Although further terms may be obtained following his method, they are much more easily found by use of the recursion formula:

$$36pK_p(m) = [(2m+2p-1)(2m-2p+3)-(m-2p-1)(m-2p-2)]K_{p-1}(m)-\tfrac{1}{6}(2m+2p-1)(m-2p+1)(m-2p+4)K_{p-2}(m),$$

which follows from (25) in conjunction with the formulas[9,16]

$$dJ_m(z)/dz=-J_{m-1}(z);\quad 2J_m(z)=(m-1)J_{m-2}(z)+zJ_{m-3}(z).$$

In order to find the value of β_0 that makes the peak intensity, $\frac{1}{2}-I(\beta_0)$, a maximum, we have $d(\frac{1}{2}-I(\beta_0))/d\beta_0=0$ or, since $dJ_3(z)/dz=-J_2(z)$,

$$\text{I.P. } J_2(i\beta_0)=0.$$

Using Laporte's expansion we find $\beta_{0m}=1.200\pi$.

[16] Differentiation of the above asymptotic expansion may be shown to be valid.

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Self-Consistent Field Calculations for Zn, Ga, Ga$^+$, Ga^{+++}, As, As$^+$, As^{++}, As^{+++} *

W. HARTREE AND D. R. HARTREE
University of Manchester, Manchester, England
AND
MILLARD F. MANNING
Department of Physics, University of Pittsburgh, Pittsburgh, Pennsylvania

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Results of self-consistent field calculations without exchange for Zn, Ga, Ga$^+$, Ga^{+++}, As, As$^+$, As^{++}, As^{+++} are reported. Tables of the wave functions and effective nuclear charges are given. The wave functions for electrons inside of the 3*d* have been assumed the same for different stages of ionization. The calculations have been carried to an estimated consistency of 0.02 in the *Z*'s. A few remarks on the relation to the structure of solids are included.

INTRODUCTION

IF the wave function for a many-electron atom is expressed as a product of one-electron wave functions, each of these functions has the form $\Phi(\phi)\Theta(\theta)P(r)/r$. The solutions for Φ and Θ are well known. The differential equation which P satisfies is

$$\frac{d^2P}{dr^2}+\left[2v-\epsilon-\frac{l(l+1)}{r^2}\right]P=0, \qquad (1)$$

where $2v$ is the potential energy of an electron at r in Rydberg units, ϵ is the negative of the energy expressed in the same units, l is the azimuthal quantum number, and r is the radius expressed in Bohr units. The square of the radial function P is a measure of the charge enclosed between a sphere of radius r and one of radius $r+dr$.

In carrying out a self-consistent field calculation one first assumes a charge distribution, from this computes the potential energy of an electron as a function of r, and then uses these values of the potential energy and the appropriate value of

TABLE I. *Values of P/r^{l+1} near origin for neutral* Zn.

r	1*s*	2*s*	2*p*	3*s*	3*p*	3*d*	4*s*
0.000	100.0	100.0	1000	100.0	1000	1000	100.0
0.005	86.1	85.8	928	85.8	928	951	85.8
0.010	74.1	73.3	861	73.2	861	906	73.2
0.015	63.8	62.2	801	62.0	799	863	62.0
0.020	55.0	52.4	745	52.1	742	823	52.0

TABLE II. *Values of ϵ and $I=\int_0^\infty P^2dr$ for* Zn.

	1*s*	2*s*	2*p*	3*s*	3*p*	3*d*	4*s*
ϵ	706	84.5	75.7	9.32	6.25	0.991	0.539
I	0.0955	1.033	1.707	7.02	12.23	13.81	178.9

* Prepared for publication by Millard F. Manning, University of Pittsburgh, Pittsburgh, Pennsylvania. Shortly after the outbreak of the war in Europe, Mr. W. Hartree sent to this country a set of the results of his recent unpublished self-consistent field calculations with the request that they be made available to interested physicists in this country. Only the wave functions and not the effective nuclear charges were received. The undersigned has calculated these and supplied the textual material. Professor Hartree has commented on the manuscript but has not seen the proof. Correspondence about this paper and requests for reprints should be addressed to the undersigned. M. F. M.

TABLE III. *Values of P for neutral* Zn.

r	1s	2s	2p	3s	3p	3d	4s	r	3s	3p	3d	4s
0.000	0.00	0.00	0.000	0.00	0.000	0.0000	0.00	1.2	1.33	−1.99	2.53	−3.09
.005	.43	.43	.023	.43	.023	.0001	.43	0.3	1.04	−1.63	2.32	−4.01
.010	.74	.73	.086	.73	.086	.0009	.73	0.4	0.81	−1.33	2.13	−4.82
.015	.96	.93	.180	.93	.180	.0029	.93					
.020	1.10	1.05	.298	1.04	.297	.0066	1.04	1.6	.48	−0.87	1.78	−6.13
.025	1.18	1.09	.433	1.08	.431	.0123	1.08	1.8	.28	−0.56	1.49	−7.06
.030	1.22	1.08	.580	1.06	.576	.0202	1.06	2.0	.16	−0.35	1.24	−7.65
.035	1.23	1.02	.735	1.00	.729	.0307	1.00	2.2	.10	−0.22	1.04	−7.98
.040	1.21	0.93	.894	0.90	.884	.0437	0.90	2.4	.06	−0.13	0.86	−8.09
								2.6	.03	−0.08	.72	−8.04
.05	1.13	0.66	1.21	0.62	1.19	.078	0.61	2.8	.02	−0.05	.60	−7.87
.06	1.01	+0.34	1.52	+0.28	1.48	.123	+0.27	3.0	.01	−0.03	.50	−7.61
.07	0.87	−0.01	1.80	−0.09	1.73	.180	−0.09	3.2		−0.02	.42	−7.29
.08	.75	−0.36	2.05	−0.45	1.95	.246	−0.45	3.4		−0.01	.35	−6.92
.09	.62	−0.69	2.27	−0.78	2.12	.322	−0.79	3.6			.29	−6.52
.10	.52	−0.99	2.44	−1.08	2.24	.407	−1.09	3.8			.24	−6.11
								4.0			.20	−5.70
.12	.35	−1.50	2.70	−1.54	2.34	.60	−1.55					
.14	.23	−1.87	2.82	−1.81	2.28	.81	−1.81	4.5			.13	−4.70
.16	.14	−2.09	2.84	−1.90	2.08	1.04	−1.89	5.0			.08	−3.79
.18	.09	−2.20	2.78	−1.83	1.76	1.27	−1.80	5.5			.05	−3.01
.20	.06	−2.22	2.67	−1.64	1.37	1.51	−1.59	6.0			.03	−2.36
.22	.03	−2.17	2.51	−1.34	0.92	1.75	−1.28	6.5			.02	−1.83
.24	.02	−2.08	2.33	−0.98	+0.44	1.98	−0.90	7.0			.01	−1.41
.26	.01	−1.95	2.14	−0.58	−0.06	2.20	−0.48	7.5				−1.08
.28	.01	−1.80	1.94	−0.15	−0.55	2.40	−0.04	8.0				−0.82
.30		−1.64	1.75	+0.28	−1.04	2.59	+0.40					
								9				−0.47
.35		−1.25	1.31	1.31	−2.13	3.00	1.43	10				−0.26
.40		−0.91	0.95	2.16	−3.01	3.30	2.25	11				−0.14
.45		−0.64	.67	2.79	−3.65	3.51	2.80	12				−0.08
.50		−0.44	.46	3.21	−4.07	3.64	3.09	13				−0.04
.55		−0.30	.32	3.44	−4.31	3.70	3.15	14				−0.02
.60		−0.20	.21	3.52	−4.39	3.71	3.01	15				−0.01
.7		−0.09	.10	3.37	−4.24	3.61	2.34					
.8		−0.04	.04	2.98	−3.85	3.43	1.13					
.9		−0.01	.02	2.53	−3.37	3.21	+0.19					
1.0			.01	2.08	−2.87	2.98	−0.96					
0.1				1.67	−2.41	2.75	−2.07					

l in Eq. (1) which is then solved subject to standard boundary conditions. The solution obtained for P usually corresponds to a charge density which is different from that originally assumed. A new charge distribution is then assumed[1] and the process repeated. This is continued until initial and final estimates agree within a certain tolerance.[2]

Actually the comparisons are usually made in terms of the effective nuclear charges, designated by Z_{nl}, of the various different groups. For a particular nl group of electrons, the effective nuclear charge is defined by

$$Z_{nl}=2(2l+1)\int_{\infty}^{r}P^2dr\Big/\int_{\infty}^{0}P^2dr. \qquad (2)$$

For these calculations the maximum discrepancy between estimated and calculated values of Z for any one type is less than 0.03. For the inner groups the discrepancy is seldom greater than 0.01 and for the entire atom the maximum discrepancy is probably not greater than 0.04.

All the various stages in a self-consistent field calculation have to be carried out either numerically or by some type of integrator such as a differential analyzer. All of these calculations were carried out by standard numerical methods.

In earlier work on copper[2] the $3d$ functions proved very troublesome. A small change in the initial field produced a much larger change in the final field. For Zn the added nuclear charge relieves this situation somewhat and for Ga and As the $3d$ functions were much more stable. Indirect evidence for this is afforded by the small change in $2Z_{3d}$ between Ga^{+++} and Ga^{+}.

[1] M. F. Manning and L. Goldberg, Phys. Rev. **53**, 662 (1938).
[2] D. R. Hartree, Proc. Roy. Soc. **A141**, 282 (1933).

TABLE IV. *Values of 2Z for neutral* Zn.

r	$(1s)^2$	$(2s)^2$	$(2p)^6$	$(3s)^2$	$(3p)^6$	$(3d)^{10}$	$(4s)^2$	r	$(3s)^2$	$(3p)^6$	$(3d)^{10}$	$(4s)^2$
0.000	4.00	4.00	12.00	4.00	12.00	20.00	4.00	0.7	1.85	5.94	12.21	3.93
.005	3.99	4.00	12.00	4.00	12.00			.8	1.27	4.33	10.41	3.92
.010	3.91	3.99	12.00	4.00	12.00			.9	0.83	3.05	8.81	3.92
.015	3.76	3.98	12.00	4.00	12.00			1.0	.53	2.09	7.42	3.92
.020	3.53	3.96	12.00	3.99	12.00			1.1	.33	1.41	6.23	3.91
.025	3.25	3.94	11.99	3.99	12.00			1.2	.20	0.94	5.21	3.90
.030	2.95	3.91	11.98	3.99	12.00			1.3	.12	.62	4.50	3.87
.035	2.63	3.89	11.97	3.98	12.00			1.4	.07	.40	3.64	3.83
.040	2.31	3.87	11.94	3.98	11.99	20.00	4.00					
								1.6	.03	.17	2.54	3.69
.05	1.73	3.85	11.87	3.98	11.98	20.00	4.00	1.8	.01	.07	1.76	3.49
.06	1.25	3.83	11.73	3.98	11.96			2.0		.03	1.22	3.25
.07	0.88	3.83	11.54	3.98	11.94			2.2		.01	0.85	2.98
.08	.60	3.83	11.28	3.98	11.91			2.4			.58	2.69
.09	.41	3.82	10.95	3.97	11.86			2.6			.40	2.40
.10	.27	3.80	10.56	3.97	11.82	20.00	4.00	2.8			.27	2.11
								3.0			.19	1.84
.12	.11	3.67	9.62	3.95	11.72	19.98	4.00	3.2			.12	1.59
.14	.05	3.44	8.54	3.92	11.61	19.97	4.00	3.4			.08	1.37
.16	.02	3.14	7.41	3.88	11.52	19.95	3.99	3.6			.06	1.17
.18		2.78	6.30	3.84	11.44	19.91	3.99	3.8			.04	0.99
.20		2.40	5.25	3.80	11.40	19.85	3.99	4.0			.02	.83
.22		2.02	4.30	3.78	11.37	19.78	3.99					
.24		1.67	3.48	3.76	11.36	19.67	3.99	4.5			.01	.53
.26		1.36	2.78	3.75	11.36	19.55	3.99	5.0				.33
.28		1.09	2.19	3.75	11.36	19.39	3.99	5.5				.20
.30		0.86	1.71	3.75	11.34	19.21	3.99	6.0				.12
								6.5				.07
.35		.45	0.89	3.73	11.21	18.64	3.99	7.0				.04
.40		.23	.45	3.64	10.88	17.92	3.98	7.5				.02
.45		.11	.22	3.46	10.33	17.07	3.98	8.0				.01
.50		.05	.10	3.20	9.59	16.14	3.97					
.55		.03	.04	2.88	8.72	15.14	3.96					
.60		.02	.02	2.53	7.79	14.16	3.94					

RESULTS

Zinc

The calculations for zinc were carried out only for the lowest state of the neutral atom. It is interesting to note that the *3d* functions are much more contracted than the corresponding functions for the Cu^+ ion and that the eigenvalue is larger numerically. As a consequence the *3d* electrons are not affected in ordinary chemical processes and Zn is divalent, whereas Cu is sometimes divalent, indicating that *3d* functions are involved. In metallic Zn the distance between nearest neighbors is 2.83 Bohr units. Reference to Table IV shows that only 0.1 of a *3d* electron lies outside of this radius. For Cu the overlap is much greater. The small overlap in Zn indicates that the ion-core repulsion is not important in determining the properties of metallic Zn. This is confirmed by the fact that the crystal structure of Zn does not correspond to a close packing of spheres.

Reference to Table IV indicates that about half the charge density of the *4s* electrons lies outside of $R=2.83$. This is in accord with a general principle formulated by Slater.[3]

TABLE V. *Values of* P/r^{l+1} *near origin for* Ga.

	Ga+							Ga
r	1s	2s	2p	3s	3p	3d	4s	4p
0.000	100.0	100.0	1000	100.0	1000	1000	100.0	1000
0.005	85.6	85.4	926	85.4	925	950	85.4	925
0.010	73.4	72.5	858	72.4	857	903	72.4	857
0.015	62.9	61.2	795	61.0	793	859	61.0	793
0.020	53.9	51.2	737	50.9	735	817	50.8	735

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

	Ga+							Ga+++	Ga	
	1s	2s	2p	3s	3p	3d	4s	3d	4s	4p
ϵ	756	92.2	82.8	11.14	7.79	2.20	1.28	3.92	0.787	0.281
I	0.0866	0.929	1.436	6.26	10.06	9.25	101.2	9.12	109.5	617

[3] J. C. Slater, Phys. Rev. **36**, 57 (1930).

TABLE VII. *Values of P for neutral and ionized* Ga.

	Ga+							Ga+++	Ga			Ga+				Ga+++	Ga	
r	$1s$	$2s$	$2p$	$3s$	$3p$	$3d$	$4s$	$3d$	$4s$	$4p$	r	$3s$	$3p$	$3d$	$4s$	$3d$	$4s$	$4p$
0.000	0.000	0.000	0.000	0.000	0.000	0.0000	0.000	same	same	0.000	1.0	1.83	−2.46	2.42	−1.52	2.41	−1.52	+0.40
.005	.428	.427	.023	.427	.023	.0001	.427	as	as	.023	1.1	1.45	−2.03	2.19	−2.60	2.18	−2.60	1.54
.010	.734	.725	.086	.724	.086	.0009	.724	for	for	.086	1.2	1.13	−1.65	1.98	−3.57	1.97	−3.57	2.64
.015	.943	.918	.179	.915	.178	.0029	.915	Ga+	Ga+	.178	1.3	0.87	−1.33	1.78	−4.40	1.77	−4.40	3.67
.020	1.078	1.024	.295	1.017	.294	.0065	1.016			.294	1.4	.66	−1.06	1.60	−5.11	1.58	−5.12	4.63
.025	1.156	1.059	.428	1.048	.425	.0122	1.046			.425								
.030	1.190	1.038	.572	1.021	.568	.0200	1.018			.568	1.6	.37	−0.67	1.28	−6.14	1.26	−6.17	6.34
.035	1.191	0.971	.723	0.947	.716	.0303	0.944			.716	1.8	.21	−0.41	1.02	−6.74	0.99	−6.79	7.75
.040	1.168	0.870	.878	0.838	.866	.0432	0.834			.866	2.0	.11	−0.25	0.81	−7.00	.77	−7.08	8.89
											2.2	.06	−0.15	.64	−6.98	.60	−7.09	9.79
.05	1.076	0.595	1.18	0.545	1.16	.077	0.539			1.16	2.4	.03	−0.09	.50	−6.77	.46	−6.92	10.5
.06	0.952	+0.263	1.48	+0.197	1.43	.121	+0.189			1.43	2.6	.02	−0.05	.40	−6.42	.35	−6.61	11.0
.07	.820	−0.088	1.74	−0.168	1.67	.176	−0.178			1.67	2.8	.01	−0.03	.31	−5.99	.26	−6.22	11.4
.08	.692	−0.435	1.98	−0.523	1.87	.240	−0.533			1.86	3.0		−0.01	.24	−5.51	.20	−5.77	11.6
.09	.575	−0.762	2.17	−0.849	2.02	.314	−0.858			2.00	3.2		−0.01	.19	−5.02	.15	−5.31	11.8
.10	.472	−1.06	2.33	−1.135	2.12	.395	−1.143			2.10	3.4			.15	−4.53	.11	−4.84	11.8
											3.6			.11	−4.05	.08	−4.38	11.8
.12	.310	−1.54	2.55	−1.56	2.18	.58	−1.56			2.16	3.8			.09	−3.59	.06	−3.94	11.7
.14	.199	−1.87	2.65	−1.79	2.09	.78	−1.78			2.05	4.0			.07	−3.17	.04	−3.53	11.5
.16	.125	−2.07	2.65	−1.83	1.86	.99	−1.81			1.81								
.18	.077	−2.15	2.57	−1.72	1.52	1.21	−1.68			1.47	4.5			.04	−2.26	.02	−2.63	10.9
.20	.047	−2.14	2.44	−1.48	1.12	1.43	−1.42			1.05	5.0			.02	−1.57	.01	−1.92	10.1
.22	.029	−2.07	2.28	−1.15	0.67	1.64	−1.08			0.59	5.5			.01	−1.07		−1.38	9.2
.24	.017	−1.95	2.10	−0.76	+0.19	1.85	−0.67			+0.10	6.0				−0.71		−0.98	8.3
.26	.010	−1.81	1.91	−0.34	−0.29	2.04	−0.24			−0.39	6.5				−0.47		−0.69	7.4
.28	.006	−1.66	1.72	+0.09	−0.77	2.22	+0.21			−0.87	7.0				−0.30		−0.48	6.5
.30	.004	−1.50	1.53	0.52	−1.22	2.39	0.65			−1.32	7.5				−0.19		−0.33	5.6
											8.0				−0.12		−0.22	4.9
.35	.001	−1.11	1.12	1.52	−2.24	2.73	1.63			−2.31								
.40		−0.79	0.80	2.31	−3.02	2.97	2.37			−3.04	9				−0.04		−0.10	3.5
.45		−0.55	.55	2.87	−3.57	3.13	2.83			−3.50	10				−0.02		−0.04	2.5
.50		−0.37	.38	3.21	−3.90	3.21	3.01			−3.70	11				−0.01		−0.02	1.7
.55		−0.25	.25	3.38	−4.05	3.23	2.97			−3.70	12						−0.01	1.2
.60		−0.16	.17	3.40	−4.07	3.21	2.75			−3.53								
											14							0.6
.7		−0.07	.07	3.16	−3.84	3.07	1.92	3.07	1.92	−2.84	16							.3
.8		−0.03	.03	2.74	−3.42	2.87	+0.82	2.87	+0.82	−1.86	18							.2
.9		−0.01	.01	2.27	−2.94	2.65	−0.36	2.64	−0.36	−0.75	20							.1

TABLE VIII. *Values of 2Z for* Ga.

	Ga+							Ga+++	Ga			Ga+				Ga+++	Ga	
r	$(1s)^2$	$(2s)^2$	$(2p)^6$	$(3s)^2$	$(3p)^6$	$(3d)^{10}$	$(4s)^2$	$(3d)^{10}$	$(4s)^2$	$(4p)$	r	$(3s)^2$	$(3p)^6$	$(3d)^{10}$	$(4s)^2$	$(3d)^{10}$	$(4s)^2$	$(4p)$
0.000	4.00	4.00	12.00	4.00	12.00	20.00	4.00	20.00	4.00	2.00	0.7	1.66	5.39	10.87	3.90	10.76	3.90	1.99
.005	3.98	4.00	12.00	4.00	12.00						0.8	1.10	3.81	8.96	3.89	8.82	3.89	1.98
.010	3.90	3.99	12.00	4.00	12.00						0.9	0.70	2.60	7.30	3.89	7.15	3.89	1.98
.015	3.74	3.98	12.00	4.00	12.00						1.0	.43	1.73	5.91	3.88	5.75	3.89	1.98
.020	3.50	3.96	12.00	3.99	12.00						1.1	.26	1.13	4.76	3.87	4.59	3.87	1.98
.025	3.21	3.93	11.99	3.99	12.00						1.2	.15	0.72	3.82	3.83	3.65	3.83	1.98
.030	2.89	3.91	11.98	3.99	12.00						1.3	.09	.46	3.05	3.76	2.88	3.78	1.98
.035	2.56	3.89	11.96	3.98	11.99						1.4	.05	.29	2.43	3.67	2.27	3.69	1.97
.040	2.24	3.86	11.94	3.98	11.99	20.00	4.00	20.00	4.00	2.00								
											1.6	.01	.11	1.53	3.42	1.38	3.46	1.95
.05	1.65	3.84	11.85	3.98	11.98	20.00	4.00	20.00	4.00	2.00	1.8		.04	0.95	3.09	0.83	3.15	1.92
.06	1.18	3.84	11.70	3.98	11.96						2.0		.01	.59	2.71	.49	2.79	1.88
.07	0.82	3.84	11.48	3.98	11.93						2.2			.36	2.32	.28	2.42	1.82
.08	.55	3.83	11.19	3.98	11.89						2.4			.22	1.94	.16	2.06	1.75
.09	.37	3.82	10.83	3.97	11.85						2.6			.13	1.60	.09	1.73	1.68
.10	.24	3.78	10.40	3.97	11.80	20.00	4.00	20.00	40.0	2.00	2.8			.08	1.29	.05	1.43	1.60
											3.0			.04	1.03	.03	1.16	1.51
.12	.10	3.63	9.39	3.94	11.68	19.98	4.00	19.98	4.00	2.00	3.2			.02	0.81	.01	0.94	1.42
.14	.04	3.37	8.25	3.91	11.57	19.96	4.00	19.96	4.00		3.4			.01	.63		.75	1.33
.16	.02	3.04	7.08	3.86	11.48	19.93	3.99	19.93	3.99		3.6				.49		.60	1.24
.18	.01	2.65	5.93	3.82	11.41	19.88	3.99	19.88	3.99		3.8				.37		.47	1.15
.20		2.26	4.88	3.79	11.37	19.80	3.99	19.80	3.99		4.0				.28		.37	1.07
.22		1.87	3.95	3.77	11.35	19.70	3.99	19.70	3.99									
.24		1.52	3.15	3.76	11.35	19.57	3.99	19.56	3.99		4.5				.13		.19	0.86
.26		1.22	2.48	3.75	11.34	19.40	3.99	19.40	3.99		5.0				.10		.10	.68
.28		0.96	1.93	3.75	11.31	19.21	3.99	19.20	3.99		5.5				.03		.05	.52
.30		.74	1.48	3.75		18.98	3.99	18.96	3.99	2.00	6.0				.01		.02	.40
											6.5						.01	.30
.35		.38	0.75	3.71	11.12	18.26	3.98	18.24	3.99	2.00	7.0							.22
.40		.18	.36	3.59	11.70	17.38	3.97	17.34	3.98	2.00	7.5							.16
.45		.08	.17	3.37	10.05	16.36	3.96	16.32	3.96	2.00	8.0							.11
.50		.04	.08	3.07	9.21	15.27	3.94	15.21	3.95	1.99								
.55		.02	.04	2.72	8.27	14.14	3.93	14.07	3.93	1.99	9							.06
.60		.01	.02	2.35	7.28	13.02	3.91	12.93	3.92	1.99	10							.03
											11							.01
											12							.01

TABLE IX. *Values of P/r^{l+1} near origin for* As^{+++} *and* As.

	As^{+++} AND As							As
r	$1s$	$2s$	$2p$	$3s$	$3p$	$3d$	$4s$	$4p$
0.000	100.0	100.0	1000	100.0	1000	1000	100.0	1000
0.005	84.8	84.5	921	84.5	921	947	84.5	921
0.010	71.9	71.0	849	70.9	848	897	70.9	848
0.015	61.0	59.1	783	58.9	781	850	58.9	781
0.020	51.8	48.7	723	48.3	720	807	48.3	720

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

	$1s$	$2s$	$2p$	$3s$	$3p$	$3d$	$4s$
ϵ	866	110.0	99.7	15.76	12.02	5.575	3.29
I	0.07155	0.750	1.0145	4.975	6.825	4.47	47.6

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

	As^{++}		As^{+}		As		
	$(4s)^2$	$(4p)$	$(4s)^2$	$(4p)^2$	$(3d)^{10}$	$(4s)^2$	$(4p)^3$
ϵ	2.481	1.734	1.768	1.0485	3.312	1.180	0.468
I	51.55	99.5	55.6	123.0	4.53	57.8	157.1

Gallium

The calculations were carried out first for Ga^+. For Ga^{+++} it was assumed that the charge densities for all the electrons inside $3d$ are the same as for Ga^+. The validity of this assumption is indicated by the fact that the maximum change in $2Z_{3d}$ between Ga^+ and Ga^{+++} is only 0.17 and inner electrons would be affected much less.

For Ga, $2Z_{3d}$ was assumed the same as for Ga^+. The reason this can be done is that the charge distribution of the added $4p$ is almost completely outside the $3d$ and also because there is a compensatory change in the $4s$ functions when the $4p$ is added. At no point where the charge density of the $3d$ is appreciable is the sum of $2Z_{4s}+2Z_{4p}$ for Ga different by more than 0.04 from $2Z_{4s}+2$ for Ga^+.

Although the charge distributions for inner electrons differ very little for different degrees of ionization, this is not true for the eigenvalues. This is because the addition of a valence electron

TABLE XII. *Values of P for* As^{+++}.

r	$1s$	$2s$	$2p$	$3s$	$3p$	$3d$	$4s$	r	$2s$	$2p$	$3s$	$3p$	$3d$	$4s$
0.000	0.000	0.000	0.000	0.000	0.000	0.0000	0.000	0.7	−0.039	0.041	2.73	−3.10	2.21	+1.03
.005	.424	.423	.023	.422	.023	.0001	.422	.8	−0.014	.016	2.26	−2.65	1.99	−0.21
.010	.719	.710	.085	.709	.085	.0009	.709	.9	−0.005	.006	1.80	−2.18	1.76	−1.43
.015	.915	.887	.176	.883	.176	.0029	.883	1.0	−0.002	.002	1.39	−1.76	1.54	−2.54
.020	1.036	.975	.289	.967	.288	.0064	.967	1.1	−0.001	.001	1.05	−1.39	1.34	−3.49
.025	1.100	.992	.417	.979	.415	.0120	.978	1.2			0.79	−1.09	1.16	−4.26
.030	1.121	.953	.555	.933	.551	.0196	.931	1.3			.58	−0.84	0.99	−4.85
.035	1.111	.870	.698	.843	.691	.0297	.840	1.4			.42	−0.65	.85	−5.27
.040	1.078	.755	.844	.718	.831	.0421	.714							
								1.6			.22	−0.37	.61	−5.68
.05	0.973	.457	1.129	.403	1.102	.074	.397	1.8			.11	−0.21	.43	−5.64
.06	.844	+0.114	1.395	+0.043	1.346	.117	+0.035	2.0			.05	−0.12	.31	−5.30
.07	.712	−0.238	1.630	−0.321	1.549	.168	−0.330	2.2			.03	−0.07	.21	−4.80
.08	.589	−0.577	1.831	−0.663	1.708	.229	−0.673	2.4			.01	−0.03	.15	−4.22
.09	.480	−0.888	1.996	−0.967	1.819	.297	−0.976	2.6				−0.02	.10	−3.62
.10	.387	−1.162	2.124	−1.223	1.882	.372	−1.229	2.8				−0.01	.07	−3.04
								3.0					.05	−2.52
.12	.244	−1.585	2.280	−1.573	1.877	.537	−1.570	3.2					.03	−2.07
.14	.150	−1.850	2.322	−1.712	1.718	.718	−1.696	3.4					.02	−1.68
.16	.091	−1.981	2.277	−1.666	1.441	.905	−1.631	3.6					.01	−1.34
.18	.054	−2.005	2.171	−1.472	1.078	1.093	−1.415	3.8					.01	−1.06
.20	.032	−1.951	2.026	−1.170	0.660	1.278	−1.088	4.0						−0.84
.22	.019	−1.846	1.858	−0.793	+0.212	1.454	−0.689	4.5						−0.45
.24	.011	−1.707	1.680	−0.374	−0.244	1.618	−0.250	5.0						−0.24
.26	.006	−1.552	1.502	+0.062	−0.692	1.770	+0.203	5.5						−0.12
.28	.003	−1.391	1.329	0.497	−1.120	1.907	0.647	6.0						−0.06
.30	.002	−1.232	1.166	0.915	−1.520	2.028	1.066	6.5						−0.03
								7.0						−0.02
.35	.001	−0.874	0.817	1.82	−2.36	2.26	1.94	7.5						−0.01
.40		−0.595	.555	2.49	−2.95	2.41	2.50	8.0						
.45		−0.394	.368	2.91	−3.32	2.48	2.75							
.50		−0.255	.241	3.12	−3.50	2.49	2.73							
.55		−0.162	.156	3.16	−3.52	2.46	2.50							
.60		−0.102	.100	3.09	−3.45	2.39	2.11							

TABLE XIII. *Values of 2Z for* As^{+++}.

r	$(1s)^2$	$(2s)^2$	$(2p)^6$	$(3s)^2$	$(3p)^6$	$(3d)^{10}$	$(4s)^2$	r	$(1s)^2$	$(2s)^2$	$(2p)^6$	$(3s)^2$	$(3p)^6$	$(3d)^{10}$	$(4s)$
0.000	4.00	4.00	12.00	4.00	12.00	20.00	4.00	0.35		0.26	0.50	3.66	10.87	17.34	3.97
.005	3.98	4.00	12.00	4.00	12.00			.40		.11	.22	3.46	10.24	16.10	3.95
.010	3.88	3.99	12.00	4.00	12.00			.45		.05	.09	3.16	9.37	14.76	3.92
.015	3.69	3.97	12.00	4.00	12.00			.50		.02	.04	2.79	8.34	13.37	3.88
.020	3.42	3.95	11.99	3.99	12.00			.55		.01	.02	2.39	7.25	11.99	3.85
.025	3.10	3.92	11.99	3.99	12.00			.60			.01	2.00	6.17	10.68	3.83
.030	2.76	3.90	11.97	3.99	12.00										
.035	2.41	3.88	11.95	3.98	11.99			.7				1.31	4.27	8.28	3.81
.040	2.07	3.86	11.92	3.98	11.99	20.00	4.00	.8				0.81	2.81	6.31	3.81
								.9				.47	1.79	4.72	3.80
.05	1.48	3.84	11.80	3.98	11.97	20.00	4.00	1.0				.27	1.10	3.50	3.77
.06	1.02	3.83	11.61	3.98	11.95	20.00		1.1				.15	0.67	2.57	3.69
.07	0.68	3.83	11.34	3.98	11.90	20.00		1.2				.08	.40	1.86	3.56
.08	.44	3.83	10.98	3.97	11.85	20.00		1.3				.04	.23	1.35	3.38
.09	.28	3.80	10.55	3.97	11.80	20.00		1.4				.02	.14	0.97	3.17
.10	.18	3.74	10.05	3.96	11.74	19.99	4.00								
								1.6				.01	.05	.49	2.65
.12	.07	3.53	8.89	3.93	11.61	19.97	4.00	1.8					.02	.24	2.11
.14	.03	3.21	7.62	3.88	11.50	19.94	3.99	2.0					.01	.12	1.60
.16	.01	2.82	6.37	3.84	11.41	19.88	3.99	2.2						.05	1.17
.18		2.39	5.19	3.80	11.35	19.79	3.98	2.4						.03	0.82
.20		1.97	4.15	3.77	11.33	19.66	3.98	2.6						.01	.56
.22		1.58	3.26	3.75	11.32	19.50	3.98	2.8							.38
.24		1.25	2.52	3.75	11.32	19.29	3.98	3.0							.25
.26		0.97	1.92	3.74	11.31	19.03	3.98	3.2							.16
.28		.73	1.44	3.74	11.28	18.72	3.98	3.4							.10
.30		.55	1.07	3.74	11.22	18.37	3.98	3.6							.06
								3.8							.04
								4.0							.02
								4.5							.01

TABLE XIV. *Values of P for* As^{++}, As^{+}, As.

	As^{++}		As^{+}		As				As^{++}		As^{+}		As		
r	$(4s)^2$	$(4p)$	$(4s)^2$	$(4p)^2$	$(3d)^{10}$	$(4s)^2$	$(4p)^3$	r	$(4s)^2$	$(4p)$	$(4s)^2$	$(4p)^2$	$(3d)^{10}$	$(4s)^2$	$(4p)^3$
0.000	same	same	same	same	same	same	0.000	0.7	+1.04	−1.61	+1.05	−1.65	2.22	+1.06	−1.67
.005	as	as	as	as	as	as	.023	.8	−0.19	−0.47	−0.18	−0.51	2.00	−0.17	−0.55
.010	for	for	for	for	for	for	.085	.9	−1.41	+0.71	−1.40	+0.66	1.78	−1.39	+0.62
.015	As^{+++}	As^{+++}	As^{+++}	As^{+++}	As^{+++}	As^{+++}	.176	1.0	−2.52	1.86	−2.51	1.81	1.56	−2.50	1.76
.020							.288	1.1	−3.48	2.92	−3.47	2.86	1.36	−3.46	2.82
.025							.415	1.2	−4.25	3.85	−4.25	3.81	1.17	−4.25	3.77
.030							.550	1.3	−4.86	4.67	−4.86	4.63	1.01	−4.86	4.60
.035							.690	1.4	−5.29	5.35	−5.31	5.34	0.87	−5.32	5.32
.040							.830								
								1.6	−5.75	6.34	−5.80	6.39	.63	−5.82	6.42
.05							1.100	1.8	−5.76	6.90	−5.85	7.02	.45	−5.89	7.12
.06							1.342	2.0	−5.47	7.09	−5.62	7.32	.32	−5.68	7.50
.07							1.543	2.2	−5.02	7.02	−5.21	7.37	.23	−5.29	7.64
.08							1.699	2.4	−4.48	6.75	−4.70	7.22	.16	−4.81	7.60
.09							1.806	2.6	−3.91	6.35	−4.17	6.95	.11	−4.29	7.45
.10							1.865	2.8	−3.36	5.87	−3.64	6.58	.08	−3.78	7.19
								3.0	−2.84	5.35	−3.14	6.16	.05	−3.29	6.88
.12	−1.570	1.848	−1.570	1.848	0.537	−1.570	1.848	3.2	−2.38	4.81	−2.68	5.71	.04	−2.84	6.53
.14	−1.696	1.674	−1.696	1.675	0.718	−1.696	1.676	3.4	−1.98	4.29	−2.27	5.24	.02	−2.44	6.16
.16	−1.631	1.382	−1.631	1.383	0.905	−1.631	1.384	3.6	−1.63	3.78	−1.91	4.78	.01	−2.08	5.78
.18	−1.415	1.003	−1.415	1.005	1.093	−1.415	1.007	3.8	−1.33	3.31	−1.60	4.32	.01	−1.77	5.40
.20	−1.088	0.570	−1.088	0.572	1.278	−1.088	0.575	4.0	−1.08	2.87	−1.33	3.89		−1.50	5.02
.22	−0.689	+0.111	−0.690	+0.114	1.455	−0.690	+0.117								
.24	−0.250	−0.353	−0.251	−0.349	1.620	−0.251	−0.346	4.5	−0.62	1.97	−0.83	2.94		−0.97	4.13
.26	+0.202	−0.805	+0.201	−0.801	1.772	+0.200	−0.798	5.0	−0.35	1.31	−0.50	2.16		−0.62	3.35
.28	0.645	−1.232	0.644	−1.228	1.909	0.643	−1.224	5.5	−0.20	0.85	−0.30	1.56		−0.39	2.69
.30	1.064	−1.624	1.063	−1.619	2.031	1.062	−1.615	6.0	−0.11	.54	−0.18	1.10		−0.25	2.13
								6.5	−0.06	.33	−0.10	0.77		−0.16	1.68
.35	1.94	−2.41	1.93	−2.41	2.27	1.93	−2.40	7.0	−0.03	.21	−0.06	.53		−0.10	1.31
.40	2.50	−2.91	2.50	−2.91	2.41	2.50	−2.91	7.5	−0.02	.12	−0.03	.37		−0.06	1.02
.45	2.76	−3.13	2.76	−3.13	2.49	2.76	−3.13	8.0	−0.01	.07	−0.02	.25		−0.04	0.79
.50	2.74	−3.11	2.74	−3.12	2.50	2.75	−3.13								
.55	2.51	−2.91	2.51	−2.93	2.47	2.52	−2.94	9		.02	−0.01	.11		−0.01	.46
.60	2.12	−2.57	2.12	−2.59	2.40	2.13	−2.61	10		.01		.05			.27
								11				.02			.16
								12				.01			.09
								13							.05
								14							.03
								15							.01
								16							.01

TABLE XV. *Values of 2Z for* As^{++}, As^{+}, As.

	As^{++}		As^{+}		As				As^{++}		As^{+}		As		
r	$(4s)^2$	$(4p)$	$(4s)^2$	$(4p)^2$	$(3d)^{10}$	$(4s)^2$	$(4p)^3$	r	$(4s)^2$	$(4p)$	$(4s)^2$	$(4p)^2$	$(3d)^{10}$	$(4s)^2$	$(4p)^3$
0.000	4.00	2.00	4.00	4.00	20.00	4.00	6.00	1.6	2.75	1.67	2.84	3.46	0.53	2.88	5.37
.10	4.00	2.00	4.00	4.00	19.99	4.00	6.00	1.8	2.23	1.49	2.35	3.17	.27	2.40	5.02
.12	4.00	2.00	4.00	3.99	19.97	4.00	5.99	2.0	1.74	1.29	1.87	2.83	.14	1.93	4.61
.14	3.99	1.99	3.99	3.99	19.94	3.99	5.99	2.2	1.31	1.09	1.45	2.48	.07	1.52	4.17
.16	3.99	1.99	3.99	3.99	19.88	3.99	5.99	2.4	0.96	0.90	1.09	2.13	.03	1.16	3.72
.18	3.98	1.99	3.98	3.99	19.79	3.99	5.99	2.6	.69	.72	0.81	1.80	.01	0.88	3.29
.20	3.98	1.99	3.98	3.99	19.67	3.98	5.99	2.8	.48	.57	.59	1.50		.65	2.88
.22	3.98	1.99	3.98	3.99	19.51	3.98	5.99	3.0	.33	.45	.42	1.24		.48	2.50
.24	3.98	1.99	3.98	3.99	19.30	3.98	5.99	3.2	.23	.34	.30	1.01		.35	2.16
.26	3.98	1.99	3.98	3.99	19.04	3.98	5.99	3.4	.15	.26	.21	0.82		.25	1.85
.28	3.98	1.99	3.98	3.99	18.74	3.98	5.99	3.6	.10	.19	.14	.65		.18	1.58
.30	3.98	1.99	3.98	3.99	18.40	3.98	5.98	3.8	.06	.14	.10	.52		.13	1.34
								4.0	.04	.10	.07	.41		.09	1.13
.35	3.97	1.99	3.97	3.98	17.37	3.97	5.98								
.40	3.95	1.98	3.95	3.97	16.15	3.95	5.96	4.5	.01	.05	.03	.22		.04	0.73
.45	3.92	1.97	3.93	3.95	14.81	3.93	5.94	5.0		.02	.01	.11		.02	.46
.50	3.89	1.96	3.90	3.94	13.43	3.90	5.93	5.5		.01		.06		.01	.29
.55	3.87	1.95	3.88	3.92	12.07	3.88	5.91	6.0				.03			.18
.60	3.84	1.94	3.86	3.91	10.75	3.86	5.89	6.5				.01			.11
								7.0				.01			.06
.7	3.82	1.94	3.84	3.90	8.38	3.84	5.88	7.5							.04
.8	3.82	1.93	3.84	3.89	6.41	3.84	5.87	8.0							.02
.9	3.81	1.93	3.83	3.89	4.82	3.84	5.87								
1.0	3.78	1.93	3.80	3.89	3.60	3.81	5.86	9							.01
1.1	3.71	1.92	3.74	3.87	2.66	3.75	5.84								
1.2	3.60	1.89	3.63	3.83	1.94	3.64	5.80								
1.3	3.43	1.86	3.48	3.77	1.42	3.50	5.73								
1.4	3.23	1.81	3.29	3.69	1.03	3.32	5.64								

raises the potential energy of an electron at all points inside.

For solid Ga the distance between closest neighbors is 3.09 Bohr units. Reference to Table VIII shows that there is a negligible overlap of the $3d$ functions but a considerable overlap of the $4s$ and $4p$ functions.

Arsenic

The calculations were carried out first for As^{+++} and then for As^{++}, As^{+}, and As. Since the maximum change in $2Z_{3d}$ between As^{+++} and As is 0.10, it is safe to assume that the Z's for intermediate stages of ionization can be found by linear interpolation. The changes in the inner electrons are of course less than for the $3d$ electrons and hence negligible.

The $4s$ and $4p$ charge distributions are quite different from one stage of ionization to the other and where the charge densities are greatest a linear interpolation between the extremes would not check the intermediate stages of ionization.

The distance between nearest neighbors in metallic arsenic is 3.20 Bohr units. Reference to Table XV shows that there is only a small overlap of the $4s$ electrons but considerable overlap of the $4p$ electrons. The latter will therefore be responsible for most of the properties of the solid.

In Tables I–XV the values of P as tabulated are not normalized but tables of normalizing factors are given.

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