·98_5$	6·00	$1·99_5$	6·00	10·00	2·00	6·00	10·00	2·00	48·21
0·015	1·61	$1·96_5$	$5·99_5$	$1·99_5$	6·00	10·00	2·00	6·00	10·00	2·00	46·96
0·020	$1·34_5$	1·94	$5·98_5$	1·99	$5·99_5$	10·00	$1·99_5$	6·00	10·00	2·00	45·80
0·025	$1·07_5$	$1·92_5$	$5·95_5$	$1·98_5$	5·99	10·00	$1·99_5$	6·00	10·00	2·00	44·73
0·030	$0·83_5$	$1·91_5$	5·91	$1·98_5$	5·98	10·00	$1·99_5$	$5·99_5$	10·00	2·00	43·72
0·035	0·63	1·91	$5·84_5$	$1·98_5$	5·97	10·00	$1·99_5$	$5·99_5$	10·00	2·00	42·76
0·040	0·47	1·91	5·75	$1·98_5$	5·95	10·00	$1·99_5$	5·99	10·00	2·00	41·84
0·05	$0·24_5$	$1·90_5$	$5·47_5$	1·98	5·90	$9·99_5$	$1·99_5$	5·98	10·00	2·00	40·10
0·06	0·12	1·88	$5·09_5$	$1·97_6$	5·83	9·99	$1·99_5$	5·97	10·00	2·00	38·48
0·07	0·06	$1·81_5$	4·64	1·96	5·76	$9·97_5$	1·99	5·96	$9·99_5$	2·00	36·98
0·08	$0·02_5$	$1·70_5$	$4·13_5$	1·94	$5·69_5$	9·95	1·99	$5·94_5$	$9·99_5$	2·00	35·58
0·09	0·01	1·57	3·61	1·92	5·64	9·91	$1·98_5$	$5·93_5$	$9·98_5$	2·00	34·27
0·10	$0·00_5$	1·41	$3·09_5$	$1·89_5$	$5·59_5$	9·85	1·98	5·93	9·98	$1·99_5$	33·06
0·12	0·00	1·06	2·17	1·86	$5·55_5$	9·67	1·97	$5·92_5$	$9·95_5$	$1·99_5$	30·88
0·14	—	$0·74_5$	$1·44_5$	1·84	5·55	9·38	1·97	$5·92_5$	$9·91_5$	$1·99_5$	28·95
0·16	—	$0·49_5$	0·92	1·84	5·54	8·99	1·97	5·92	9·87	$1·99_5$	27·20
0·18	—	0·31	0·57	$1·83_5$	5·48	$8·49_5$	1·97	$5·90_5$	9·81	$1·99_5$	25·60
0·20	—	0·19	0·34	$1·81_5$	5·35	7·92	1·96	$5·87_5$	$9·74_5$	$1·99_5$	24·14
0·225	—	0·10	$0·17_5$	1·75	5·07	7·13	$1·94_5$	5·82	9·67	$1·99_5$	22·47
0·250	—	0·05	$0·08_5$	1·64	$4·67_5$	$6·29_5$	1·92	5·75	$9·59_5$	1·99	20·98
0·275	—	$0·02_5$	0·04	1·49	$4·19_5$	$5·46_5$	$1·89_5$	5·68	9·54	$1·98_5$	19·66
0·300	—	0·01	0·02	$1·31_5$	$3·67_5$	4·67	1·87	5·62	9·50	$1·98_5$	18·50
0·35	—	0·00	$0·00_5$	0·95	2·64	$3·27_5$	$1·83_5$	$5·54_5$	9·46	1·98	16·54
0·40	—	—	0·00	0·63	1·76	$2·19_5$	$1·82_5$	$5·52_5$	$9·45_5$	1·98	14·98
0·45	—	—	—	0·39	1·11	$1·41_5$	1·82	5·52	$9·44_5$	1·98	13·66
0·50	—	—	—	0·23	0·67	$0·88_5$	$1·80_5$	$5·47_5$	9·38	$1·97_5$	12·50
0·55	—	—	—	0·13	0·39	0·54	$1·75_5$	5·35	$9·23_5$	1·97	11·46
0·60	—	—	—	0·07	0·22	$0·32_5$	1·67	5·13	9·00	1·96	10·51
0·65	—	—	—	0·04	0·12	0·19	1·55	$4·81_5$	$8·67_5$	$1·94_5$	9·65
0·70	—	—	—	0·02	$0·06_5$	0·11	1·40	$4·43_5$	8·27	1·93	8·87
0·8	—	—	—	$0·00_5$	0·02	$0·03_5$	$1·07_5$	$3·56_5$	7·29	$1·90_5$	7·55
0·9	—	—	—	0·00	$0·00_5$	0·01	$0·76_5$	$2·69_5$	6·21	1·89	6·52
1·0	—	—	—	—	0·00	$0·00_5$	0·52	1·95	5·15	$1·88_5$	5·74
1·1	—	—	—	—	—	0·00	$0·33_5$	1·36	$4·17_5$	$1·88_5$	5·15
1·2	—	—	—	—	—	—	0·21	0·92	$3·32_5$	1·88	4·70
1·3	—	—	—	—	—	—	0·13	0·61	$2·61_5$	1·86	4·37
1·4	—	—	—	—	—	—	0·08	0·40	2·03	1·82	4·10
1·6	—	—	—	—	—	—	$0·02_5$	0·16	1·19	$1·68_5$	3·74
1·8	—	—	—	—	—	—	0·01	$0·06_5$	$0·67_5$	$1·48_5$	3·50
2·0	—	—	—	—	—	—	$0·00_5$	$0·02_5$	$0·37_5$	1·25	3·34
2·2	—	—	—	—	—	—	0·00	0·01	$0·20_5$	1·01	3·23
2·4	—	—	—	—	—	—	—	$0·00_5$	0·11	$0·78_5$	3·15
2·6	—	—	—	—	—	—	—	0·00	0·06	$0·59_5$	3·10
2·8	—	—	—	—	—	—	—	—	0·03	$0·43_5$	3·07
3·0	—	—	—	—	—	—	—	—	$0·01_5$	$0·31_5$	3·04
3·2	—	—	—	—	—	—	—	—	0·01	0·22	3·03
3·4	—	—	—	—	—	—	—	—	$0·00_5$	0·15	3·02
3·6	—	—	—	—	—	—	—	—	0·00	$0·10_5$	3·01
3·8	—	—	—	—	—	—	—	—	—	0·07	3·01
4·0	—	—	—	—	—	—	—	—	—	$0·04_5$	3·00
4·5	—	—	—	—	—	—	—	—	—	$0·01_5$	3·00
5·0	—	—	—	—	—	—	—	—	—	$0·00_5$	3·00
5·5	—	—	—	—	—	—	—	—	—	0·00	3·00
6·0	—	—	—	—	—	—	—	—	—	—	3·00
6·5	—	—	—	—	—	—	—	—	—	—	3·00
ΔZ	0·005	0·005	0·006	0·01	0·02	0·01	0·005	0·01	0·01	0·005	

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