I. Minimal Atomic Primitive basis sets for elements 1 to 54, Supplementary Material

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Supplementary material for the article "Minimal Atomic Primitive basis sets for elements 1 to 54".

I. TABLES OF EXPONENTS

Table I: Elements 1 to 36

Z	Atom	1s	2s	2p	3s	3p	3d	4s	4p
1	H	1.000000	—	—	—	—	—	—	—
2	He	1.687502	—	—	—	—	—	—	—
3	Li	2.693722	0.766686	—	—	—	—	—	—
4	Be	3.707671	1.159534	—	—	—	—	—	—
5	B	4.710990	1.579218	1.187182	—	—	—	—	—
6	C	5.711933	1.981429	1.546196	—	—	—	—	—
7	N	6.711682	2.376750	1.896216	—	—	—	—	—
8	O	7.711801	2.780614	2.205807	—	—	—	—	—
9	F	8.711213	3.178804	2.529365	—	—	—	—	—
10	Ne	9.710137	3.573487	2.858856	—	—	—	—	—
11	Na	10.705262	4.073095	3.383370	0.936581	—	—	—	—
12	Mg	11.701055	4.597624	3.898911	1.284556	—	—	—	—
13	Al	12.697604	5.118831	4.415321	1.663127	1.196582	—	—	—
14	Si	13.694116	5.636225	4.933955	1.999983	1.521695	—	—	—
15	P	14.691196	6.150096	5.455256	2.318181	1.829309	—	—	—
16	S	15.688973	6.662367	5.977871	2.633291	2.094983	—	—	—
17	Cl	16.686279	7.171912	6.502968	2.936768	2.370669	—	—	—
18	Ar	17.684133	7.679366	7.030633	3.234001	2.648909	—	—	—
19	K	18.683036	8.192091	7.548673	3.624961	3.062779	—	0.945539	—
20	Ca	19.682454	8.704996	8.063251	4.032424	3.459484	—	1.259072	—
21	Sc	20.682035	9.212633	8.574560	4.363612	3.785991	2.106735	1.331486	—
22	Ti	21.681554	9.718086	9.083306	4.663420	4.078148	2.540534	1.370045	—
23	V	22.680296	10.222936	9.590605	4.956695	4.363488	2.845245	1.405519	—
24	Cr	23.681034	10.727151	10.097294	5.246069	4.643488	3.117084	1.441161	—
25	Mn	24.679868	11.229622	10.602085	5.527008	4.917329	3.380100	1.468892	—
26	Fe	25.679509	11.732542	11.107194	5.813616	5.197415	3.600251	1.500036	—
27	Co	26.679478	12.235096	11.611747	6.096106	5.472295	3.828376	1.530045	—
28	Ni	27.680272	12.737319	12.115797	6.375551	5.744260	4.056032	1.557136	—
29	Cu	28.679464	13.238558	12.618752	6.651793	6.014222	4.281122	1.580615	—
30	Zn	29.680343	13.740131	13.121703	6.926485	6.281434	4.508920	1.607333	—
31	Ga	30.683746	14.242997	13.624191	7.261469	6.592868	4.924418	2.040701	1.525604
32	Ge	31.700036	14.751793	14.126348	7.596417	6.920801	5.325472	2.398180	1.863751
33	As	32.709359	15.249769	14.624879	7.958496	7.258370	5.705089	2.730393	2.176995
34	Se	33.698842	15.758374	15.122462	8.305893	7.609294	6.080494	3.013013	2.390673
35	Br	34.732976	16.259106	15.629240	8.657271	7.970487	6.452438	3.280007	2.658711
36	Kr	35.744778	16.768605	16.128661	9.005626	8.336293	6.816574	3.550695	2.908975

Table II: Elements 37 to 54

Z	Atom	1s	2s	2p	3s	3p	3d
37	Rb	36.682187	17.238749	16.621287	9.321820	8.692536	7.169531
38	Sr	37.682717	17.740437	17.122230	9.687469	9.057851	7.522048
39	Y	38.714164	18.258637	17.633780	10.071503	9.421560	7.882265
40	Zr	39.691863	18.747313	18.126582	10.405408	9.773349	8.240299
41	Nb	40.683871	19.243289	18.624540	10.746949	10.123748	8.602727
42	Mo	41.684240	19.743385	19.124876	11.094124	10.472772	8.968688
43	Tc	42.684469	20.244084	19.625003	11.439097	10.819885	9.336555
44	Ru	43.684407	20.743575	20.125165	11.784029	11.166972	9.703985
45	Rh	44.684989	21.243957	20.625324	12.128160	11.512328	10.073353
46	Pd	45.685390	21.744236	21.125685	12.471294	11.856300	10.443929
47	Ag	46.685073	22.243889	21.625460	12.812676	12.199441	10.815815
48	Cd	47.685950	22.743707	22.125372	13.153341	12.541450	11.189297
49	In	48.687466	23.244780	22.625998	13.499918	12.886859	11.554953
50	Sn	49.686714	23.745683	23.126862	13.844558	13.233057	11.917240
51	Sb	50.685800	24.245432	23.627814	14.189781	13.580090	12.276307
52	Te	51.686237	24.746517	24.129271	14.535850	13.927809	12.633214
53	I	52.687494	25.248422	24.631069	14.882280	14.276339	12.988047
54	Xe	53.688848	25.749559	25.133464	15.228510	14.625272	13.340843

Z	Atom	4s	4p	4d	5s	5p
37	Rb	3.840370	3.259506	—	1.022718	—
38	Sr	4.215132	3.618527	—	1.343339	—
39	Y	4.567649	3.942727	2.022470	1.538832	—
40	Zr	4.828797	4.213019	2.403524	1.521661	—
41	Nb	5.078696	4.466535	2.767116	1.525853	—
42	Mo	5.332942	4.715491	3.067395	1.547262	—
43	Tc	5.580156	4.956052	3.345319	1.566893	—
44	Ru	5.825975	5.198928	3.574433	1.590671	—
45	Rh	6.067229	5.434998	3.808113	1.610825	—
46	Pd	6.303299	5.666646	4.038913	1.630954	—
47	Ag	6.535604	5.895111	4.266306	1.649808	—
48	Cd	6.763356	6.119422	4.493548	1.667563	—
49	In	7.038805	6.386353	4.862655	2.073268	1.630105
50	Sn	7.318894	6.666079	5.210775	2.393323	1.950531
51	Sb	7.601792	6.956454	5.544434	2.671913	2.237940
52	Te	7.889710	7.254092	5.867813	2.937915	2.468644
53	I	8.179709	7.559399	6.182514	3.188955	2.704618
54	Xe	8.468346	7.870467	6.489983	3.423725	2.938461

II. POLYNOMIALS

Example of the $5s$ polynomial coefficients as functions of the exponents ξ_i. k_{ij} is defined as $k_{ij} = \xi_i/(\xi_i + \xi_j) \neq k_{ji}$. For determining the variables $a_{5s} \ldots d_{5s}$ the coefficients of the lower polynomials $a_{2s} \ldots c_{4s}$ are already known.

$$
\begin{aligned}
1 + 3\,k_{51}\,[\mathbf{a_{5s}} + 4\,k_{51}\,[\mathbf{b_{5s}} + 5k_{51}\,[\mathbf{c_{5s}} + 6k_{51}\,\mathbf{d_{5s}}]]] &= 0 \\
(1 + 3a_{2s}\,k_{25}) + 3k_{52}\,[(1 + 4\,k_{25}\,a_{2s})\,\mathbf{a_{5s}} + 4\,k_{52}\,[\,(1 + 5\,k_{25}\,a_{2s})\,\mathbf{b_{5s}} & \\
+5\,k_{52}\,[(1 + 6\,k_{25}\,a_{2s})\,\mathbf{c_{5s}} + 6\,k_{52}\,(1 + 7\,k_{25}\,a_{2s})\,\mathbf{d_{5s}}]]] &= 0 \\
(1 + 3\,k_{35}\,(a_{3s} + 4\,k_{35}\,b_{3s})) + 3\,k_{53}\,[(1 + 4\,k_{35}\,(a_{3s} + 5\,k_{35}\,b_{3s}))\,\mathbf{a_{5s}} & \\
+4\,k_{53}\,[(1 + 5\,k_{35}(a_{3s} + 6\,k_{35}\,[b_{3s}))\,\mathbf{b_{5s}} + 5k_{53}\,[(1 + 6\,k_{35} & \\
(a_{3s} + 7\,k_{35}\,b_{3s}))\,\mathbf{c_{5s}} + 6k_{53}\,(1 + 7\,k_{35}(a_{3s} + 8\,k_{35}\,b_{3s}))\,\mathbf{d_{5s}}]]] &= 0 \\
(1 + 3\,k_{45}(a_{4s} + 4\,k_{45}\,(b_{4s} + 5\,k_{45}\,c_{4s}))) & \\
+3k_{54}\,[(1 + 4\,k_{45}(a_{4s} + 5\,k_{45}(b_{4s} + 6\,k_{45}\,c_{4s})))\,\mathbf{a_{5s}} & \\
+\,4k_{54}\,[\,(1 + 5\,k_{45}\,(a_{4s} + 6\,k_{45}(\,b_{4s} + 7\,k_{45}\,c_{4s})))\,\mathbf{b_{5s}} & \\
+5k_{54}\,\Big[\,\Big(1 + 6\,k_{45}(\,a_{4s} + 7\,k_{45}(\,b_{4s}^2 + 8\,k_{45}\,c_{4s}))\Big)\,\mathbf{c_{5s}} & \\
+\;6k_{54}\,(1 + 7\,k_{45}(\,a_{4s} + 8\,k_{45}(\,b_{4s} + 9\,k_{45}\,c_{4s})))\,\mathbf{d_{5s}}]]] &= 0 \qquad (1)
\end{aligned}
$$

As example for the coefficients we give a Chromium atom. The primitive $r^{n-1}e^{-\xi r}$ is assumed to be normalized.

basis set and orbitals

sym	n-1	exp	coeff
S	0	23.6810340000	1.0000000000
S	0	10.7271510000	0.9046377106
S	1	10.7271510000	-1.6752955348
S	0	5.2460690000	0.4765433385
S	1	5.2460690000	-2.1817486029
S	2	5.2460690000	2.5092104017
S	0	1.4411610000	0.0184270805
S	1	1.4411610000	-0.2896594042
S	2	1.4411610000	1.4009472823
S	3	1.4411610000	-2.0519464210
P	1	10.0972940000	1.0000000000
P	1	4.6434880000	1.0854565962
P	2	4.6434880000	-1.8873362673
D	2	3.1170840000	1.0000000000

III. TOTAL ENERGIES

Calculated total energies for the exponents of Table I, in atomic units.

Table III: Total energies in a.u. for the main-group elements.

period	s^1	s^2	s^2p^1	s^2p^2	s^2p^3	s^2p^4	s^2p^5	s^2p^6
1	H	He	—	—	—	—	—	—
	−0.5000	−2.8477	—	—	—	—	—	—
2	Li	Be	B	C	N	O	F	Ne
	−7.4139	−14.5300	−24.4506	−37.5471	−54.1597	−74.3931	−98.7503	−127.5695
3	Na	Mg	Al	Si	P	S	Cl	Ar
	−160.8612	−198.5549	−240.7413	−287.6068	−339.3179	−395.8788	−457.5753	−524.5736
4	K	Ca	Ga	Ge	As	Se	Br	Kr
	−596.7993	−674.2442	−1913.2412	−2065.0558	−2223.6071	−2388.8428	−2560.9651	−2740.0761
5	Rb	Sr	In	Sn	Sb	Te	I	Xe
	−2926.0977	−3118.9607	−5718.6231	−6000.7732	−6290.6878	−6588.2973	−6893.7730	−7207.1795

Table IV: Total energies in a.u. for the transition elements. The electronic state is the one with highest L and highest spin.

period	s^2d^1	s^2d^2	s^2d^3	s^2d^4	s^2d^5
4	Sc	Ti	V	Cr	Mn
	−756.8904	−845.1598	−939.1657	−1039.0409	−1144.9715
5	Y	Zr	Nb	Mo	Tc
	−3318.6585	−3525.3994	−3739.3406	−3960.5424	−4189.1286

period	s^2d^6	s^2d^7	s^2d^8	s^2d^9	s^2d^{10}
4	Fe	Co	Ni	Cu	Zn
	−1256.7813	−1374.8903	−1499.3759	−1630.3692	−1768.0729
5	Ru	Rh	Pd	Ag	Cd
	−4424.9391	−4668.2842	−4919.2073	−5177.7917	−5444.1740