Potentials for atomic negative ions

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For the purpose of astrophysical, aeronomical, and laboratory applications, we seek a precise independent-particle model for electrons in atomic negative ions from $Z=3$ up to $Z=85$. We obtain analytic potentials whose inner energy levels are close to the experimental levels of neutral atoms but whose last electron eigenvalue is adjusted so as to be in precise agreement with the electron affinity of negative ions. Systematic trends in the potential parameters are discussed.

I. INTRODUCTION

Negative ions play important roles in astrophysical, aeronomical, and laboratory phenomena.[1-4] For example, H^- is the major source of opacity in the continuum of the sun and many stars and plays a part in many stellar reactions. The negative ions O^- and O_2^- and others in Earth's upper atmosphere have important effects in determining the density of free electrons which influence radio communications and other aeronomical phenomena. In the laboratory, negative ions influence radiation from shock waves, the shape of gaseous discharge pulses and other experimental observations. Negative ions are used in tandem Van de Graaff accelerators for multiplying the energy of the accelerated particles. Although in most situations the abundance of negative ions is usually small compared to that of neutrals, the fact that they are electrically charged and that electron affinities of negative ions are small often amplifies their influence. In order to provide theoretical explanations of negative-ion phenomena it is desirable to have simple but accurate characterizations of their properties. The present work addresses this objective and is devoted to independent-particle model (IPM) descriptions of negative atomic ions from $Z=3$ up to $Z=85$.

In pure atomic physics one is usually interested in finding the most precise theoretical characterization of one, two, or a few properties of the system. On the other hand, in applications of atomic physics very often approximate characterizations of many or all of the properties of the system are needed. In this context a negative ion may be regarded as the bound-state limit of the electron-neutral atomic system. For example, the scattering of electrons from an atom A, and the bound-state properties of the negative ion A^-, can be considered as physical manifestations of the negative-energy (shell-model) and positive-energy (optical-model) states of the e-A system. Such a unified characterization is useful not only for the calculation of cross sections for photodetachment ($h\nu + A^- \rightarrow A + e$) but also for the calculation of differential, total elastic, and various inelastic cross sections for electrons impacting on A atoms. These cross sections are needed as input data for various problems in applied physics. The IPM of electrons in central potentials is the simplest model for calculating the bound-state properties (e.g., energy levels) and the scattering properties (e.g., cross sections) of atomic systems. Here all the physical results are extracted from the radial Schrödinger equation

$$-u''(r)+[V(r)+l(l+1)/r^2]u(r)=Eu(r)\ , \tag{1}$$

where $V(r)$ is the potential of an electron in a negative ion, and E is the energy eigenvalue. For bound-state (shell-model) problems E is a negative number, for scattering problems (optical model) E is positive. In this work $V(r)$ is assumed to have the form[5]

$$V(r)=-(2Z/r)\Omega(r)\ , \tag{2}$$

where $\Omega(r)$ is the two-parameter ($\mathscr{H}$ and d) screening function

$$\Omega(r)=[\mathscr{H}(e^{r/d}-1)+1]^{-1}\ . \tag{3}$$

For a neutral atom an electron at large distances moves in the potential of the positive ion it leaves behind. Thus the potential for large r is Coulombic, behaving like $-2/r$. For a negative ion an electron at large distances leaves behind a neutral atom. From Eqs. (2) and (3) the potential for large r is a Yukawa, behaving as $-(2Z/\mathscr{H})r^{-1}e^{-r/d}$. This potential falls off more rapidly than a Coulomb potential.

II. BINDING ENERGIES

The analytic IPM approach used in this work is similar to the approach which has been used to calculate electronic binding energies of neutral atoms[6] and positive ions.[7] One approach for determining the potential parameters d and $\mathscr{H}$ is to tune the parameters so that the energy eigenvalues from Eq. (1) agree with the experimental values of the excited-state energies. This approach was used by Ganas and Green[8] to achieve an IPM description of the rare-gas atoms. Unfortunately, excited states for negative ions are extremely rare, so that the procedure used by Ganas and Green cannot be applied to negative ions. Furthermore, no experimental information is available on the inner energy levels of negative ions, though some theoretical information on these levels does exist.[9] In attempting to achieve a realistic IPM description of atomic negative ions, we have adopted the following procedure. We utilize the electronic binding energies of neutral atoms for which

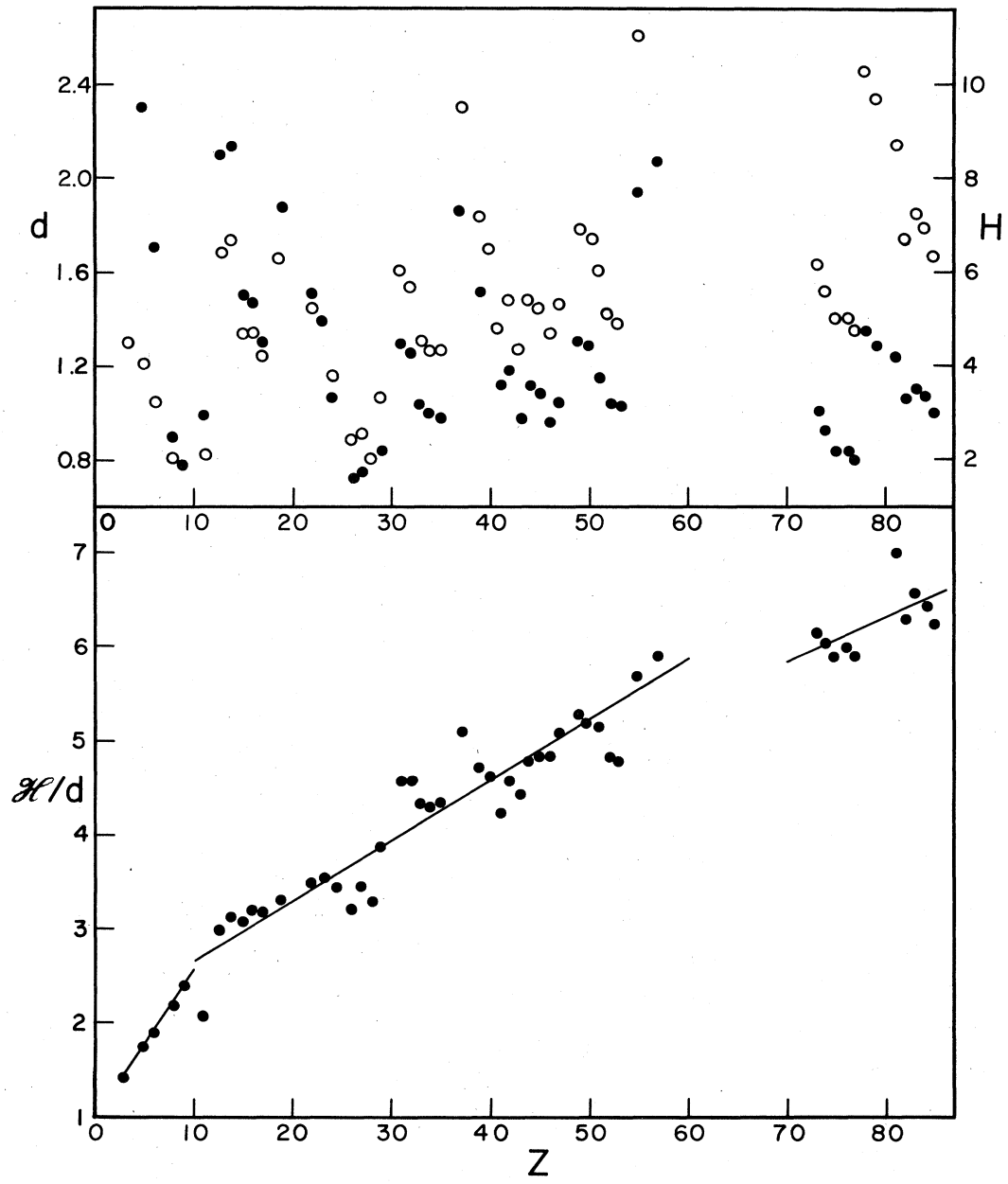

FIG. 1. Plots of d (●), $\mathscr{H}$ (○), $\mathscr{H}/d$ (●) vs Z. The straight lines through the $\mathscr{H}/d$ data are the best linear fits for low ($Z<10$), medium ($10<Z<60$), and high ($Z>60$) values of Z.

abundant experimental information exists.[10] We assume that if we take a neutral atom and add an electron to the last unfilled subshell to form a negative ion, the addition of the last electron does not significantly modify the binding energies of the inner electrons of the neutral atom. We determine the potential parameters d and $\mathscr{H}$ by requiring the energy eigenvalues to be approximately equal to the binding energies of the inner electrons of the neutral atom, and the last electron eigenvalue to be precisely equal to the electron affinity of the negative ion. An automatic search for the best parameters was performed using a nonlinear least-squares search routine which adjusts the parameters in such a way as to minimize the quantity

$$\sum_i [w(E_e - E_c)^2]_i \ . \tag{4}$$

Here E_e is the experimental electronic binding energy, E_c is the calculated energy eigenvalue, and w is the weight. In order to achieve the desired precision in matching the last electron eigenvalue to the electron affinity, it was necessary to use a weighting of $w=1/E_e^3$ in this work. The potential parameters obtained in this way are plotted in Fig. 1. In Table I a comparison is given between the last electron eigenvalues obtained in this work, the values obtained from Hartree-Fock (HF) calculations,[9] and the recommended values of electron affinities.[4] It is clear that

TABLE I. Comparison of last electron eigenvalues obtained in the present work [IPM(2) and IPM(1)] with the recommended values of electron affinities (EA), and the values from Hartree-Fock calculations (HF). IPM(2) and IPM(1) denote the results of two-parameter searches (d and $\mathscr{K}$) and one-parameter searches (d), respectively. All values are in rydbergs.

Atom	Configuration: Neutral atom	Configuration: Negative ion	IPM(2)	IPM(1)	EA	HF
$_{3}$Li	$2s$	$2s^2$	0.0456	0.0456	0.0456	0.0291
$_{5}$B	$2p$	$2p^2$	0.0206	0.0206	0.0206	0.0319
$_{6}$C	$2p^2$	$2p^3$	0.0932	0.0932	0.0932	0.0972
$_{8}$O	$2p^4$	$2p^5$	0.1075	0.1075	0.1075	0.2585
$_{9}$F	$2p^5$	$2p^6$	0.2499	0.2499	0.2499	0.3617
$_{11}$Na	$3s$	$3s^2$	0.0401	0.0401	0.0401	0.0250
$_{13}$Al	$3p$	$3p^2$	0.0338	0.0338	0.0338	0.0268
$_{14}$Si	$3p^2$	$3p^3$	0.1018	0.1016	0.1018	0.0783
$_{15}$P	$3p^3$	$3p^4$	0.0546	0.0546	0.0546	0.1409
$_{16}$S	$3p^4$	$3p^5$	0.1527	0.1525	0.1527	0.2148
$_{17}$Cl	$3p^5$	$3p^6$	0.2659	0.2657	0.2659	0.2998
$_{19}$K	$4s$	$4s^2$	0.0368	0.0368	0.0368	0.0204
$_{22}$Ti	$3d^24s^2$	$3d^34s^2$	0.0147	0.0147	0.0147	0.1175
$_{23}$V	$3d^34s^2$	$3d^44s^2$	0.0368	0.0368	0.0368	0.2714
$_{24}$Cr	$3d^54s$	$3d^54s^2$	0.0485	0.0485	0.0485	0.0066
$_{26}$Fe	$3d^64s^2$	$3d^74s^2$	0.0183	0.0184	0.0184	0.4605
$_{27}$Co	$3d^74s^2$	$3d^84s^2$	0.0515	0.0515	0.0515	0.4968
$_{28}$Ni	$3d^84s^2$	$3d^94s^2$	0.0845	0.0845	0.0845	0.4710
$_{29}$Cu	$3d^{10}4s$	$3d^{10}4s^2$	0.0901	0.0901	0.0901	0.0411
$_{31}$Ga	$4p$	$4p^2$	0.0221	0.0221	0.0221	0.0017
$_{32}$Ge	$4p^2$	$4p^3$	0.0882	0.0877	0.0882	0.0856
$_{33}$As	$4p^3$	$4p^4$	0.0588	0.0588	0.0588	0.1342
$_{34}$Se	$4p^4$	$4P^5$	0.1485	0.1484	0.1485	0.2025
$_{35}$Br	$4P^5$	$4p^6$	0.2473	0.2493	0.2473	0.2776
$_{37}$Rb	$5s$	$5s^2$	0.0357	0.0357	0.0357	0.0131
$_{39}$Y	$4d5s^2$	$4d^25s^2$	0.0050	0.0010	0.0	0.0098
$_{40}$Zr	$4d^25s^2$	$4d^35s^2$	0.0368	0.0368	0.0368	0.1004
$_{41}$Nb	$4d^45s$	$4d^45s^2$	0.0735	0.0735	0.0735	0.0309
$_{42}$Mo	$4d^55s$	$4d^55s^2$	0.0735	0.0735	0.0735	0.0109
$_{43}$Tc	$4d^55s^2$	$4d^65s^2$	0.0515	0.0515	0.0515	0.3387
$_{44}$Ru	$4d^75s$	$4d^75s^2$	0.0809	0.0809	0.0809	
$_{45}$Rh	$4d^85s$	$4d^85s^2$	0.0882	0.0882	0.0882	0.0377
$_{46}$Pd	$4d^{10}$	$4d^95s^2$	0.0441	0.0441	0.0441	0.0382
$_{47}$Ag	$4d^{10}5s$	$4d^{10}5s^2$	0.0958	0.0958	0.0958	0.0383
$_{49}$In	$5p$	$5p^2$	0.0221	0.0221	0.0221	0.0419
$_{50}$Sn	$5p^2$	$5p^3$	0.0919	0.0919	0.0919	0.1210
$_{51}$Sb	$5p^3$	$5p^4$	0.0772	0.0772	0.0772	0.1445
$_{52}$Te	$5p^4$	$5p^5$	0.1449	0.1451	0.1449	0.1929
$_{53}$I	$5p^5$	$5p^6$	0.2250	0.2257	0.2250	0.2583
$_{55}$Cs	$6s$	$6s^2$	0.0347	0.0347	0.0347	
$_{57}$La	$5d6s^2$	$5d^26s^2$	0.0368	0.0368	0.0368	
$_{73}$Ta	$5d^36s^2$	$5d^46s^2$	0.0441	0.0441	0.0441	
$_{74}$W	$5d^46s^2$	$5d^56s^2$	0.0441	0.0441	0.0441	
$_{75}$Re	$5d^56s^2$	$5d^66s^2$	0.0110	0.0110	0.0110	
$_{76}$Os	$5d^66s^2$	$5d^76s^2$	0.0809	0.0809	0.0809	
$_{77}$Ir	$5d^76s^2$	$5d^86s^2$	0.1176	0.1176	0.1176	
$_{78}$Pt	$5d^96s$	$5d^96s^2$	0.1564	0.1564	0.1564	
$_{79}$Au	$5d^{10}6s$	$5d^{10}6s^2$	0.1697	0.1697	0.1697	
$_{81}$Tl	$6p$	$6p^2$	0.0221	0.0221	0.0221	
$_{82}$Pb	$6p^2$	$6p^3$	0.0809	0.0809	0.0809	
$_{83}$Bi	$6p^3$	$6p^4$	0.0809	0.0809	0.0809	
$_{84}$Po	$6p^4$	$6p^5$	0.1397	0.1399	0.1397	
$_{85}$At	$6p^5$	$6p^6$	0.2058	0.2062	0.2058	

3 Li 0.0456	4 Be < 0	5 B 0.0206	6 C 0.0932	7 N ⩽ 0	8 O 0.1075	9 F 0.2499	10 Ne < 0
11 Na 0.0401	12 Mg < 0	13 Al 0.0338	14 Si 0.1018	15 P 0.0546	16 S 0.1527	17 Cl 0.2659	18 Ar < 0
19 K 0.0368	20 Ca < 0	31 Ga 0.0221	32 Ge 0.0882	33 As 0.0588	34 Se 0.1485	35 Br 0.2473	36 Kr < 0
37 Rb 0.0357	38 Sr < 0	49 In 0.0221	50 Sn 0.0919	51 Sb 0.0772	52 Te 0.1449	53 I 0.2250	54 Xe < 0
55 Cs 0.0347	56 Ba < 0	81 Tl 0.0221	82 Pb 0.0809	83 Bi 0.0809	84 Po 0.1397	85 At 0.2058	86 Rn < 0

21 Sc <0	22 Ti 0.0147	23 V 0.0368	24 Cr 0.0485	25 Mn < 0	26 Fe 0.0184	27 Co 0.0515	28 Ni 0.0845	29 Cu 0.0901	30 Zn <0
39 Y =0	40 Zn 0.0368	41 Nb 0.0735	42 Mo 0.0735	43 Tc 0.0515	44 Ru 0.0809	45 Rh 0.0882	46 Pd 0.0441	47 Ag 0.0958	48 Cd <0
57 La 0.0368	72 Hf <0	73 Ta 0.0441	74 W 0.0441	75 Re 0.0110	76 Os 0.0809	77 Ir 0.1176	78 Pt 0.1564	79 Au 0.1697	80 Hg <0

FIG. 2. Periodic chart showing best electron affinities (in rydbergs) for atomic negative ions.

TABLE II. Computed IPM electronic binding energies (in rydbergs) in atomic negative ions, from the one-parameter search (d).

Negative ion	$1s$	$2s$	$2p$	$3s$	$3p$
$_3Li^-$	3.7219	0.0456			
$_5B^-$	12.894	0.3935	0.0206		
$_6C^-$	19.547	0.6666	0.0932		
$_8O^-$	36.702	1.1404	0.1075		
$_9F^-$	47.516	1.5814	0.2499		
$_{11}Na^-$	75.445	4.7239	2.7021	0.0401	
$_{13}Al^-$	111.55	8.8190	6.1362	0.4192	0.0338
$_{14}Si^-$	131.99	10.987	7.9590	0.5955	0.1016
$_{15}P^-$	153.83	12.958	9.5714	0.6079	0.0546
$_{16}S^-$	177.76	15.635	11.892	0.8365	0.1525
$_{17}Cl^-$	203.40	18.526	14.421	1.0798	0.2657
$_{19}K^-$	261.01	26.799	21.966	2.6329	1.4452
$_{22}Ti^-$	359.17	39.210	33.212	4.2194	2.5726
$_{23}V^-$	395.29	43.709	37.312	4.7124	2.9056
$_{24}Cr^-$	432.98	48.185	41.385	5.0462	3.0802
$_{26}Fe^-$	513.95	58.513	50.890	6.2007	3.8823
$_{27}Co^-$	557.03	64.017	55.976	6.7890	4.2865
$_{28}Ni^-$	601.84	69.766	61.301	7.3958	4.7037
$_{29}Cu^-$	648.83	76.555	67.651	8.5798	5.6794
$_{31}Ga^-$	748.86	92.480	82.645	12.276	8.9375
$_{32}Ge^-$	801.09	100.11	89.809	13.661	10.107
$_{33}As^-$	854.74	107.41	96.651	14.616	10.846
$_{34}Se^-$	910.51	115.68	104.44	16.166	12.171
$_{35}Br^-$	968.02	124.20	112.48	17.752	13.528
$_{37}Rb^-$	1090.1	145.54	132.73	24.021	19.324
$_{39}Y^-$	1217.4	164.65	150.80	27.700	22.518
$_{40}Zr^-$	1283.6	174.61	160.23	29.605	24.172

TABLE II. (*Continued*).

Negative ion	3*d*	4*s*	4*p*	4*d*	5*s*
$_{3}Li^{-}$					
$_{5}B^{-}$					
$_{6}C^{-}$					
$_{8}O^{-}$					
$_{9}F^{-}$					
$_{11}Na^{-}$					
$_{13}Al^{-}$					
$_{14}Si^{-}$					
$_{15}P^{-}$					
$_{16}S^{-}$					
$_{17}Cl^{-}$					
$_{19}K^{-}$		0.0368			
$_{22}Ti^{-}$	0.0147	0.0864			
$_{23}V^{-}$	0.0368	0.0824			
$_{24}Cr^{-}$		0.0485			
$_{26}Fe^{-}$	0.0184	0.0455			
$_{27}Co^{-}$	0.0515	0.0395			
$_{28}Ni^{-}$	0.0845	0.0297			
$_{29}Cu^{-}$	0.5940	0.0901			
$_{31}Ga^{-}$	2.9232		0.0221		
$_{32}Ge^{-}$	3.6575		0.0877		
$_{33}As^{-}$	3.9543		0.0588		
$_{34}Se^{-}$	4.8263		0.1484		
$_{35}Br^{-}$	5.7241	1.1294	0.2493		
$_{37}Rb^{-}$	10.650	2.9192	1.6600		0.0357
$_{39}Y^{-}$	12.881	3.4832	2.0518	0.0010	0.0553
$_{40}Zr^{-}$	14.039	3.7641	2.2449	0.0368	0.0633

	1*s*	2*s*	2*p*	3*s*	3*p*
$_{41}Nb^{-}$	1351.7	184.89	169.98	31.594	25.906
$_{42}Mo^{-}$	1421.4	195.34	179.89	33.530	27.584
$_{43}Tc^{-}$	1492.8	205.88	189.89	35.347	29.136
$_{44}Ru^{-}$	1566.2	217.21	200.66	37.675	31.196
$_{45}Rh^{-}$	1641.2	228.64	211.52	39.882	33.130
$_{46}Pd^{-}$	1717.7	239.62	221.97	41.483	34.451
$_{47}Ag^{-}$	1796.6	252.29	234.03	44.408	37.095
$_{49}In^{-}$	1960.3	279.76	260.23	51.653	43.768
$_{50}Sn^{-}$	2044.5	293.42	273.26	54.905	46.726
$_{51}Sb^{-}$	2130.1	306.57	285.80	57.458	48.978
$_{52}Te^{-}$	2217.7	320.70	299.29	60.725	51.942
$_{53}I^{-}$	2307.2	335.14	313.08	64.076	54.984
$_{55}Cs^{-}$	2492.6	367.65	344.15	73.662	63.949
$_{57}La^{-}$	2683.8	398.58	373.72	80.838	70.477
$_{73}Ta^{-}$	4544.1	726.78	695.46	160.24	145.21
$_{74}W^{-}$	4673.4	748.95	717.03	165.50	150.12
$_{75}Re^{-}$	4804.5	771.30	738.79	170.67	154.94
$_{76}Os^{-}$	4937.6	794.49	761.34	176.47	160.39
$_{77}Ir^{-}$	5072.4	817.83	784.07	182.17	165.73
$_{78}Pt^{-}$	5210.0	843.76	809.23	190.44	173.64
$_{79}Au^{-}$	5348.5	867.87	832.70	196.42	179.25
$_{81}Tl^{-}$	5631.9	919.48	882.86	211.29	193.39
$_{82}Pb^{-}$	5776.2	945.33	908.01	218.36	200.08
$_{83}Bi^{-}$	5921.9	970.77	932.79	224.68	206.02
$_{84}Po^{-}$	6069.8	997.15	958.48	231.77	212.73
$_{85}At^{-}$	6219.4	1023.9	984.49	238.95	219.53

TABLE II. (*Continued*).

Negative ion	3*d*	4*s*	4*p*	4*d*	4*f*
$_{41}Nb^-$	15.267	4.0667	2.4565	0.0838	
$_{42}Mo^-$	16.425	4.3159	2.6176	0.0965	
$_{43}Tc^-$	17.441	4.4748	2.6941	0.0515	
$_{44}Ru^-$	18.971	4.8873	3.0024	0.1562	
$_{45}Rh^-$	20.359	5.2089	3.2257	0.2040	
$_{46}Pd^-$	21.099	5.1726	3.1167	0.0257	
$_{47}Ag^-$	23.199	5.8369	3.6535	0.2800	
$_{49}In^-$	28.805	7.9365	5.4592	1.4312	
$_{50}Sn^-$	31.197	8.7514	6.1445	1.8595	
$_{51}Sb^-$	32.845	9.1127	6.3970	1.9196	
$_{52}Te^-$	35.220	9.8852	7.0401	2.3124	
$_{53}I^-$	37.664	10.684	7.7078	2.7279	
$_{55}Cs^-$	45.503	14.095	10.795	5.1542	
$_{57}La^-$	50.768	15.835	12.266	6.1244	
$_{73}Ta^-$	115.75	33.254	27.267	16.247	2.5683
$_{74}W^-$	119.96	34.397	28.245	16.904	2.7631
$_{75}Re^-$	124.06	35.431	29.114	17.450	2.8505
$_{76}Os^-$	128.08	36.882	30.393	18.393	3.3000
$_{77}Ir^-$	133.42	38.220	31.558	19.222	3.6393
$_{78}Pt^-$	140.67	41.433	34.579	21.869	5.6991
$_{79}Au^-$	145.55	42.894	35.864	22.810	6.1433
$_{81}Tl^-$	158.27	47.910	40.505	26.727	8.9963
$_{82}Pb^-$	164.23	50.077	42.486	28.348	10.097
$_{83}Bi^-$	169.40	51.612	43.838	29.344	10.580
$_{84}Po^-$	175.37	53.710	45.748	30.887	11.598
$_{85}At^-$	181.40	55.828	47.675	32.446	12.628

	5*s*	5*p*	5*d*	6*s*	6*p*
$_{41}Nb^-$	0.0735				
$_{42}Mo^-$	0.0735				
$_{43}Tc^-$	0.0586				
$_{44}Ru^-$	0.0809				
$_{45}Rh^-$	0.0882				
$_{46}Pd^-$	0.0441				
$_{47}Ag^-$	0.0958				
$_{49}In^-$	0.4346	0.0221			
$_{50}Sn^-$	0.5771	0.0919			
$_{51}Sb^-$	0.5738	0.0772			
$_{52}Te^-$	0.7020	0.1451			
$_{53}I^-$	0.8414	0.2257			
$_{55}Cs^-$	1.9041	1.0405		0.0347	
$_{57}La^-$	2.2754	1.3115	0.0368		
$_{73}Ta^-$	4.5046	2.6958	0.0441		
$_{74}W^-$	4.6495	2.7849	0.0441		
$_{75}Re^-$	4.7333	2.8187	0.0110		
$_{76}Os^-$	5.0142	3.0286	0.0809		
$_{77}Ir^-$	5.2320	3.1816	0.1176		
$_{78}Pt^-$	6.4035	4.2033	0.7549	0.1564	
$_{79}Au^-$	6.6729	4.4039	0.8313	0.1697	
$_{81}Tl^-$	8.3305	5.8432	1.7951		0.0221
$_{82}Pb^-$	8.9744	6.3942	2.1589	0.5813	0.0809
$_{83}Bi^-$	9.2532	6.6026	2.2426	0.5947	0.0809
$_{84}Po^-$	9.8443	7.1042	2.5687	0.7036	0.1399
$_{85}At^-$	10.441	7.6115	2.9016	0.8176	0.2062

TABLE III. Values of d which give rise to the binding energies in Table II.

Negative ion	d	Negative ion	d
$_3Li^-$	3.2891	$_{41}Nb^-$	1.2737
$_5B^-$	2.1956	$_{42}Mo^-$	1.2169
$_6C^-$	1.6823	$_{43}Tc^-$	1.1384
$_8O^-$	0.8920	$_{44}Ru^-$	1.1283
$_9F^-$	0.7755	$_{45}Rh^-$	1.0931
$_{11}Na^-$	1.4316	$_{46}Pd^-$	0.9887
$_{13}Al^-$	1.8644	$_{47}Ag^-$	1.0194
$_{14}Si^-$	1.7455	$_{49}In^-$	1.2229
$_{15}P^-$	1.3457	$_{50}Sn^-$	1.2705
$_{16}S^-$	1.2850	$_{51}Sb^-$	1.2088
$_{17}Cl^-$	1.2065	$_{52}Te^-$	1.2332
$_{19}K^-$	1.7766	$_{53}I^-$	1.2575
$_{22}Ti^-$	1.4563	$_{55}Cs^-$	1.8123
$_{23}V^-$	1.3077	$_{57}La^-$	1.8457
$_{24}Cr^-$	1.1203	$_{73}Ta^-$	0.9356
$_{26}Fe^-$	0.9556	$_{74}W^-$	0.9126
$_{27}Co^-$	0.8823	$_{75}Re^-$	0.8829
$_{28}Ni^-$	0.8172	$_{76}Os^-$	0.8775
$_{29}Cu^-$	0.8300	$_{77}Ir^-$	0.8641
$_{31}Ga^-$	1.0170	$_{78}Pt^-$	0.9594
$_{32}Ge^-$	1.0147	$_{79}Au^-$	0.9459
$_{33}As^-$	0.9366	$_{81}Tl^-$	1.0513
$_{34}Se^-$	0.9386	$_{82}Pb^-$	1.0787
$_{35}Br^-$	0.9349	$_{83}Bi^-$	1.0561
$_{37}Rb^-$	1.4323	$_{84}Po^-$	1.0725
$_{39}Y^-$	1.3559	$_{85}At^-$	1.0877
$_{40}Zr^-$	1.3119		

the present eigenvalues are in precise agreement with the recommended values of electron affinities, while the HF values are very inaccurate for the most part. Figure 2 is a periodic chart giving the recommended values of the electron affinities of negative ions in the main body of the periodic table.

III. SYSTEMATIC TRENDS

We have examined the potential parameters d and $\mathscr{H}$ for systematic trends throughout the periodic table, and we find that although d and $\mathscr{H}$ individually do not show any regular behavior throughout the periodic table, the ratio $\mathscr{H}/d$ is quite regular (see Fig. 1). For any given row in Fig. 2, the values of $\mathscr{H}/d$ are appreciably constant for the most part; and as we go from row to row (Z increasing) the values of $\mathscr{H}/d$ increase systematically in an almost linear fashion. As shown in Fig. 1, the values of $\mathscr{H}/d$ considered as a function of Z are scattered around the straight lines

$$\mathscr{H}/d = \begin{cases} 0.1639Z + 0.9096, & Z < 10 \quad (5) \\ 0.0637Z + 2.0043, & 10 < Z < 60 \quad (6) \\ 0.0478Z + 2.4695, & Z > 60 \quad (7) \end{cases}$$

which are the best linear fits to the values of $\mathscr{H}/d$ for low ($Z<10$), medium ($10<Z<60$), and high ($Z>60$) values of Z. The approximate linear behavior of the ratio $\mathscr{H}/d$ with increasing Z suggests that the previous fitting can be done by varying one independent parameter, d, while $\mathscr{H}$ is constrained to have the following dependences on Z and d:

$$\mathscr{H} = \begin{cases} (0.1639Z + 0.9096)d, & Z < 10 \quad (8) \\ (0.0637Z + 2.0043)d, & 10 < Z < 60 \quad (9) \\ (0.0478Z + 2.4695)d, & Z > 60 \; . \quad (10) \end{cases}$$

The energy eigenvalues obtained from these one-parameter searches are given in Table II, and the corresponding values of d are given in Table III. From Table I it can be seen that the one-parameter searches reproduce the electron affinities very precisely. The values of d obtained from the one-parameter searches are close to unity in most cases.

IV. CONCLUSION

In this article we have dwelt on IPM descriptions of the bound states of atomic negative ions. Starting with a simple analytic potential containing two adjustable parameters we have arrived at a realistic set of binding energies of every stable negative ion from $Z=3$ to $Z=85$.

The IPM potentials obtained in this work may be used in starting points for electron-atom[11] and electron-molecule[12] scattering problems. These potentials should also be applicable to the calculation of photodetachment cross sections. The fact that they are precisely tuned to the electronic affinities should give these IPM's a substantial advantage over Hartree-Fock calculations.

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[1]H. S. W. Massey, *Negative Ions* (Cambridge University, Cambridge, England, 1950).

[2]L. M. Branscomb, in *Atomic and Molecular Processes,* edited by D. R. Bates (Academic, New York, 1962).

[3]E. W. McDaniel, *Collision Phenomena in Ionized Gases* (Wiley, New York, 1964), Chap. 5.

[4]H. Hotop and W. C. Lineberger, J. Phys. Chem. Ref. Data **4**, 539 (1975).

[5]P. S. Ganas, J. Talman, and A. E. S. Green, Phys. Rev. A **22**, 336 (1980).

[6]A. E. S. Green, D. L. Sellin, and A. S. Zachor, Phys. Rev. **184**, 1 (1969).

[7]R. H. Garvey, C. H. Jackman, and A. E. S. Green, Phys. Rev. A **12**, 1144 (1975).

[8]P. S. Ganas and A. E. S. Green, Phys. Rev. A **4**, 182 (1971).

[9]E. Clementi and C. Roetti, At. Data Nucl. Data Tables **14**, 177 (1974).

[10]Kai Siegbahn *et al.*, ESCA: Atomic, Molecular and Solid State Structure Studied by Means of Electron Spectroscopy, Uppsala, 1967.

[11]A. E. S. Green, P. F. Schippnick, D. E. Rio, and P. S. Ganas, Int. J. Quantum Chem. Symp. **14**, 71 (1980).

[12]P. S. Ganas and A. E. S. Green, J. Chem. Phys. **76**, 1819 (1982).