

Supporting Information

Atomic / Ionic Radius as Mathematical Limit of System Energy Evolution

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Table S1. Experimental static dipole polarizabilities of ions, in a_0^3 . *) The polarizability of Li^{-1} is predicted value.

Ion	Static Dipole Polarizability
H	-1 211.49 ¹ , 230.1 ^{2,3} , 212 ⁴ , 203.8 ⁵
Li	-1 1050.0 ^{*,6}
	+1 0.193 ¹ , 0.202 ⁷ , 0.1883 ⁸ , 0.159 ⁹ , 0.191 ¹⁰⁻¹² , 0.216 ¹³ , 0.202 ¹⁴ , 0.16 ¹⁵ , 0.169 ¹⁶ ,
Be	+2 0.0398 ⁹ , 0.047 ^{1,15,16} , 0.027 ¹⁷
B	+3 0.019 ⁹ , 0.013 ^{15,17} , 0.0223 ^{1,16}
C	+4 0.0088 ⁹ , 0.00999 ¹² , 0.0067 ¹⁵ , 0.00810 ¹⁷ , 0.0101 ^{1,16}
N	+4 1.606 ¹⁸
O	-2 3.4-21.6 ⁷ , 18.56 ¹⁷ , 52.37 ¹⁹
F	-1 4.32 ⁷ , 10.53 ¹¹ , 6.68 ^{1,22} , 6.61 ¹⁷ , 12.41 ¹⁹ , 13.56 ¹⁹ , 7.33 ^{17,20,21} , 8.01 ^{21,22}
Ne	+1 1.3028 ²³ , 1.310 ²³
Na	+1 1.147 ^{1,16} , 0.9987 ^{10,11,27} , 1.316 ¹³ , 1.181 ¹⁵ , 1.32 ¹⁷ , 0.30 ^{17,20,21} , 0.11 ^{21,22} , 1.49 ^{21,22} , 0.978 ²⁴ , 1.0015 ²⁵ , 0.9980 ²⁶
Mg	+1 34.62 ²⁸ , 33.0 ²⁹ , 33.8 ³⁰ , 35.02 ³¹
	+2 0.675 ^{1,16} , 0.63 ¹⁵ , 0.742 ¹⁷ , 0.810 ¹⁷ , 0.489 ²⁴ , 0.486 ³² ,
Al	+1 24.20 ³³
	+2 12.18 ³⁴
	+3 0.36 ¹⁵ , 0.452 ¹⁷ , 0.358 ^{1,16,35}
Si	+2 11.666 ³⁶ , 11.669 ³⁷
	+3 6.858 ³⁸ , 7.404 ³⁹
	+4 0.22 ¹⁵ , 0.27 ¹⁷ , 0.29 ^{1,22}
P	+3 6.312 ⁴⁰
	+4 3.699 ⁴¹
	+5 0.14 ¹⁵

S	-2	32.4-39.8 ⁷ , 58.04 ¹⁷ ,
	+4	4.49 ³³
	+5	2.45 ⁴²
Cl	-1	19.98 ⁷ , 29.76 ¹¹ , 23.82 ¹⁷ , 32.93 ¹⁹ , 23.69 ^{17,20,21} , 21.74 ^{21,22} , 22.93 ^{21,22} , 20.58 ^{1,22}
	+5	2.77 ³³
	+6	1.62 ⁴³
Ar	+6	2.00 ³³
K	+1	5.47 ^{11,24} , 5.54 ¹⁵ , 5.932 ¹⁷ , 5.94 ¹⁷ , 5.40 ^{1,16}
Ca	+1	70.89 ²⁸ , 75.3 ⁴⁴ , 72.5 ⁴⁵ , 73.89 ⁴⁶ , 74.05 ⁴⁷ , 76.1 ⁴⁸
	+2	3.16 ¹⁵ , 3.64 ^{1,16} , 3.44 ¹⁷ , 3.017 ¹⁷ , 3.26 ²⁴ , 3.17 ⁴⁹ , 7.42 ⁴⁹
Sc	+3	1.94 ¹⁵ , 2.36 ¹⁷
Ti	+4	1.24 ¹⁵ , 1.59 ¹⁷
V	+5	0.823 ¹⁵
Cr	+6	0.57 ¹⁵
Ni	+1	7.92 ⁵⁰ , 7.949 ⁵¹
Cu	+1	10.8 ⁵²
Zn	+2	1.91 ¹⁵ , 1.95 ²¹
Ga	+1	18.14 ³³
	+3	1.32 ¹⁵
Ge	+2	10.68 ³³
	+4	0.924 ¹⁵
As	+3	6.19 ³³
	+5	0.674 ¹⁵
Se	-2	40.5-50.6 ⁷ , 75.58 ¹⁷
	+4	4.61 ³³
	+6	0.49 ¹⁵
Br	-1	28.07 ⁷ , 39.41 ¹¹ , 33.54 ¹⁷ , 32.83 ^{17,20,21} , 29.91 ^{21,22} , 31.91 ^{21,22}
	+5	3.37 ³³
Kr	+6	2.70 ³³
	+7	2.69 ⁵³
Rb	+1	9.25 ¹¹ , 9.697 ¹⁵ , 10.1 ¹⁶ , 10.53 ¹⁷ , 9.63 ^{17,21,22} , 10.20 ^{21,22} , 11.09 ^{21,22} , 9.0 ⁵⁴ , 9.05 ⁵⁵
Sr	+2	5.81 ¹⁵ , 6.7 ¹⁶ , 5.959 ¹⁷ , 5.80 ¹⁷ , 5.20 ⁵⁵
Y	+3	3.67 ¹⁵
Zr	+4	2.41 ¹⁵
Nb	+5	1.63 ¹⁵
Mo	+6	1.14 ¹⁵
Ag	+1	11.01 ¹⁵ , 11.71 ²¹
Cd	+2	7.11 ¹⁵ , 7.41 ²¹

In	+1	18.8 ³³
	+3	4.46 ¹⁵
Sn	+2	11.9 ³³
	+4	3.23 ¹⁵
Sb	+3	7.19 ³³
	+5	2.25 ¹⁵
Te	-2	56.0-68.8 ⁷ , 105.95 ¹⁷ ,
	+4	5.50 ³³
	+6	1.63 ¹⁵
I	-1	43.39 ⁷ , 60.13 ¹¹ , 50.95 ¹⁷ , 48.87 ^{17,21,22} , 43.92 ^{21,22} , 46.03 ^{21,22} ,
	+5	4.04 ³³
Xe	+6	3.28 ³³
Cs	+1	16.53 ¹¹ , 15.86 ¹⁶ , 17.28 ¹⁷ , 16.69 ^{17,21,22} , 16.85 ^{21,22} , 17.36 ^{21,22} , 15.3 ⁵⁶
Ba	+2	10.76 ¹⁵ , 11.34 ¹⁷ , 10.1 ⁵⁶
La	+3	7.099 ¹⁵ , 8.77 ¹⁷
Ce	+4	4.74 ¹⁵
Yb	+1	47 ⁵⁷
Hf	+4	2.48 ¹⁵
Ta	+5	1.25 ¹⁵
W	+6	0.99 ¹⁵
Au	+1	13.95 ¹⁵
Hg	+2	9.32 ¹⁵ , 8.49 ²¹
Tl	+1	12.7 ³³
Pb	+2	24.45 ¹⁵ , 7.8 ³³ , 13.62 ⁵⁸ , 13.38 ⁵⁹
	+3	13.38 ⁵⁹
	+4	3.61 ⁵⁸ , 3.63 ⁶⁰
Bi	+3	5.7 ³³
Po	+4	4.3 ³³
At	+5	3.33 ³³
Rn	+6	2.64 ³³
Fr	+7	2.15 ³³
Ra	+8	1.78 ³³
Ac	+9	1.49 ³³
Th	+3	15.42 ⁶¹
	+4	7.702 ⁶¹ , 7.61 ⁶² , 7.02 ⁶³ , 7.72 ⁶⁴
	+10	1.26 ³³
Pa	+11	1.08 ³³
U	+12	0.94 ³³

Table S2. Hardness of cations calculated from experimental ionization potentials⁶⁵, in Hartree.

	I	II	III	IV	V	VI	VII	VIII	IX	X	XI	XII
2 He	0.548											
3 Li	1.291	0.860										
4 Be	0.163	2.493	1.173									
5 B	0.310	0.235	4.069	1.486								
6 C	0.241	0.432	0.305	6.019	1.799							
7 N	0.277	0.328	0.552	0.375	8.345	2.113						
8 O	0.395	0.364	0.413	0.670	0.445	11.046	2.428					
9 F	0.322	0.510	0.449	0.498	0.789	0.515	14.125	2.742				
10 Ne	0.356	0.413	0.619	0.535	0.583	0.907	0.585	17.579	3.057			
11 Na	0.774	0.447	0.501	0.726	0.621	0.667	1.024	0.654	21.411	3.373		
12 Mg	0.136	1.196	0.535	0.588	0.836	0.703	0.752	1.141	0.725	25.620	3.691	
13 Al	0.236	0.177	1.682	0.622	0.674	0.942	0.788	0.835	1.261	0.795	30.207	4.009
14 Si	0.151	0.315	0.214	2.235	0.707	0.758	1.048	0.874	0.923	1.378	0.865	35.173
15 P	0.171	0.192	0.390	0.250	2.855	0.793	0.846	1.149	0.960	1.012	1.495	0.936
16 S	0.238	0.210	0.228	0.466	0.284	3.544	0.878	0.933	1.249	1.053	1.096	1.613
17 Cl	0.199	0.290	0.255	0.263	0.537	0.315	4.301	0.951	1.021	1.353	1.152	1.189
18 Ar	0.218	0.241	0.350	0.279	0.294	0.612	0.352	5.126	1.033	1.107	1.457	1.247
19 K	0.501	0.260	0.278	0.400	0.308	0.334	0.686	0.385	6.027	1.119	1.189	1.566
20 Ca	0.106	0.717	0.301	0.317	0.446	0.338	0.368	0.759	0.418	6.994	1.200	1.275
21 Sc	0.115	0.220	0.895	0.334	0.350	0.502	0.369	0.403	0.830	0.452	8.040	1.274
22 Ti	0.124	0.256	0.290	1.030	0.372	0.391	0.544	0.399	0.438	0.903	0.486	9.120
23 V	0.145	0.269	0.320	0.341	1.155	0.413	0.419	0.595	0.454	0.463	0.963	0.518
24 Cr	0.179	0.266	0.334	0.373	0.389	1.278	0.451	0.452	0.645	0.485	0.500	1.044
25 Mn	0.151	0.331	0.322	0.390	0.426	0.434	1.384	0.502	0.487	0.693	0.522	0.537
26 Fe	0.152	0.266	0.444	0.371	0.443	0.476	0.479	1.517	0.524	0.516	0.746	0.555
27 Co	0.169	0.302	0.327	0.518	0.413	0.494	0.531	0.521	1.640	0.544	0.570	0.790
28 Ni	0.193	0.313	0.362	0.389	0.587	0.459	0.533	0.570	0.581	1.771	0.570	0.588
29 Cu	0.231	0.304	0.377	0.412	0.426	0.661	0.496	0.606	0.606	0.612	1.905	0.588
30 Zn	0.157	0.400	0.362	0.426	0.467	0.478	0.735	0.533	0.643	0.661	0.676	2.001
31 Ga	0.267	0.187	0.612									
32 Ge	0.148	0.336	0.211	0.878								
33 As	0.163	0.179	0.400	0.230	1.194							
34 Se	0.210	0.177	0.223	0.466	0.246	1.354						
35 Br	0.183	0.261	0.208	0.228	0.531	0.265	1.650					
36 Kr	0.190	0.231	0.286	0.224	0.254	0.597	0.272	1.930	0.686	0.731	0.772	0.753
37 Rb	0.425	0.234	0.232	0.338	0.246	0.272	0.676	0.257	2.335			
38 Sr	0.098	0.585	0.259	0.268	0.353	0.279	0.300	0.729	0.276	2.703		
39 Y	0.111	0.152	0.736	0.301	0.294	0.423	0.239	0.316	0.823	0.276	3.087	
40 Zr	0.119	0.181	0.209	0.845								
41 Nb	0.139	0.197	0.244	0.225	0.946	0.422						
42 Mo	0.167	0.202	0.354	0.149	0.263	1.044	0.330	0.377	0.409	0.421	0.385	0.897
43 Tc	0.147	0.262										
44 Ru	0.173	0.215										
45 Rh	0.195	0.239										

46	Pd	0.204	0.248						
47	Ag	0.256	0.245						
48	Cd	0.145	0.378						
49	In	0.240	0.168	0.477					
50	Sn	0.134	0.292	0.188	0.580				
51	Sb	0.146	0.161	0.347	0.217	0.955			
52	Te	0.176	0.172	0.174	0.392	0.220	1.218		
53	I	0.159	0.255						
54	Xe	0.167	0.201						
55	Cs	0.354							
56	Ba	0.088							
57	La	0.101	0.149	0.565	0.214				
58	Ce	0.098	0.172	0.304	0.529	0.221			
59	Pr	0.093	0.203	0.319	0.341				
60	Nd	0.096	0.209	0.336					
61	Pm	0.098	0.209	0.345					
62	Sm	0.100	0.227	0.331					
63	Eu	0.102	0.251	0.327					
64	Gd	0.109	0.157	0.429					
65	Tb	0.104	0.191	0.329					
66	Dy	0.105	0.205	0.343					
67	Ho	0.106	0.203	0.361					
68	Er	0.107	0.199	0.367					
69	Tm	0.108	0.214	0.349					
70	Yb	0.109	0.237	0.340					
71	Lu	0.156	0.130	0.446	0.396				
72	Hf	0.148	0.154	0.184					
	...								
78	Pt	0.176	0.173						
79	Au	0.207	0.175						
80	Hg	0.153	0.284						
81	Tl	0.263	0.173						
82	Pb	0.140	0.311	0.191	0.487				
83	Bi	0.173	0.163	0.363	0.197	0.593	-1.622		
	...								
88	Ra	0.089							
89	Ac	0.127							
90	Th	0.095	0.156	0.162					

Table S3. Experimental vs. theoretical polarizabilities in Zn²⁺, Ag⁺, Tl⁺ isoelectronic series.

Ions	Expr.	Theoretical
Zn 2	+ 1.91 ¹⁵ , 1.95 ²¹	2.24 ⁶⁶ , 2.294 ⁶⁷ , 2.132 ⁶⁸ , 2.658 ⁶⁸ , 2.206 ⁶⁸ , 2.732 ⁶⁸
Ga 3	+ 1.32 ¹⁵	1.35 ²¹ , 1.228 ⁶⁶ , 1.242 ⁶⁷
Ge 4	+ 0.924 ¹⁵	0.97 ²¹ , 0.762 ⁶⁷
As 5	+ 0.674 ¹⁵	0.70 ²¹ , 0.506 ⁶⁷
Se 6	+ 0.49 ¹⁵	0.51 ²¹ , 0.358 ⁶⁷
A g 1	+ 11.71 ²¹ , 11.01 ¹⁵	8.27 ⁶⁶ , 7.78 ⁶⁹ , 8.23 ⁶⁹ , 8.40 ⁶⁹ , 8.93 ⁶⁹ , 8.68 ⁶⁹ , 9.20 ⁶⁹ , 8.47 ⁶⁹ , 9.00 ⁶⁹ , 6.88 ⁶⁹ , 7.29 ⁶⁹ , 7.56 ⁶⁹ , 7.96 ⁶⁹ , 10.598 ⁷⁰
Cd 2	+ 7.41 ²¹ , 7.11 ¹⁵	4.70 ⁶⁶ , 4.974 ⁶⁷ , 4.450 ⁶⁸ , 4.776 ⁶⁸ , 4.668 ⁶⁸ , 4.994 ⁶⁸
In 3	+ 4.46 ¹⁵	4.98 ²¹ , 3.220 ⁶⁷ , 3.345 ⁷¹
Sn 4	+ 3.23 ¹⁵	3.41 ²¹ , 2.261 ⁶⁷
Sb 5	+ 2.25 ¹⁵	2.46 ²¹ , 1.680 ⁶⁷
Te 6	+ 1.63 ¹⁵	1.78 ²¹
Tl 1	+ 12.7 ³³	35.1 ⁷² , 21.43 ⁷³ ,
Pb 2	+ 24.45 ¹⁵ , 7.8 ³³ , 13.62 ⁵⁸ , 13.38 ⁵⁹	17.88 ⁶⁷
Bi 3	+ 5.7 ³³	10.18 ⁷²

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