Self-Consistent Field Calculations for Ge^{++} and Ge*

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Results of self-consistent field calculations for Ge^{++} and Ge are reported. Tables of the wave functions and effective nuclear charges are given. The wave functions inside of the $3d$ have been assumed the same for the two stages of ionization. The calculations have been carried to a consistency of 0.02 electronic unit in the Z's.

IN the previous paper results of self-consistent field calculations for Zn, Ga, As and some of their ions have been reported. In this paper results for Ge^{++} and Ge are reported (see Tables I–IV). Before this series of calculations was begun there were no results available for atoms between Cu and Rb. The first atom in this region for which calculations were made was As. For this atom the initial fields were estimated between Cu and Rb by a method described by Hartree.[1] After the results for As were obtained, values for Ga were interpolated between Cu and As. In a similar manner the initial fields for Zn and Ge were estimated from the available results for their neighbors. It should be remarked that at large values of r a linear interpolation between the Z's for As and Ge did not give satisfactory values for the Z's for Ge.

RESULTS

The maximum difference between the values of $2Z_{3d}$ for Ge^{++} and Ge is only 0.04, so that it is safe to assume that the $3p$ and other inner wave functions would show negligible changes. This is partly because most of the $3d$ charge density is inside of the region of appreciable charge density of the valence electrons and partly because the addition of the two $4p$ electrons causes a redistribution of the charge density of the $4s$ electrons which partially compensates for the changes in total charge density caused by introduction of the $4p$ electrons. Since the valence electrons in Ge and neighboring atoms have small l values, the process of obtaining a self-consistent solution of the equations is much more rapid than for elements with a nearly filled d shell or for elements with only one electron outside of a filled d shell.

* Prepared for publication by Millard F. Manning, University of Pittsburgh, Pittsburgh, Pennsylvania. For explanation see previous paper. These results were received from Professor Hartree after the others were ready for publication. The tables are reproduced here in the same form as when received. The textual material has been supplied by the undersigned. Correspondence about this paper and requests for reprints should also be addressed to him.—M. F. M.

[1] D. R. Hartree, Physik. Zeits. **30**, 517 (1929).

TABLE I. *Values of* ϵ *and* $I=\int_0^\infty P^2dr$ *for* Ge^{++} *and* Ge.

	Ge^{++}							Ge		
	$1s$	$2s$	$2p$	$3s$	$3p$	$3d$	$4s$	$3d$	$4s$	$4p$
ϵ	810.8	100.8	91.0	13.26	9.75	3.73	2.21	2.44	0.989	0.386
I	0.314	3.334	1.199	22.34	8.26	6.365	266	6.395	308	268

TABLE II. *Values of* P/r^{l+1} *for* Ge^{++} *and* Ge.

	Ge^{++}							Ge
r	$1s$	$2s$	$2p$	$3s$	$3p$	$3d$	$4s$	$4p$
0.000	200.0	200.0	1000	200.0	1000	1000	200.0	1000
0.005	170.4	169.9	923	169.9	923	948	169.9	923
0.010	145.3	143.5	853	143.3	852	900	143.3	852
0.015	123.9	120.3	789	119.9	787	855	119.8	787
0.020	105.6	99.9	730	99.3	727	812	99.2	727

TABLE III. *Values of P for* Ge^{++} *and* Ge.

	Ge^{++}							Ge				Ge^{++}				Ge		
r	$1s$	$2s$	$2p$	$3s$	$3p$	$3d$	$4s$	$3d$	$4s$	$4p$	r	$3s$	$3p$	$3d$	$4s$	$3d$	$4s$	$4p$
0.000	0.00	0.00	0.000	0.00	0.000	0.0000	0.00	Same	Same	0.000	1.1	2.50	−1.69	1.73	−6.20	1.73	−6.13	2.27
.005	0.85	.85	.023	.85	.023	.0001	.85	as	as	.023	1.2	1.91	−1.35	1.53	−7.95	1.53	−7.91	3.31
.010	1.45	1.44	.085	1.43	.085	.0009	1.43	for	for	.085	1.3	1.45	−1.08	1.35	−9.40	1.35	−9.38	4.26
.015	1.86	1.80	.177	1.80	.177	.0029	1.80	Ge^{++}	Ge^{++}	.177	1.4	1.08	−0.84	1.18	−10.54	1.19	−10.56	5.11
.020	2.11	2.00	.292	1.98	.291	.0065	1.98			.291								
.025	2.25	2.05	.422	2.03	.420	.0121	2.02			.420	1.6	0.59	−0.505	0.90	−11.98	0.91	−12.11	6.51
.030	2.31	1.99	.563	1.95	.559	.0198	1.95			.559	1.8	.32	−0.30	.68	−12.51	.69	−12.78	7.56
.035	2.30	1.84	.711	1.79	.703	.0300	1.78			.703	2.0	.17	−0.175	.51	−12.36	.52	−12.79	8.29
.040	2.24	1.62	.860	1.55	.849	.0426	1.55			.848	2.2	.09	−0.10	.38	−11.74	.39	−12.34	8.75
											2.4	.05	−0.055	.28	−10.84	.29	−11.60	9.01
.050	2.05	1.05	1.155	0.94	1.13	.0755	0.93			1.13	2.6	.03	−0.03	.21	−9.78	.22	−10.70	9.09
.06	1.79	+0.37	1.435	+0.23	1.39	.119	+0.22			1.385	2.8	.01	−0.015	.15	−8.67	.16	−9.72	9.06
.07	1.53	−0.34	1.685	−0.50	1.61	.172	−0.51			1.605	3.0		−0.01	.11	−7.57	.12	−8.72	8.92
.08	1.28	−1.02	1.90	−1.19	1.785	.234	−1.21			1.78	3.2			.08	−6.53	.09	−7.76	8.69
.09	1.05	−1.66	2.08	−1.82	1.915	.305	−1.84			1.905	3.4			.06	−5.58	.07	−6.84	8.41
.10	0.85	−2.23	2.225	−2.37	1.995	.383	−2.38			1.98	3.6			.045	−4.72	.05	−6.02	8.09
											3.8			.03	−3.96	.035	−5.25	7.74
.12	.55	−3.14	2.41	−3.15	2.025	.56	−3.14			2.00	4.0			.02	−3.30	.025	−4.57	7.37
.14	.34	−3.73	2.48	−3.51	1.895	.75	−3.48			1.86								
.16	.21	−4.06	2.45	−3.51	1.64	.95	−3.45			1.59	4.5			.01	−2.04	.01	−3.16	6.42
.18	.13	−4.16	2.36	−3.20	1.29	1.15	−3.10			1.225	5.0			.005	−1.22	.005	−2.15	5.50
.20	.08	−4.10	2.22	−2.66	0.875	1.35	−2.51		−2.52	0.80	5.5				−0.70		−1.45	4.64
.22	.05	−3.92	2.055	−1.95	+0.42	1.55	−1.76		−1.77	+0.335	6.0				−0.39		−0.96	3.86
.24	.03	−3.67	1.875	−1.14	−0.045	1.73	−0.92		−0.92	−0.14	6.5				−0.21		−0.62	3.19
.26	.02	−3.37	1.69	−0.28	−0.51	1.90	−0.02		−0.03	−0.615	7.0				−0.11		−0.42	2.61
.28	.01	−3.05	1.51	+0.59	−0.965	2.06	+0.87		+0.86	−1.065	7.5				−0.06		−0.27	2.12
.30		−2.73	1.335	1.45	−1.39	2.20	1.73		1.72	−1.49	8.0				−0.03		−0.18	1.72
.35		−1.98	0.955	3.36	−2.315	2.49	3.60		3.60	−2.38	9				−0.01		−0.08	1.11
.40		−1.38	.665	4.82	−3.00	2.68	4.91		4.92	−2.99	10						−0.04	0.70
.45		−0.93	.45	5.80	−3.45	2.79	5.62		5.63	−3.325	11						−0.02	.43
.50		−0.62	.30	6.35	−3.695	2.83	5.79		5.82	−3.42	12						−0.01	.27
.55		−0.40	.20	6.55	−3.785	2.82	5.51		5.53	−3.32	13							.16
.60		−0.26	.13	6.49	−3.75	2.78	4.89		4.92	−3.065	14							.09
											15							.05
.7		−0.11	.055	5.90	−3.455	2.61	2.96	2.61	3.01	−2.24	16							.03
.8		−0.04	.025	5.01	−3.015	2.40	+0.59	2.40	+0.66	−1.17	17							.02
.9		−0.02	.01	4.08	−2.535	2.17	−1.84	2.17	−1.76	−0.01	18							.01
1.0		−0.01	.005	3.23	−2.085	1.94	−4.14	1.95	−4.06	+1.15								

TABLE IV. *Values of 2Z for* Ge^{++} *and* Ge.

	Ge^{++}							Ge				Ge^{++}				Ge		
r	$(1s)^2$	$(2s)^2$	$(2p)^6$	$(3s)^2$	$(3p)^6$	$(3d)^{10}$	$(4s)^2$	$(3d)^{10}$	$(4s)^2$	$(4p)^2$	r	$(3s)^2$	$(3p)^6$	$(3d)^{10}$	$(4s)^2$	$(3d)^{10}$	$(4s)^2$	$(4p)^2$
0.000	4.00	4.00	12.00	4.00	12.00	20.00	4.00	20.00	4.00	4.00	0.7	1.49	4.82	9.55	3.84	9.59	3.86	3.94
.005	3.98	4.00	12.00	4.00	12.00						0.8	0.95	3.29	7.57	3.84	7.61	3.86	3.94
.010	3.91	3.99	12.00	4.00	12.00						0.9	.58	2.16	5.94	3.84	5.97	3.86	3.94
.015	3.72	3.99	12.00	4.00	12.00						1.0	.34	1.40	4.61	3.82	4.64	3.85	3.94
.020	3.46	3.95	12.00	3.99	12.00						1.1	.20	0.88	3.55	3.78	3.59	3.81	3.93
.025	3.16	3.95	12.00	3.99	12.00						1.2	.11	.54	2.71	3.70	2.75	3.75	3.92
.030	2.82	3.90	11.98	3.99	12.00						1.3	.06	.33	2.06	3.59	2.09	3.65	3.90
.035	2.49	3.90	11.98	3.99	12.00						1.4	.03	.20	1.56	3.44	1.60	3.52	3.86
.040	2.16	3.86	11.93	3.98	11.99	20.00	4.00	20.00	4.00	4.00								
											1.6	.01	.07	0.88	3.05	0.91	3.18	3.76
.05	1.56	3.84	11.82	3.98	11.97	20.00	4.00	20.00	4.00	4.00	1.8		.02	.49	2.60	.52	2.77	3.61
.06	1.09	3.84	11.66	3.98	11.95	20.00	4.00	20.00	4.00		2.0		.01	.27	2.13	.28	2.34	3.42
.07	0.75	3.84	11.41	3.98	11.92	20.00	4.00	20.00	4.00		2.2			.15	1.69	.16	1.93	3.20
.08	.49	3.83	11.08	3.98	11.88	20.00	4.00	20.00	4.00		2.4			.08	1.30	.09	1.56	2.96
.09	.32	3.81	10.69	3.97	11.83	20.00	3.99	20.00	3.99		2.6			.04	0.97	.05	1.24	2.72
.10	.20	3.76	10.22	3.96	11.77	19.99	3.99	19.99	3.99	4.00	2.8			.02	.72	.03	0.96	2.47
											3.0			.01	.52	.02	.74	2.23
.12	.08	3.58	9.14	3.93	11.65	19.98	3.99	19.98	3.99	4.00	3.2				.37	.01	.56	2.00
.14	.03	3.29	7.94	3.90	11.54	19.95	3.99	19.95	3.99	4.00	3.4				.26		.43	1.78
.16	.01	2.93	6.71	3.85	11.45	19.90	3.98	19.90	3.98	4.00	3.6				.18		.32	1.57
.18		2.52	5.55	3.81	11.38	19.84	3.98	19.84	3.98	4.00	3.8				.12		.24	1.39
.20		2.12	4.50	3.78	11.35	19.74	3.98	19.74	3.98	4.00	4.0				.08		.18	1.22
.22		1.73	3.58	3.76	11.33	19.60	3.98	19.60	3.98	4.00								
.24		1.39	2.81	3.75	11.33	19.43	3.98	19.44	3.98	4.00	4.5				.03		.08	0.86
.26		1.09	2.17	3.75	11.33	19.22	3.98	19.23	3.98	4.00	5.0				.01		.04	.60
.28		0.84	1.66	3.75	11.31	18.98	3.98	18.98	3.98	4.00	5.5						.02	.40
.30		.64	1.26	3.74	11.27	18.69	3.98	18.69	3.98	3.99	6.0						.01	.27
											6.5							.18
.35		.31	0.60	3.69	11.01	17.82	3.97	17.82	3.98	3.99	7.0							.12
.40		.14	.28	3.53	10.49	16.76	3.96	16.77	3.97	3.98	7.5							.08
.45		.06	.12	3.28	9.73	15.58	3.94	15.59	3.95	3.98	8.0							.05
.50		.03	.05	2.94	8.80	14.33	3.91	14.35	3.92	3.97								
.55		.01	.02	2.57	7.77	13.08	3.89	13.09	3.90	3.96	9							.02
.60			.01	2.19	6.74	11.84	3.87	11.87	3.89	3.95	10							.01