Spatial distribution of atomic electronic density for elements 1 to 54 as coming from a Hartree-Fock treatment within the minimum atomic parameters (MAP) paradigm, Supplementary Material

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Supplementary material for the article "Spatial distribution of atomic electronic density for elements 1 to 54 as coming from a Hartree-Fock treatment within the minimum atomic parameters (MAP) paradigm.".

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I. FULL DATA FOR TABLE I

Table I of the article shows MAP exponents for a Iodine atom, fitted to Bunge orbitals while respecting the position of the nodes. In Tables I to III we give exponents for all elements considered.

Table I. Optimized exponents for MAP orbitals fitted to Bunge orbitals. The overlap of the individual orbitals is maximized, for nodes fixed as given by Bunge's orbitals, leaving one single free parameter. Elements from $Z = 3$ to $Z = 36$.

Z	1s	2s	2p	3s	3p	3d	4s	4p	element
3	2.618301	0.735590	—	—		—	—	—	Li
4	3.615282	1.082930	—	—		—	—	—	Be
5	7.554751	2.550073	—	—	2.048265	—	—	—	O
6	4.603976	1.461440	—	—	1.137523	—	—	—	B
7	5.588829	1.824320	—	—	1.465192	—	—	—	C
8	6.571642	2.180983	—	—	1.784493	—	—	—	N
9	8.536688	2.913120	—	—	2.332038	—	—	—	F
10	9.517860	3.272287	—	—	2.625017	—	—	—	Ne
11	10.501953	3.760018	0.937670	—	3.155584	—	—	—	Na
12	11.488033	4.257317	1.239726	—	3.669802	—	—	—	Mg
13	12.475241	4.753206	1.583534	—	4.179680	1.131980	—	—	Al
14	13.463386	5.247135	1.889385	—	4.683952	1.430329	—	—	Si
15	14.452311	5.738954	2.177959	—	5.184686	1.709834	—	—	P
16	15.441997	6.229721	2.465678	—	5.680703	1.937655	—	—	S
17	16.432224	6.718670	2.743959	—	6.173880	2.178595	—	—	Cl
18	17.422890	7.206079	3.015977	—	6.671309	2.422863	—	—	Ar
19	18.414468	7.696050	3.386124	0.979230	7.164534	2.827555	—	—	K
20	19.406713	8.187131	3.756825	1.244847	7.657791	3.211642	—	—	Ca
21	20.400453	8.678090	4.048814	1.325242	8.150887	3.496916	—	2.140720	Sc
22	21.394933	9.167894	4.323794	1.385491	8.642321	3.762758	—	2.453277	Ti
23	22.389934	9.656769	4.591749	1.440382	9.132457	4.021318	—	2.708123	V
24	23.385401	10.144830	4.854644	1.491603	9.621504	4.274547	—	2.942090	Cr
25	24.381248	10.632073	5.112215	1.537121	10.109507	4.522579	—	3.175999	Mn
26	25.377321	11.119115	5.375716	1.593164	10.597197	4.778185	—	3.358628	Fe
27	26.373724	11.605515	5.634258	1.643537	11.084077	5.028366	—	3.555080	Co
28	27.370394	12.091442	5.890491	1.691612	11.570354	5.276243	—	3.752573	Ni
29	28.367272	12.576941	6.144686	1.738071	12.056124	5.521977	—	3.950238	Cu
30	29.364396	13.061994	6.396209	1.780201	12.541332	5.765158	—	4.151688	Zn
31	30.361085	13.546643	6.697242	2.107294	13.026053	6.073459	1.464235	4.560164	Ga
32	31.357780	14.031439	7.006824	2.384571	13.511100	6.392247	1.776096	4.951297	Ge
33	32.354455	14.516471	7.321959	2.640275	13.996505	6.717806	2.049857	5.329503	As
34	33.351169	15.001837	7.640949	2.892518	14.482284	7.045200	2.258240	5.699197	Se
35	34.347926	15.487492	7.962305	3.132794	14.968445	7.374413	2.477488	6.061179	Br
36	35.344730	15.973428	8.285168	3.365074	15.455007	7.709538	2.697687	6.417111	Kr

Table II. Optimized exponents for MAP orbitals fitted to Bunge orbitals, with fixed nodes, for $Z = 37$ to 54, orbitals $1s$ to $3d$.

Z	1s	2s	2p	3s	3p	3d	element
37	36.341620	16.460109	15.941984	8.610971	8.042434	6.771523	Rb
38	37.338656	16.947375	16.429368	8.938583	8.376163	7.123607	Sr
39	38.335884	17.434940	16.917133	9.265667	8.709720	7.474247	Y
40	39.333286	17.922824	17.405189	9.592488	9.042479	7.821814	Zr
41	40.330777	18.411003	17.893495	9.919090	9.374447	8.166584	Nb
42	41.328367	18.899468	18.382064	10.245379	9.705585	8.508964	Mo
43	42.326031	19.388184	18.870851	10.571215	10.035787	8.849716	Tc
44	43.323850	19.877214	19.359914	10.897023	10.365569	9.187067	Ru
45	44.321693	20.366443	19.849170	11.222300	10.694442	9.522859	Rh
46	45.319498	20.856751	20.338457	11.550924	11.021549	9.854714	Pd
47	46.317647	21.345560	20.828228	11.871542	11.349875	10.188601	Ag
48	47.315732	21.835401	21.317997	12.195435	11.676438	10.526847	Cd
49	48.313737	22.325567	21.808073	12.520453	12.003905	10.858612	In
50	49.311735	22.815952	22.298400	12.845593	12.331580	11.189925	Sn
51	50.309735	23.306547	22.788949	13.170868	12.659431	11.520868	Sb
52	51.307819	23.797374	23.279718	13.496305	12.987391	11.851557	Te
53	52.305877	24.288416	23.770726	13.821877	13.315464	12.181961	I
54	53.304001	24.779632	24.261927	14.147560	13.643731	12.512112	Xe

Table III. Optimized exponents for MAP orbitals fitted to Bunge orbitals, with fixed nodes, for $Z = 37$ to 54. Orbitals $4s$ to $5p$.

Z	4s	4p	4d	5s	5p	element
37	3.693094	3.066030	—	1.104737	—	Rb
38	4.019019	3.406375	—	1.371649	—	Sr
39	4.291626	3.679281	2.044428	1.483754	—	Y
40	4.544717	3.928882	2.380410	1.560535	—	Zr
41	4.787258	4.166925	2.650623	1.625276	—	Nb
42	5.022335	4.397249	2.894705	1.682084	—	Mo
43	5.250465	4.620428	3.131809	1.730212	—	Tc
44	5.479137	4.844944	3.322481	1.787925	—	Ru
45	5.702334	5.063786	3.521456	1.837509	—	Rh
46	5.949507	5.250657	3.548081	3.804374	—	Pd
47	6.138373	5.491152	3.915438	1.924892	—	Ag
48	6.351661	5.700043	4.111720	1.961979	—	Cd
49	6.608266	5.966092	4.457461	2.265380	1.644920	In
50	6.868528	6.236860	4.788138	2.518486	1.940877	Sn
51	7.130739	6.510581	5.107861	2.748888	2.196822	Sb
52	7.394013	6.782563	5.420731	2.973725	2.387778	Te
53	7.657479	7.054029	5.726611	3.186302	2.587723	I
54	7.920674	7.330701	6.026811	3.390525	2.787198	Xe

II. FIT OF MAP PARAMETERS TO BUNGE ORBITALS VIA THE FROBENIUS INNER PRODUCT

We give here all exponens as obtained from a fit of the MAP parameters to Bunge orbitals via minimization of the Frobenius angle of the respecive subspaces.

Table IV. Minimization of the Frobenius angle between MAP and Bunge orbitals via a multi-dimensional simplex optimization. Elements from $Z = 3$ to $Z = 36$.

Z	1s	2s	2p	3s	3p	3d	4s	4p	cos(angle)	element
3	2.658803	0.743259	—	—	—	—	—	—	0.999	Li
4	3.683335	1.096211	—	—	—	—	—	—	0.998	Be
5	4.698410	1.478538	1.137456	—	—	—	—	—	0.996	O
6	5.707192	1.845994	1.465050	—	—	—	—	—	0.996	B
7	6.720973	2.206308	1.784282	—	—	—	—	—	0.995	C
8	7.734178	2.577791	2.048604	—	—	—	—	—	0.994	N
9	8.724014	2.945277	2.332398	—	—	—	—	—	0.993	F
10	9.736118	3.308738	2.624991	—	—	—	—	—	0.992	Ne
11	10.735619	3.894043	3.155567	0.960254	—	—	—	—	0.993	Na
12	11.746989	4.427527	3.670237	1.273662	—	—	—	—	0.994	Mg
13	12.692781	4.954379	4.317799	1.626251	1.156346	—	—	—	0.991	Al
14	13.774102	5.467379	4.854114	1.938603	1.463236	—	—	—	0.992	Si
15	14.767466	5.973986	5.380821	2.232444	1.749557	—	—	—	0.992	P
16	15.621862	6.493006	5.906530	2.524890	1.984333	—	—	—	0.991	S
17	16.656732	6.995178	6.425346	2.806815	2.232319	—	—	—	0.991	Cl
18	17.650473	7.494420	6.940708	3.081402	2.483475	—	—	—	0.991	Ar
19	18.358516	8.078647	7.437483	3.560264	2.887415	—	1.010864	—	0.992	K
20	19.813407	8.520199	7.947041	3.955257	3.265011	—	1.290746	—	0.992	Ca
21	20.466055	9.084528	8.451021	4.262027	3.551927	2.140698	1.375294	—	0.986	Sc
22	21.465826	9.584717	8.963597	4.545035	3.820012	2.452907	1.437152	—	0.987	Ti
23	22.623021	10.057585	9.484253	4.817421	4.077975	2.707884	1.494977	—	0.987	V
24	23.346199	10.608462	10.032966	5.053706	4.277886	2.672506	1.455172	—	0.982	Cr
25	24.580294	11.239466	10.426524	5.351120	4.593624	3.178378	1.596229	—	0.987	Mn
26	25.702156	11.526694	10.991215	5.633301	4.845661	3.358964	1.653121	—	0.986	Fe
27	26.922249	12.063658	11.488707	5.895007	5.094339	3.555172	1.704863	—	0.986	Co
28	27.764010	12.540011	11.995888	6.166956	5.345327	3.752657	1.754024	—	0.985	Ni
29	29.052749	12.995875	12.497190	6.351786	5.551277	3.731074	1.574682	—	0.982	Cu
30	29.448899	13.840731	12.971130	6.673612	5.844058	4.152170	1.842333	—	0.985	Zn
31	30.965355	14.431454	13.526595	7.002877	6.343085	4.555167	2.187864	1.505642	0.983	Ga
32	31.758451	14.578197	14.088098	7.364913	6.673671	4.952081	2.482812	1.834431	0.985	Ge
33	32.544144	15.251371	14.595978	7.674868	7.027529	5.330043	2.750539	2.123143	0.987	As
34	33.823002	15.562959	15.038573	8.039455	7.387486	5.699944	3.007447	2.343051	0.987	Se
35	34.671315	16.398011	15.542795	8.433088	7.743890	6.057820	3.243532	2.573199	0.988	Br
36	35.776698	16.599964	16.016314	8.707546	8.091643	6.417659	3.493249	2.804816	0.989	Kr

Table V. Minimization of the Frobenius angle between MAP and Bunge orbitals via a multi-dimensional simplex optimization. Elements from $Z = 37$ to $Z = 54$, orbitals 1s to 3d.

Z	1s	2s	2p	3s	3p	3d	element
37	37.054404	17.184319	16.578873	9.053774	8.449835	6.771833	Rb
38	37.458054	17.657208	17.108165	9.411691	8.801685	7.124385	Sr
39	38.297384	18.145588	17.562346	9.776031	9.152382	7.785615	Y
40	39.622564	18.676852	18.011443	10.119084	9.499279	8.172191	Zr
41	40.991889	19.228150	18.707861	10.432617	9.839622	8.526450	Nb
42	41.940362	19.933907	19.158303	11.038642	10.166137	8.882643	Mo
43	42.908727	20.138397	19.567883	11.142889	10.526772	9.290488	Tc
44	44.435820	19.865028	20.308877	11.588036	10.876025	9.640192	Ru
45	44.840588	21.165039	20.614345	11.776566	11.213767	10.004516	Rh
46	47.214572	21.110677	22.138989	12.134314	11.370959	10.336606	Pd
47	48.295660	21.730447	21.310710	12.605081	11.943686	10.738390	Ag
48	47.627070	22.729494	21.946425	12.741093	12.284267	11.064694	Cd
49	48.628638	23.900068	22.584486	13.157948	12.626582	11.443093	In
50	49.520806	23.188559	23.292967	13.497879	12.868677	11.729162	Sn
51	50.933474	24.308765	23.595967	13.814699	13.283846	12.119666	Sb
52	51.487641	24.725350	24.330376	14.216822	13.593213	12.480086	Te
53	52.378111	25.750162	24.623552	14.571927	13.975430	12.842064	I
54	53.698294	26.005186	25.183708	14.814301	14.322030	13.185916	Xe

Table VI. Minimization of the Frobenius angle between MAP and Bunge orbitals via a multi-dimensional simplex optimization. Elements from $Z = 37$ to $Z = 54$, orbitals 4s to 5p.

Z	4s	4p	4d	5s	5p	cos(angle)	element
37	3.959514	3.180932	—	1.142926	—	0.989	Rb
38	4.329526	3.524389	—	1.427188	—	0.990	Sr
39	4.610438	3.801981	2.104538	1.546052	—	0.983	Y
40	4.874206	4.055887	2.456363	1.626870	—	0.984	Zr
41	5.088831	4.257234	2.516543	1.668069	—	0.982	Nb
42	5.331609	4.483481	2.795738	1.723558	—	0.983	Mo
43	5.590900	4.751519	3.239196	1.806878	—	0.986	Tc
44	5.812215	4.938844	3.255313	1.765764	—	0.983	Ru
45	6.004844	5.159015	3.474652	1.771900	—	0.984	Rh
46	6.306775	5.332985	3.521571	3.541070	—	0.963	Pd
47	6.408297	5.588549	3.906130	1.773781	—	0.984	Ag
48	6.731155	5.832023	4.261631	2.044124	—	0.986	Cd
49	6.991495	6.293326	4.601338	2.382114	1.707832	0.983	In
50	7.346419	6.611645	4.945294	2.639923	2.020531	0.985	Sn
51	7.567620	6.906217	5.252558	2.881962	2.291078	0.986	Sb
52	7.849668	7.203409	5.559006	3.116575	2.499282	0.987	Te
53	8.112024	7.488656	5.848317	3.338582	2.706284	0.987	I
54	8.384167	7.774153	6.141158	3.560267	2.920427	0.988	Xe

III. FULL DATA FOR TABLE II

Table II of the article shows exponents for a Iodine atom only. In the following tables VII to XIV we show optimized exponents for all elements considered. The first subsection shows fitting of primitive radial functions to Bunge orbitals, using the n of the principal number (Tables VII to IX), and the second subsection gives the same kind of fit for MAP orbitals (Tables XI to XIII). For shells with principal numbers 4 and 5 we give as well data following Slater's suggestion of an effective n^* (Tables X and XIV).

$$R_{n\ell}^{\text{Slater}}(r; Z_{n_\ell}^*) = N_n \; r^{n-1} e^{-\frac{Z_{n_\ell}^*}{n} r}$$

The optimization criterion is here the maximization of the overlap integral

$$S(Z_{n\ell}^*) = \int_0^\infty \phi_r^{\text{Bunge}}(r) R_{n\ell}^{\text{Slater}}(r; Z_{n\ell}^*) \, r^2 \, dr$$

easily evaluated by the overlap of two primitive Slater orbitals.

A. Slater to fit Bunge

Table VII. Fit of primitve Slater functions to Bunge orbitals, for $Z = 3$ to 36. For the $4s$ and the $4p$ shell $n = 4$ is used.

Z	1s	2s	2p	3s	3p	3d	4s	4p	element
3	2.618301	0.629133	—	—	—	—	—	—	Li
4	3.615282	0.914305	—	—	—	—	—	—	Be
5	4.603976	1.218585	1.137523	—	—	—	—	—	B
6	5.588828	1.511274	1.465192	—	—	—	—	—	C
7	6.571642	1.799368	1.784493	—	—	—	—	—	N
8	7.554750	2.095244	2.048264	—	—	—	—	—	O
9	8.536687	2.386963	2.332038	—	—	—	—	—	F
10	9.517859	2.676043	2.625017	—	—	—	—	—	Ne
11	10.501951	3.051785	3.155584	0.818519	—	—	—	—	Na
12	11.488032	3.432269	3.669801	1.048428	—	—	—	—	Mg
13	12.475240	3.810759	4.179680	1.295613	1.002363	—	—	—	Al
14	13.463385	4.187231	4.683952	1.512264	1.240317	—	—	—	Si
15	14.452310	4.561850	5.184686	1.715290	1.460261	—	—	—	P
16	15.441995	4.935495	5.680703	1.915362	1.641373	—	—	—	S
17	16.432224	5.307748	6.173880	2.108766	1.830180	—	—	—	Cl
18	17.422890	5.678858	6.671309	2.297818	2.022194	—	—	—	Ar
19	18.414466	6.051745	7.164534	2.540229	2.314436	—	0.840976	—	K
20	19.406713	6.425380	7.657790	2.780304	2.588102	—	1.032930	—	Ca
21	20.400452	6.798837	8.150887	2.977697	2.799753	2.140720	1.101685	—	Sc
22	21.394934	7.171509	8.642320	3.166259	2.999462	2.453277	1.156915	—	Ti
23	22.389933	7.543558	9.132457	3.351172	3.194600	2.708123	1.208199	—	V
24	23.385400	7.915083	9.621503	3.533384	3.386316	2.942090	1.256570	—	Cr
25	24.381248	8.286075	10.109507	3.713042	3.575033	3.175999	1.300973	—	Mn
26	25.377321	8.656981	10.597197	3.895484	3.767825	3.358627	1.352203	—	Fe
27	26.373725	9.027468	11.084076	4.075414	3.957374	3.555080	1.399370	—	Co
28	27.370396	9.397666	11.570354	4.254153	4.145491	3.752573	1.444775	—	Ni
29	28.367274	9.767593	12.056124	4.431732	4.332237	3.950238	1.488778	—	Cu
30	29.364397	10.137239	12.541332	4.608232	4.517561	4.151687	1.529822	—	Zn
31	30.361086	10.506730	13.026052	4.810800	4.742234	4.560163	1.759787	1.308725	Ga
32	31.357782	10.876375	13.511099	5.017270	4.972479	4.951297	1.949761	1.548184	Ge
33	32.354456	11.246233	13.996505	5.226124	5.206257	5.329503	2.122071	1.752084	As
34	33.351170	11.616364	14.482285	5.436603	5.440349	5.699197	2.288746	1.906223	Se
35	34.347927	11.986734	14.968444	5.647973	5.675099	6.061179	2.446308	2.065262	Br
36	35.344734	12.357321	15.455007	5.859867	5.913824	6.417111	2.597779	2.224172	Kr

Table VIII. Fit of primitve Slater functions to Bunge orbitals, for $Z = 37$ to 54, Orbitals from $4s$ to $5p$. For shells with $n = 4$ or 5 this n is used.

Z	1s	2s	2p	3s	3p	3d	element
37	36.341624	12.728444	15.941984	6.073266	6.150682	6.771522	Rb
38	37.338659	13.099982	16.429368	6.287571	6.387991	7.123607	Sr
39	38.335891	13.471760	16.917131	6.501721	6.625268	7.474247	Y
40	39.333290	13.843778	17.405187	6.715714	6.862033	7.821813	Zr
41	40.330784	14.216015	17.893494	6.929575	7.098312	8.166584	Nb
42	41.328373	14.588469	18.382063	7.143255	7.334091	8.508964	Mo
43	42.326036	14.961122	18.870849	7.356688	7.569326	8.849716	Tc
44	43.323861	15.333995	19.359913	7.570108	7.804333	9.187067	Ru
45	44.321700	15.707031	19.849169	7.783268	8.038834	9.522858	Rh
46	45.319505	16.080731	20.338456	7.998007	8.272300	9.854713	Pd
47	46.317654	16.453582	20.828228	8.208939	8.506580	10.188600	Ag
48	47.315744	16.827067	21.317997	8.421425	8.739830	10.526847	Cd
49	48.313748	17.200776	21.808073	8.634527	8.973741	10.858612	In
50	49.311747	17.574637	22.298399	8.847753	9.207858	11.189924	Sn
51	50.309750	17.948658	22.788948	9.061111	9.442167	11.520868	Sb
52	51.307831	18.322841	23.279716	9.274631	9.676629	11.851557	Te
53	52.305892	18.697171	23.770725	9.488288	9.911250	12.181959	I
54	53.304019	19.071633	24.261926	9.702067	10.146074	12.512112	Xe

Table IX. Fit of primitve Slater functions to Bunge orbitals, for $Z = 37$ to 54, Orbitals from $1s$ to $3d$. For shells with $n = 4$ or 5 this n is used.

Z	4s	4p	4d	5s	5p	element
37	2.798649	2.469246	—	0.960136	—	Rb
38	2.993565	2.689154	—	1.153700	—	Sr
39	3.158337	2.866748	1.853069	1.240986	—	Y
40	3.312533	3.029957	2.120875	1.305059	—	Zr
41	3.461024	3.185951	2.334036	1.361110	—	Nb
42	3.605613	3.337076	2.525312	1.411651	—	Mo
43	3.746732	3.483914	2.709812	1.456207	—	Tc
44	3.887666	3.630810	2.859778	1.506710	—	Ru
45	4.025951	3.774435	3.014827	1.551783	—	Rh
46	4.171955	3.898228	3.048967	2.518972	—	Pd
47	4.297373	4.055584	3.319609	1.633684	—	Ag
48	4.430969	4.193412	3.472980	1.669946	—	Cd
49	4.584522	4.359641	3.720011	1.876364	1.446225	In
50	4.739189	4.527246	3.952813	2.044331	1.663133	Sn
51	4.894248	4.695588	4.175410	2.194706	1.844816	Sb
52	5.049418	4.862034	4.391409	2.338446	1.979239	Te
53	5.204361	5.027639	4.601209	2.473191	2.116984	I
54	5.358946	5.196221	4.806118	2.601790	2.253851	Xe

Table X. Using n^*

Z	4s	4p	4d	5s	5p	element
	3.7	3.7	3.7	4.0	4.0	
19	0.782454	—	—	—	—	K
20	0.960145	—	—	—	—	Ca
21	1.023982	—	—	—	—	Sc
22	1.075306	—	—	—	—	Ti
23	1.122974	—	—	—	—	V
24	1.167905	—	—	—	—	Cr
25	1.209239	—	—	—	—	Mn
26	1.256835	—	—	—	—	Fe
27	1.300674	—	—	—	—	Co
28	1.342878	—	—	—	—	Ni
29	1.383721	—	—	—	—	Cu
30	1.421948	—	—	—	—	Zn
31	1.635158	1.217309	—	—	—	Ga
32	1.811326	1.439290	—	—	—	Ge
33	1.971138	1.628345	—	—	—	As
34	2.125698	1.770777	—	—	—	Se
35	2.271829	1.917985	—	—	—	Br
36	2.412327	2.065242	—	—	—	Kr
37	2.599231	2.293251	—	0.778289	—	Rb
38	2.780457	2.497536	—	0.932731	—	Sr
39	2.933343	2.662240	1.721244	1.002764	—	Y
40	3.076379	2.813576	1.969723	1.054290	—	Zr
41	3.214133	2.958250	2.167330	1.099461	—	Nb
42	3.348255	3.098385	2.344600	1.140193	—	Mo
43	3.479147	3.234523	2.515693	1.176129	—	Tc
44	3.609903	3.370763	2.654217	1.216705	—	Ru
45	3.738190	3.503951	2.797658	1.253028	—	Rh
46	3.873365	3.618148	2.826479	2.032875	—	Pd
47	3.989991	3.764675	3.079744	1.319166	—	Ag
48	4.113912	3.892473	3.221848	1.348649	—	Cd
49	4.256631	4.047014	3.452070	1.514412	1.170095	In
50	4.400358	4.202792	3.668714	1.649451	1.344034	Sn
51	4.544419	4.359240	3.875686	1.770431	1.489922	Sb
52	4.688561	4.513817	4.076442	1.886001	1.596703	Te
53	4.832468	4.667572	4.271350	1.994406	1.706767	I
54	4.976025	4.824242	4.461652	2.097916	1.816578	Xe

B. Slater to fit MAP

The same optimization of overlap integrals, now between MAP orbitals and primitive Slater functions, as

$$S(Z^*_{n\ell}) = \int_0^\infty \phi_r^{\rm MAP}(r) R_{n\ell}^{\rm Slater}(r; Z^*_{n\ell})\, r^2\, dr$$

Table XI. Using n, elements 3 - 36

Z	1s	2s	2p	3s	3p	3d	4s	4p	element
3	2.693715	0.651134	—	—	—	—	—	—	Li
4	3.707670	0.970025	—	—	—	—	—	—	Be
5	4.710990	1.305450	1.187159	—	—	—	—	—	B
6	5.711930	1.627907	1.546191	—	—	—	—	—	C
7	6.711659	1.945352	1.896201	—	—	—	—	—	N
8	7.711796	2.268279	2.205804	—	—	—	—	—	O
9	8.711201	2.587235	2.529366	—	—	—	—	—	F
10	9.710125	2.903778	2.858858	—	—	—	—	—	Ne
11	10.705261	3.288554	3.383365	0.811182	—	—	—	—	Na
12	11.701054	3.688407	3.898911	1.078054	—	—	—	—	Mg
13	12.697368	4.085216	4.415184	1.355758	1.047165	—	—	—	Al
14	13.694101	4.478873	4.933953	1.599835	1.306937	—	—	—	Si
15	14.691186	4.869907	5.455231	1.828388	1.550119	—	—	—	P
16	15.688627	5.259544	5.977812	2.052407	1.761951	—	—	—	S
17	16.686279	5.647216	6.502967	2.268527	1.979891	—	—	—	Cl
18	17.684097	6.033344	7.030642	2.479508	2.198875	—	—	—	Ar
19	18.682890	6.422521	7.548635	2.742415	2.506154	—	0.7513030	—	K
20	19.682189	6.811667	8.063154	3.011632	2.798375	—	0.9665291	—	Ca
21	20.681320	7.197722	8.574493	3.237883	3.043995	2.1020434	1.0256797	—	Sc
22	21.680566	7.582221	9.083118	3.446622	3.266725	2.5393582	1.0618914	—	Ti
23	22.680004	7.966036	9.590477	3.651671	3.485052	2.8447162	1.0963290	—	V
24	23.679531	8.349324	10.096859	3.853804	3.699775	3.1166665	1.1287616	—	Cr
25	24.679296	8.732026	10.602047	4.052486	3.910497	3.3801505	1.1579860	—	Mn
26	25.679101	9.114756	11.107204	4.253628	4.124934	3.6000061	1.1879161	—	Fe
27	26.678984	9.497041	11.611572	4.452163	4.335877	3.8282548	1.2161244	—	Co
28	27.679023	9.879723	12.116903	4.658872	4.558839	3.9914841	1.2457120	—	Ni
29	28.679062	10.260831	12.618681	4.845048	4.752910	4.2811233	1.2674230	—	Cu
30	29.679286	10.642334	13.121538	5.039428	4.958898	4.5086433	1.2915039	—	Zn
31	30.680008	11.022867	13.620655	5.257650	5.189129	4.9261301	1.5767688	1.203700	Ga
32	31.680039	11.403501	14.120030	5.481666	5.430165	5.3240789	1.8010966	1.457863	Ge
33	32.680781	11.783973	14.619586	5.708201	5.679040	5.7086190	1.9976979	1.673501	As
34	33.680781	12.164636	15.119424	5.937228	5.932918	6.0839439	2.1839800	1.845988	Se
35	34.681444	12.545006	15.619501	6.166482	6.191474	6.4517817	2.3569774	2.019877	Br
36	35.681405	12.925516	16.120196	6.396315	6.453975	6.8138005	2.5224370	2.191973	Kr

Table XII. Using n, elements 37 – 54

Z	1s	2s	2p	3s	3p	3d	element
37	36.681610	13.306832	16.621211	6.632982	6.716794	7.169553	Rb
38	37.681796	13.688615	17.122410	6.871199	6.978802	7.522132	Sr
39	38.682069	14.070476	17.623823	7.109769	7.239838	7.872158	Y
40	39.682049	14.459611	18.126148	7.346707	7.495495	8.238870	Zr
41	40.682578	14.832127	18.624604	7.565973	7.745573	8.602946	Nb
42	41.682890	15.212655	19.124913	7.793958	7.997157	8.968894	Mo
43	42.683164	15.593384	19.624841	8.021493	8.247500	9.336549	Tc
44	43.683515	15.973915	20.125410	8.248400	8.497686	9.703986	Ru
45	44.683671	16.354729	20.625376	8.474982	8.746618	10.073319	Rh
46	45.684028	16.735494	21.125705	8.700580	8.994957	10.443748	Pd
47	46.684335	17.116013	21.625572	8.925788	9.242491	10.815744	Ag
48	47.684550	17.496156	22.125329	9.150178	9.489291	11.189233	Cd
49	48.684687	17.878063	22.626413	9.377292	9.738351	11.555113	In
50	49.685250	18.258082	23.127249	9.604405	9.987220	11.917211	Sn
51	50.685661	18.638646	23.627810	9.830429	10.236464	12.276307	Sb
52	51.686215	19.019876	24.129242	10.057380	10.486291	12.633210	Te
53	52.686249	19.401566	24.631513	10.284720	10.736623	12.988135	I
54	53.686540	19.783126	25.133649	10.511597	10.986955	13.341070	Xe

Table XIII. Using n, elements 37 – 54

Z	4s	4p	4d	5s	5p	element
37	2.740580	2.438156	—	0.719538	—	Rb
38	2.961670	2.665857	—	0.912539	—	Sr
39	3.178230	2.880677	2.130386	1.138760	—	Y
40	3.339914	3.049011	1.931308	1.064394	—	Zr
41	3.477990	3.205029	2.248327	1.042651	—	Nb
42	3.631234	3.364101	2.469204	1.063206	—	Mo
43	3.780730	3.518202	2.672256	1.081908	—	Tc
44	3.929893	3.673155	2.841512	1.102921	—	Ru
45	4.075232	3.823566	3.013798	1.121428	—	Rh
46	4.218282	3.971906	3.183083	1.139164	—	Pd
47	4.359324	4.117765	3.350010	1.156720	—	Ag
48	4.497958	4.261578	3.516737	1.172661	—	Cd
49	4.658164	4.426260	3.771141	1.412739	1.150484	In
50	4.820130	4.596507	4.009531	1.595247	1.343337	Sn
51	4.982018	4.771279	4.237043	1.750281	1.512515	Sb
52	5.146157	4.948948	4.456772	1.896515	1.647559	Te
53	5.310803	5.129731	4.670043	2.033367	1.783780	I
54	5.474498	5.312218	4.877902	2.160544	1.917014	Xe

Table XIV. Using n^*

Z	4s*	5s*	4p*	5p*	4d*	
19	0.805817	—	—	—	—	K
20	1.036991	—	—	—	—	Ca
21	1.100405	—	—	—	—	Sc
22	1.139174	—	—	—	—	Ti
23	1.176046	—	—	—	—	V
24	1.210771	—	—	—	—	Cr
25	1.242057	—	—	—	—	Mn
26	1.274104	—	—	—	—	Fe
27	1.304307	—	—	—	—	Co
28	1.335990	—	—	—	—	Ni
29	1.359228	—	—	—	—	Cu
30	1.385009	—	—	—	—	Zn
31	1.691376	—	1.290744	—	—	Ga
32	1.932393	—	1.563638	—	—	Ge
33	2.143673	—	1.795251	—	—	As
34	2.343905	—	1.980532	—	—	Se
35	2.529877	—	2.167354	—	—	Br
36	2.707762	—	2.352278	—	—	Kr
37	2.942459	0.881549	2.617031	—	—	Rb
38	3.180412	1.118881	2.861981	—	—	Sr
39	3.413553	1.397761	3.093131	—	2.285767	Y
40	3.587492	1.305230	3.274195	—	2.071449	Zr
41	3.735998	1.278076	3.442001	—	2.412078	Nb
42	3.900871	1.303084	3.613112	—	2.649431	Mo
43	4.061704	1.325835	3.778873	—	2.867657	Tc
44	4.222187	1.351446	3.945566	—	3.049528	Ru
45	4.378545	1.373990	4.107365	—	3.234680	Rh
46	4.532437	1.395599	4.266936	—	3.416615	Pd
47	4.684162	1.416998	4.423835	—	3.596021	Ag
48	4.833289	1.436421	4.578528	—	3.775225	Cd
49	5.005750	1.731619	4.755787	1.409359	4.049017	In
50	5.180124	1.956269	4.939081	1.646454	4.305623	Sn
51	5.354431	2.147223	5.127286	1.854626	4.550562	Sb
52	5.531182	2.327433	5.318642	2.020822	4.787153	Te
53	5.708490	2.496139	5.513387	2.188548	5.016819	I
54	5.884782	2.652942	5.709997	2.352652	5.240677	Xe