Tables of Atomic Densities from H to Kr

Pere Constans*
New York, February 2001

The following tables of atomic densities from hydrogen to krypton compile simplified 1S Gaussian representations of the electron density. Such expansions are accurate approximations of the densities derived from the ground-state HF/6-311G wavefunctions albeit significantly more appealing in computational settings.

I. ATOMIC SHELL APPROXIMATION

The tabulated atomic densities have the general form

$$\rho_{ASA}(\boldsymbol{r}) = \sum n_i c_i e^{-\xi_i(\boldsymbol{R}-\boldsymbol{r})^2} = \sum q_i e^{-\xi_i(\boldsymbol{R}-\boldsymbol{r})^2}, \qquad (1)$$

for an atom centered at $\boldsymbol{R}$. Coefficients n_i are shell occupations, provided that the relations

$$n_i \geq 0 \quad \forall i \qquad (2)$$

and normalization to the number of electrons N_e,

$$\sum n_i = N_e \qquad (3)$$

hold. Coefficient q_i in the right-hand side of equation 1 collect occupations and shell normalizations c_i.

Expansion coefficients are obtained variationally through the *Atomic Shell Approximation* (ASA) algorithm described in Ref. 1. The integral squared error with respect to an *ab initio* density ρ,

$$\Delta^2(\boldsymbol{n}) = \int (\rho - \rho_{ASA})^2 \, d\boldsymbol{r}, \qquad (4)$$

is minimized under constraints 2 and 3.

Atomic ground-state wavefunctions and densities are computed at the HF/6-311G level of theory [2]. The restricted density fitting is performed using *ASAC* program [3]. The tables list the shell occupations n_i, coefficients q_i and shell exponents ξ_i. As a measure of accuracy, integral square errors Δ^2 are reported. Additionally, *ab initio* versus ASA values for the density expectation $\langle\rho|\rho\rangle$, and the density values at nucleus coordinates $\rho(0)$ are included. Maximum relative deviations for $\langle\rho|\rho\rangle$ and $\rho(0)$ appear to be 0.063 and 1.801 percent, respectively, while the average relative differences are 0.009 and 0.236.

REFERENCES

[1] P. Constans and R. Carbó, J. Chem. Inf. Comput. Sci. **35**, 1046 (1995).
[2] M. J. Frisch et al., *Gaussian 98, revision a.7*, Gaussian, Inc., Pittsburgh PA (1998).
[3] P. Constans and R. Carbó, *ASA Calculations, v2.1*, Institute of Computational Chemistry, University of Girona (1995).

*Electronic address: constans@molspaces.com

TABLE I: Shell expansion for H atom density, Z= 1. Expansion fitted to HF/6-311G density, $N_s = 7$, $\Delta^2 = 0.00$.

i	n_i	q_i	ξ_i		ρ_{SCF}	ρ_{ASA}	%
1	0.305	0.7338114403E-02	0.2616315470E+00	$\langle\rho\|\rho\rangle$	0.04	0.04	-0.012
2	0.476	0.4765480102E-01	0.6769499354E+00	$\rho(0)$	0.29	0.29	1.408
3	0.173	0.7203538925E-01	0.1751551830E+01				
4	0.038	0.6578492194E-01	0.4531995136E+01				
5	0.006	0.4355973335E-01	0.1172616166E+02				
6	0.001	0.2976029125E-01	0.3034047105E+02				
7	0.000	0.2541473249E-01	0.7850345323E+02				

TABLE II: Shell expansion for He atom density, Z= 2. Expansion fitted to HF/6-311G density, $N_s = 7$, $\Delta^2 = 0.00$.

i	n_i	q_i	ξ_i		ρ_{SCF}	ρ_{ASA}	%
1	0.263	0.1339611021E-01	0.4317198298E+00	$\langle\rho\|\rho\rangle$	0.76	0.76	-0.034
2	0.927	0.2162248704E+00	0.1190028478E+01	$\rho(0)$	3.19	3.24	1.801
3	0.606	0.6466233125E+00	0.3280293560E+01				
4	0.166	0.8123574583E+00	0.9042074237E+01				
5	0.033	0.7310526092E+00	0.2492432614E+02				
6	0.003	0.3508868964E+00	0.6870348740E+02				
7	0.001	0.4743789182E+00	0.1893800119E+03				

TABLE III: Shell expansion for Li atom density, Z= 3. Expansion fitted to HF/6-311G density, $N_s = 13$, $\Delta^2 = 0.00$.

i	n_i	q_i	ξ_i		ρ_{SCF}	ρ_{ASA}	%
1	0.031	0.1665729492E-04	0.2083084777E-01	$\langle\rho\|\rho\rangle$	3.14	3.14	0.000
2	0.056	0.9745336554E-04	0.4565360242E-01	$\rho(0)$	13.04	13.10	0.496
3	0.958	0.5446492128E-02	0.1000560052E+00				
4	0.015	0.2857733697E-03	0.2192861823E+00				
5	0.037	0.7245688861E-02	0.1053288836E+01				
6	0.699	0.4403406975E+00	0.2308424039E+01				
7	0.694	0.1419116341E+01	0.5059221518E+01				
8	0.357	0.2366958653E+01	0.1108796388E+02				
9	0.112	0.2414647104E+01	0.2430076300E+02				
10	0.032	0.2203716889E+01	0.5325838796E+02				
11	0.006	0.1325899461E+01	0.1167229148E+03				
12	0.002	0.1559658208E+01	0.2558139545E+03				
13	0.000	0.1356734990E+01	0.1228741271E+04				

TABLE IV: Shell expansion for Be atom density, Z= 4. Expansion fitted to HF/6-311G density, $N_s = 11$, $\Delta^2 = 0.00$.

i	n_i	q_i	ξ_i		ρ_{SCF}	ρ_{ASA}	%
1	1.698	0.2161966025E-01	0.1713171620E+00	$\langle\rho\|\rho\rangle$	8.39	8.39	-0.010
2	0.405	0.1685559514E-01	0.3771383255E+00	$\rho(0)$	33.44	33.61	0.503
3	0.513	0.7428803438E+00	0.4023463445E+01				
4	0.845	0.4001985008E+01	0.8857269457E+01				
5	0.360	0.5572848053E+01	0.1949843047E+02				
6	0.139	0.7022829866E+01	0.4292392737E+02				
7	0.030	0.4890916793E+01	0.9449291538E+02				
8	0.008	0.4180287505E+01	0.2080171039E+03				
9	0.002	0.3482955210E+01	0.4579297329E+03				
10	0.000	0.1773670554E+00	0.1008088452E+04				
11	0.000	0.3497308374E+01	0.2219210186E+04				

TABLE V: Shell expansion for B atom density, Z= 5. Expansion fitted to HF/6-311G density, $N_s = 12$, $\Delta^2 = 0.01$.

i	n_i	q_i	ξ_i		ρ_{SCF}	ρ_{ASA}	%
1	0.054	0.1319485301E-03	0.5698947912E-01	$\langle\rho\|\rho\rangle$	17.53	17.52	-0.048
2	2.131	0.5524848106E-01	0.2751706846E+00	$\rho(0)$	68.12	68.33	0.312
3	0.938	0.7922889777E-01	0.6046525695E+00				
4	0.443	0.1293047009E+01	0.6415302183E+01				
5	0.887	0.8430422562E+01	0.1409681033E+02				
6	0.363	0.1123085619E+02	0.3097594716E+02				
7	0.144	0.1448840224E+02	0.6806570281E+02				
8	0.030	0.9784419742E+01	0.1495657219E+03				
9	0.008	0.8420573718E+01	0.3286516447E+03				
10	0.002	0.7205861438E+01	0.7221701749E+03				
11	0.000	0.1592407667E+00	0.1586877078E+04				
12	0.000	0.7183722783E+01	0.3486960480E+04				

TABLE VI: Shell expansion for C atom density, Z= 6. Expansion fitted to HF/6-311G density, $N_s = 11$, $\Delta^2 = 0.02$.

i	n_i	q_i	ξ_i		ρ_{SCF}	ρ_{ASA}	%
1	0.154	0.6567872501E-03	0.8271981671E-01	$\langle\rho\|\rho\rangle$	31.82	31.80	-0.059
2	2.324	0.1055103194E+00	0.3998354269E+00	$\rho(0)$	121.04	121.10	0.056
3	1.658	0.2453764468E+00	0.8790571803E+00				
4	0.412	0.2114777833E+01	0.9341673580E+01				
5	0.896	0.1497679669E+02	0.2053811314E+02				
6	0.373	0.2031178873E+02	0.4515401741E+02				
7	0.143	0.2536741327E+02	0.9927325232E+02				
8	0.031	0.1785059947E+02	0.2182569612E+03				
9	0.008	0.1417578764E+02	0.4798482975E+03				
10	0.002	0.1332561141E+02	0.1054969277E+04				
11	0.000	0.1262974596E+02	0.5099311243E+04				

TABLE VII: Shell expansion for N atom density, Z= 7. Expansion fitted to HF/6-311G density, $N_s = 12$, $\Delta^2 = 0.00$.

i	n_i	q_i	ξ_i		ρ_{SCF}	ρ_{ASA}	%
1	0.041	0.2841963653E-03	0.1142888927E+00	$\langle\rho\|\rho\rangle$	52.59	52.59	-0.001
2	0.420	0.9518018691E-02	0.2517228121E+00	$\rho(0)$	195.64	195.91	0.135
3	2.250	0.1668140374E+00	0.5544228549E+00				
4	2.432	0.5892981571E+00	0.1221123741E+01				
5	0.422	0.3572595712E+01	0.1304714007E+02				
6	0.885	0.2449108965E+02	0.2873650022E+02				
7	0.374	0.3382750952E+02	0.6329252544E+02				
8	0.137	0.4035856909E+02	0.1394026324E+03				
9	0.030	0.2922816098E+02	0.3070361593E+03				
10	0.007	0.2224058135E+02	0.6762512406E+03				
11	0.002	0.2134368542E+02	0.1489452387E+04				
12	0.000	0.2008127752E+02	0.7225430447E+04				

TABLE VIII: Shell expansion for O atom density, Z= 8. Expansion fitted to HF/6-311G density, $N_s = 13$, $\Delta^2 = 0.04$.

i	n_i	q_i	ξ_i		ρ_{SCF}	ρ_{ASA}	%
1	0.856	0.2862447807E-01	0.3259849203E+00	$\langle\rho\|\rho\rangle$	81.47	81.42	-0.058
2	1.994	0.2173775825E+00	0.7170185313E+00	$\rho(0)$	296.46	296.79	0.114
3	3.258	0.1158948961E+01	0.1577114591E+01				
4	0.038	0.4374536834E-01	0.3468934656E+01				
5	0.395	0.4872088042E+01	0.1678270104E+02				
6	0.880	0.3544180241E+02	0.3691430769E+02				
7	0.398	0.5230232669E+02	0.8119468428E+02				
8	0.138	0.5935687799E+02	0.1785913692E+03				
9	0.033	0.4680869540E+02	0.3928197695E+03				
10	0.007	0.3157704095E+02	0.8640247958E+03				
11	0.002	0.3432598986E+02	0.1900461498E+04				
12	0.000	0.2899488839E+02	0.9194430084E+04				
13	0.000	0.1665912244E+01	0.2022356356E+05				

TABLE IX: Shell expansion for F atom density, Z= 9. Expansion fitted to HF/6-311G density, $N_s = 13$, $\Delta^2 = 0.07$.

i	n_i	q_i	ξ_i		ρ_{SCF}	ρ_{ASA}	%
1	1.054	0.5124095375E-01	0.4186050296E+00	$\langle\rho\|\rho\rangle$	120.04	119.96	-0.063
2	2.249	0.3561251666E+00	0.9196509638E+00	$\rho(0)$	426.98	427.52	0.126
3	3.670	0.1892605065E+01	0.2020419812E+01				
4	0.192	0.3231215831E+00	0.4438745108E+01				
5	0.374	0.6659144019E+01	0.2142384329E+02				
6	0.881	0.5107710357E+02	0.4706694076E+02				
7	0.400	0.7549628559E+02	0.1034033382E+03				
8	0.138	0.8500491805E+02	0.2271711348E+03				
9	0.034	0.6768568317E+02	0.4990818032E+03				
10	0.007	0.4463067652E+02	0.1096453766E+04				
11	0.002	0.4996067913E+02	0.2408845311E+04				
12	0.000	0.4034940867E+02	0.1162642216E+05				
13	0.000	0.4033921763E+01	0.2554257494E+05				

TABLE X: Shell expansion for Ne atom density, Z= 10. Expansion fitted to HF/6-311G density, $N_s = 13$, $\Delta^2 = 0.00$.

i	n_i	q_i	ξ_i		ρ_{SCF}	ρ_{ASA}	%
1	1.198	0.8002735773E-01	0.5173342811E+00	$\langle\rho\|\rho\rangle$	170.10	170.09	-0.007
2	2.495	0.5423626651E+00	0.1135751247E+01	$\rho(0)$	590.17	590.90	0.123
3	4.106	0.2902991083E+01	0.2493418552E+01				
4	0.384	0.8830315195E+00	0.5474029717E+01				
5	0.345	0.8393791585E+01	0.2638341929E+02				
6	0.883	0.6993364890E+02	0.5792193256E+02				
7	0.405	0.1043833942E+03	0.1271613143E+03				
8	0.140	0.1173911388E+03	0.2791688594E+03				
9	0.034	0.9387341651E+02	0.6128849212E+03				
10	0.007	0.6189599868E+02	0.1345522303E+04				
11	0.002	0.6908198730E+02	0.2953948131E+04				
12	0.000	0.5600114586E+02	0.1423727238E+05				
13	0.000	0.5534328604E+01	0.3125638575E+05				

TABLE XI: Shell expansion for Na atom density, Z= 11. Expansion fitted to HF/6-311G density, $N_s = 16$, $\Delta^2 = 0.00$.

i	n_i	q_i	ξ_i		ρ_{SCF}	ρ_{ASA}	%
1	1.004	0.3516790513E-02	0.7246944518E-01	$\langle\rho\|\rho\rangle$	233.74	233.73	0.000
2	0.025	0.2790723333E-03	0.1555555872E+00	$\rho(0)$	805.67	808.73	0.378
3	0.804	0.8764199429E-01	0.7167157877E+00				
4	2.756	0.9445124864E+00	0.1538429678E+01				
5	4.270	0.4601715784E+01	0.3302237673E+01				
6	0.329	0.1116080885E+01	0.7088249662E+01				
7	0.342	0.1144872423E+02	0.3265881047E+02				
8	0.866	0.9126815737E+02	0.7010210203E+02				
9	0.402	0.1333315036E+03	0.1504740877E+03				
10	0.155	0.1615278719E+03	0.3229924696E+03				
11	0.033	0.1082503846E+03	0.6933029934E+03				
12	0.011	0.1176577061E+03	0.1488174140E+04				
13	0.001	0.3616123991E+02	0.3194364213E+04				
14	0.001	0.8288611073E+02	0.6856699396E+04				
15	0.000	0.3637210507E+02	0.3159195241E+05				
16	0.000	0.2307053541E+02	0.6781209235E+05				

TABLE XII: Shell expansion for Mg atom density, Z= 12. Expansion fitted to HF/6-311G density, $N_s = 16$, $\Delta^2 = 0.00$.

i	n_i	q_i	ξ_i		ρ_{SCF}	ρ_{ASA}	%
1	1.570	0.1056541802E-01	0.1119931034E+00	$\langle\rho\|\rho\rangle$	312.87	312.87	-0.001
2	0.653	0.1356519906E-01	0.2375019538E+00	$\rho(0)$	1058.54	1063.21	0.440
3	0.592	0.1174603920E+00	0.1068117428E+01				
4	3.447	0.2110141931E+01	0.2265139268E+01				
5	3.916	0.7403592664E+01	0.4803644023E+01				
6	0.024	0.1383699028E+00	0.1018700979E+02				
7	0.501	0.2788102492E+02	0.4581403450E+02				
8	0.801	0.1377995932E+03	0.9715707822E+02				
9	0.333	0.1770071493E+03	0.2060394364E+03				
10	0.127	0.2081874665E+03	0.4369444835E+03				
11	0.026	0.1309155764E+03	0.9266210634E+03				
12	0.010	0.1507477824E+03	0.1965070226E+04				
13	0.001	0.3952103802E+02	0.4167292486E+04				
14	0.001	0.1069116883E+03	0.8837509432E+04				
15	0.000	0.4291887253E+02	0.3974492714E+05				
16	0.000	0.3152951047E+02	0.8428642090E+05				

TABLE XIII: Shell expansion for Al atom density, Z= 13. Expansion fitted to HF/6-311G density, $N_s = 16$, $\Delta^2 = 0.00$.

i	n_i	q_i	ξ_i		ρ_{SCF}	ρ_{ASA}	%
1	0.231	0.3664493195E-03	0.4270753197E-01	$\langle\rho\|\rho\rangle$	408.97	408.97	-0.001
2	2.899	0.4266354854E-01	0.1886505074E+00	$\rho(0)$	1358.87	1364.23	0.393
3	0.519	0.7092028396E-01	0.8333193772E+00				
4	0.296	0.1230134098E+00	0.1751411641E+01				
5	5.331	0.6761308874E+01	0.3680992932E+01				
6	1.983	0.7662937338E+01	0.7736450212E+01				
7	0.789	0.8628681322E+02	0.7182439714E+02				
8	0.609	0.2029977128E+03	0.1509554304E+03				
9	0.241	0.2450396686E+03	0.3172674313E+03				
10	0.076	0.2364570641E+03	0.6668102143E+03				
11	0.018	0.1660641060E+03	0.1401454477E+04				
12	0.005	0.1568376682E+03	0.2945477752E+04				
13	0.001	0.5838839559E+02	0.6190596506E+04				
14	0.000	0.1124574201E+03	0.1301095724E+05				
15	0.000	0.5806518719E+02	0.5747285250E+05				
16	0.000	0.2697199071E+02	0.1207923705E+06				

TABLE XIV: Shell expansion for Si atom density, Z= 14. Expansion fitted to HF/6-311G density, $N_s = 19$, $\Delta^2 = 0.01$.

i	n_i	q_i	ξ_i		ρ_{SCF}	ρ_{ASA}	%
1	0.307	0.8165497218E-03	0.6024434214E-01	$\langle\rho\|\rho\rangle$	523.51	523.50	-0.001
2	0.104	0.8339032688E-03	0.1259798301E+00	$\rho(0)$	1712.62	1716.49	0.225
3	3.864	0.9383946396E-01	0.2634424584E+00				
4	0.125	0.9168782116E-02	0.5508971462E+00				
5	0.183	0.4059062572E-01	0.1152007416E+01				
6	0.679	0.4562345531E+00	0.2409017899E+01				
7	5.673	0.1151828359E+02	0.5037612744E+01				
8	1.345	0.8256573779E+01	0.1053439336E+02				
9	0.047	0.2651975950E+01	0.4606584430E+02				
10	0.891	0.1512383432E+03	0.9633049401E+02				
11	0.492	0.2524037096E+03	0.2014413112E+03				
12	0.216	0.3348211699E+03	0.4212435768E+03				
13	0.054	0.2519487557E+03	0.8808826251E+03				
14	0.017	0.2363595284E+03	0.1842055860E+04				
15	0.003	0.1457685321E+03	0.3852011261E+04				
16	0.001	0.1049329688E+03	0.8055125297E+04				
17	0.000	0.1113220623E+03	0.1684445843E+05				
18	0.000	0.8570286817E+02	0.7365912517E+05				
19	0.000	0.1896458545E+02	0.1540321256E+06				

TABLE XV: Shell expansion for P atom density, Z= 15. Expansion fitted to HF/6-311G density, $N_s = 17$, $\Delta^2 = 0.00$.

i	n_i	q_i	ξ_i		ρ_{SCF}	ρ_{ASA}	%
1	0.409	0.1607832458E-02	0.7824713795E-01	$\langle\rho\|\rho\rangle$	658.55	658.55	0.000
2	4.878	0.1729329331E+00	0.3390127104E+00	$\rho(0)$	2119.68	2121.93	0.106
3	0.345	0.3674212266E-01	0.7056506424E+00				
4	0.632	0.6070968707E+00	0.3057294403E+01				
5	5.979	0.1723700538E+02	0.6363719392E+01				
6	1.039	0.8993886275E+01	0.1324600093E+02				
7	0.107	0.8345753395E+01	0.5738948151E+02				
8	0.900	0.2110121938E+03	0.1194554754E+03				
9	0.446	0.3137605254E+03	0.2486450519E+03				
10	0.200	0.4220636680E+03	0.5175515113E+03				
11	0.045	0.2887476285E+03	0.1077276884E+04				
12	0.016	0.3059455606E+03	0.2242338125E+04				
13	0.003	0.1477186777E+03	0.4667398271E+04				
14	0.001	0.1549459494E+03	0.9715130104E+04				
15	0.000	0.1135797923E+03	0.2022191968E+05				
16	0.000	0.1230943784E+03	0.8761327224E+05				
17	0.000	0.5664821770E+01	0.1823659112E+06				

TABLE XVI: Shell expansion for S atom density, Z= 16. Expansion fitted to HF/6-311G density, $N_s = 17$, $\Delta^2 = 0.01$.

i	n_i	q_i	ξ_i		ρ_{SCF}	ρ_{ASA}	%
1	0.504	0.2809966448E-02	0.9881202479E-01	$\langle\rho\|\rho\rangle$	815.87	815.86	-0.002
2	5.895	0.2916762468E+00	0.4234282006E+00	$\rho(0)$	2590.41	2594.74	0.167
3	0.339	0.4995948497E-01	0.8765259318E+00				
4	0.461	0.6021913655E+00	0.3756079272E+01				
5	6.241	0.2430135706E+02	0.7775346278E+01				
6	0.847	0.9817942838E+01	0.1609550954E+02				
7	0.149	0.1529416878E+02	0.6897230024E+02				
8	0.894	0.2740588206E+03	0.1427774760E+03				
9	0.420	0.3836733690E+03	0.2955593415E+03				
10	0.189	0.5138978378E+03	0.6118284679E+03				
11	0.043	0.3444029984E+03	0.1266527636E+04				
12	0.015	0.3662379454E+03	0.2621800614E+04				
13	0.003	0.1819484328E+03	0.5427310279E+04				
14	0.001	0.1773358282E+03	0.1123491112E+05				
15	0.000	0.1458261619E+03	0.2325705025E+05				
16	0.000	0.1359912420E+03	0.9966085564E+05				
17	0.000	0.2100782958E+02	0.2063049278E+06				

TABLE XVII: Shell expansion for Cl atom density, Z= 17. Expansion fitted to HF/6-311G density, $N_s = 17$, $\Delta^2 = 0.02$.

i	n_i	q_i	ξ_i		ρ_{SCF}	ρ_{ASA}	%
1	0.554	0.4144328959E-02	0.1201774150E+00	$\langle\rho\|\rho\rangle$	997.59	997.57	-0.002
2	6.851	0.4513847345E+00	0.5124666668E+00	$\rho(0)$	3123.97	3127.92	0.126
3	0.452	0.8829384728E-01	0.1058246898E+01				
4	0.250	0.4295669059E+00	0.4512630435E+01				
5	6.491	0.3315786703E+02	0.9318610300E+01				
6	0.692	0.1049025014E+02	0.1924298902E+02				
7	0.193	0.2576981299E+02	0.8205693596E+02				
8	0.888	0.3517742609E+03	0.1694480901E+03				
9	0.395	0.4645215839E+03	0.3499113745E+03				
10	0.178	0.6222795242E+03	0.7225691945E+03				
11	0.039	0.4001386936E+03	0.1492109942E+04				
12	0.014	0.4436454816E+03	0.3081216439E+04				
13	0.002	0.2025390347E+03	0.6362731373E+04				
14	0.001	0.2234649407E+03	0.1313908040E+05				
15	0.000	0.1620048441E+03	0.2713228387E+05				
16	0.000	0.1713539667E+03	0.1156988697E+06				
17	0.000	0.1580404188E+02	0.2389188955E+06				

TABLE XVIII: Shell expansion for Ar atom density, Z= 18. Expansion fitted to HF/6-311G density, $N_s = 17$, $\Delta^2 = 0.00$.

i	n_i	q_i	ξ_i		ρ_{SCF}	ρ_{ASA}	%
1	0.557	0.5473904910E-02	0.1442207120E+00	$\langle\rho\|\rho\rangle$	1205.58	1205.57	0.000
2	7.944	0.6829939177E+00	0.6119681072E+00	$\rho(0)$	3725.89	3729.14	0.087
3	0.463	0.1177066792E+00	0.1260605990E+01				
4	0.052	0.1164532302E+00	0.5349097580E+01				
5	6.724	0.4416586452E+02	0.1101871874E+02				
6	0.550	0.1067763036E+02	0.2269769075E+02				
7	0.238	0.4037436211E+02	0.9631253829E+02				
8	0.876	0.4393893376E+03	0.1983962257E+03				
9	0.375	0.5563267702E+03	0.4086805628E+03				
10	0.169	0.7430814518E+03	0.8418496968E+03				
11	0.036	0.4609451848E+03	0.1734143917E+04				
12	0.014	0.5336556378E+03	0.3572199570E+04				
13	0.002	0.2203764729E+03	0.7358449114E+04				
14	0.001	0.2800829655E+03	0.1515782428E+05				
15	0.000	0.1771944629E+03	0.3122392140E+05				
16	0.000	0.2143058729E+03	0.1324916776E+06				
17	0.000	0.7643772860E+01	0.2729223965E+06				

TABLE XIX: Shell expansion for K atom density, Z= 19. Expansion fitted to HF/6-311G density, $N_s = 20$, $\Delta^2 = 0.01$.

i	n_i	q_i	ξ_i		ρ_{SCF}	ρ_{ASA}	%
1	1.254	0.4364240199E-02	0.7215282918E-01	$\langle\rho\|\rho\rangle$	1442.31	1442.31	0.000
2	2.018	0.1557994284E+00	0.5696810168E+00	$\rho(0)$	4423.79	4426.94	0.071
3	6.710	0.9630654722E+00	0.8612067488E+00				
4	2.732	0.1617047819E+02	0.1027925132E+02				
5	4.572	0.5029781114E+02	0.1553950429E+02				
6	0.021	0.1492845396E+01	0.5368638860E+02				
7	0.180	0.4402121590E+02	0.1226918017E+03				
8	0.580	0.2633173080E+03	0.1854774944E+03				
9	0.364	0.3073106736E+03	0.2803928255E+03				
10	0.245	0.3842054931E+03	0.4238796565E+03				
11	0.161	0.4693313129E+03	0.6407937251E+03				
12	0.099	0.5351956540E+03	0.9687103210E+03				
13	0.013	0.1320403451E+03	0.1464433326E+04				
14	0.041	0.7681362212E+03	0.2213835158E+04				
15	0.004	0.2466280743E+03	0.5059372238E+04				
16	0.004	0.5044279513E+03	0.7648430241E+04				
17	0.000	0.3431811195E+03	0.2642404740E+05				
18	0.000	0.1134620853E+03	0.3994615809E+05				
19	0.000	0.4317030217E+02	0.1380072958E+06				
20	0.000	0.2034266793E+03	0.2086304635E+06				

TABLE XX: Shell expansion for Ca atom density, Z= 20. Expansion fitted to HF/6-311G density, $N_s = 20$, $\Delta^2 = 0.01$.

i	n_i	q_i	ξ_i		ρ_{SCF}	ρ_{ASA}	%
1	2.158	0.7512418933E-02	0.7215282918E-01	$\langle\rho\|\rho\rangle$	1709.77	1709.76	-0.001
2	6.168	0.8852854870E+00	0.8612067488E+00	$\rho(0)$	5185.01	5185.57	0.011
3	2.821	0.7526916288E+00	0.1301916410E+01				
4	0.101	0.5950503862E+00	0.1027925132E+02				
5	6.912	0.7603694558E+02	0.1553950429E+02				
6	0.109	0.4136818891E+01	0.3551309425E+02				
7	0.072	0.5068746658E+01	0.5368638860E+02				
8	0.619	0.2806199649E+03	0.1854774944E+03				
9	0.372	0.3140240102E+03	0.2803928255E+03				
10	0.311	0.4876819626E+03	0.4238796565E+03				
11	0.142	0.4129569040E+03	0.6407937251E+03				
12	0.152	0.8224921549E+03	0.9687103210E+03				
13	0.051	0.9511672535E+03	0.2213835158E+04				
14	0.005	0.1569795033E+03	0.3346732158E+04				
15	0.001	0.7220616909E+02	0.5059372238E+04				
16	0.006	0.7532363282E+03	0.7648430241E+04				
17	0.000	0.3324176925E+03	0.2642404740E+05				
18	0.000	0.2261860528E+03	0.3994615809E+05				
19	0.000	0.2807626432E+03	0.2086304635E+06				
20	0.000	0.7352990626E+01	0.3153939799E+06				

TABLE XXI: Shell expansion for Sc atom density, Z= 21. Expansion fitted to HF/6-311G density, $N_s = 19$, $\Delta^2 = 0.05$.

i	n_i	q_i	ξ_i		ρ_{SCF}	ρ_{ASA}	%
1	1.368	0.4761031644E-02	0.7215282918E-01	$\langle\rho\|\rho\rangle$	2006.50	2006.44	-0.003
2	0.965	0.6243786797E-02	0.1090759594E+00	$\rho(0)$	6037.95	6040.37	0.040
3	4.316	0.6194473277E+00	0.8612067488E+00				
4	5.445	0.1452727348E+01	0.1301916410E+01				
5	5.022	0.5524276908E+02	0.1553950429E+02				
6	2.222	0.4543787727E+02	0.2349161299E+02				
7	0.332	0.1503835865E+03	0.1854774944E+03				
8	0.766	0.6462875995E+03	0.2803928255E+03				
9	0.401	0.1167565006E+04	0.6407937251E+03				
10	0.041	0.2206290891E+03	0.9687103210E+03				
11	0.063	0.6346524815E+03	0.1464433326E+04				
12	0.040	0.7538087948E+03	0.2213835158E+04				
13	0.009	0.3035444867E+03	0.3346732158E+04				
14	0.002	0.1601993532E+03	0.5059372238E+04				
15	0.007	0.8424562614E+03	0.7648430241E+04				
16	0.001	0.4920214821E+03	0.2642404740E+05				
17	0.000	0.1975575443E+03	0.3994615809E+05				
18	0.000	0.5229426083E+02	0.1380072958E+06				
19	0.000	0.3162100696E+03	0.2086304635E+06				

TABLE XXII: Shell expansion for Ti atom density, Z= 22. Expansion fitted to HF/6-311G density, $N_s = 20$, $\Delta^2 = 0.07$.

i	n_i	q_i	ξ_i		ρ_{SCF}	ρ_{ASA}	%
1	0.379	0.1317481482E-02	0.7215282918E-01	$\langle\rho\|\rho\rangle$	2332.89	2332.83	-0.003
2	1.597	0.1920746295E-01	0.1648939487E+00	$\rho(0)$	6961.29	6962.98	0.024
3	0.364	0.8131978642E-02	0.2492759584E+00				
4	2.162	0.3103283145E+00	0.8612067488E+00				
5	8.581	0.2289259213E+01	0.1301916410E+01				
6	3.139	0.3453278113E+02	0.1553950429E+02				
7	4.120	0.8424798010E+02	0.2349161299E+02				
8	0.145	0.6587519012E+02	0.1854774944E+03				
9	0.887	0.7482819234E+03	0.2803928255E+03				
10	0.410	0.1195030853E+04	0.6407937251E+03				
11	0.084	0.4534772333E+03	0.9687103210E+03				
12	0.058	0.5864610441E+03	0.1464433326E+04				
13	0.047	0.8865379061E+03	0.2213835158E+04				
14	0.016	0.5429165883E+03	0.3346732158E+04				
15	0.009	0.1028409153E+04	0.7648430241E+04				
16	0.001	0.1158616960E+03	0.1156239992E+05				
17	0.001	0.4046391873E+03	0.2642404740E+05				
18	0.000	0.3947529008E+03	0.3994615809E+05				
19	0.000	0.3870363998E+03	0.2086304635E+06				
20	0.000	0.3228646845E+02	0.3153939799E+06				

TABLE XXIII: Shell expansion for V atom density, Z= 23. Expansion fitted to HF/6-311G density, $N_s = 20$, $\Delta^2 = 0.11$.

i	n_i	q_i	ξ_i		ρ_{SCF}	ρ_{ASA}	%
1	1.429	0.9244202511E-02	0.1090759594E+00	$\langle\rho\|\rho\rangle$	2699.81	2699.71	-0.004
2	1.447	0.1739537681E-01	0.1648939487E+00	$\rho(0)$	7989.65	7997.33	0.096
3	9.011	0.2403877366E+01	0.1301916410E+01				
4	2.340	0.1160460041E+01	0.1968152643E+01				
5	0.847	0.9316548848E+01	0.1553950429E+02				
6	6.258	0.1279533154E+03	0.2349161299E+02				
7	0.094	0.4285779149E+02	0.1854774944E+03				
8	0.778	0.6559332071E+03	0.2803928255E+03				
9	0.154	0.2413301239E+03	0.4238796565E+03				
10	0.373	0.1087929947E+04	0.6407937251E+03				
11	0.108	0.5874268476E+03	0.9687103210E+03				
12	0.087	0.8777260532E+03	0.1464433326E+04				
13	0.036	0.6644358808E+03	0.2213835158E+04				
14	0.028	0.9583565069E+03	0.3346732158E+04				
15	0.007	0.8903261524E+03	0.7648430241E+04				
16	0.002	0.4884201992E+03	0.1156239992E+05				
17	0.000	0.1779348810E+03	0.2642404740E+05				
18	0.000	0.6958373810E+03	0.3994615809E+05				
19	0.000	0.3110745413E+03	0.2086304635E+06				
20	0.000	0.1768842897E+03	0.3153939799E+06				

TABLE XXIV: Shell expansion for Cr atom density, Z= 24. Expansion fitted to HF/6-311G density, $N_s = 19$, $\Delta^2 = 0.02$.

i	n_i	q_i	ξ_i		ρ_{SCF}	ρ_{ASA}	%
1	0.534	0.1859930708E-02	0.7215282918E-01	$\langle\rho\|\rho\rangle$	3096.80	3096.79	0.000
2	2.083	0.4655966214E-01	0.2492759584E+00	$\rho(0)$	9109.08	9115.04	0.065
3	7.852	0.2094666714E+01	0.1301916410E+01				
4	4.772	0.2366350066E+01	0.1968152643E+01				
5	6.171	0.1261890162E+03	0.2349161299E+02				
6	0.935	0.3552851982E+02	0.3551309425E+02				
7	0.673	0.5677914174E+03	0.2803928255E+03				
8	0.380	0.5947804732E+03	0.4238796565E+03				
9	0.195	0.5670681309E+03	0.6407937251E+03				
10	0.275	0.1488456732E+04	0.9687103210E+03				
11	0.020	0.2055847310E+03	0.1464433326E+04				
12	0.071	0.1336940924E+04	0.2213835158E+04				
13	0.026	0.8885551994E+03	0.3346732158E+04				
14	0.009	0.1108328598E+04	0.7648430241E+04				
15	0.003	0.5626277845E+03	0.1156239992E+05				
16	0.000	0.1893915456E+03	0.2642404740E+05				
17	0.001	0.8472200544E+03	0.3994615809E+05				
18	0.000	0.3603942801E+03	0.2086304635E+06				
19	0.000	0.2316770896E+03	0.3153939799E+06				

TABLE XXV: Shell expansion for Mn atom density, Z= 25. Expansion fitted to HF/6-311G density, $N_s = 19$, $\Delta^2 = 0.05$.

i	n_i	q_i	ξ_i		ρ_{SCF}	ρ_{ASA}	%
1	0.315	0.1096831890E-02	0.7215282918E-01	$\langle\rho\|\rho\rangle$	3540.68	3540.64	-0.001
2	1.930	0.2320775464E-01	0.1648939487E+00	$\rho(0)$	10322.07	10330.93	0.086
3	0.858	0.1918197805E-01	0.2492759584E+00				
4	4.224	0.1126823356E+01	0.1301916410E+01				
5	8.873	0.4399802591E+01	0.1968152643E+01				
6	4.636	0.9480165082E+02	0.2349161299E+02				
7	2.532	0.9621412900E+02	0.3551309425E+02				
8	0.354	0.2988361634E+03	0.2803928255E+03				
9	0.766	0.1201251132E+04	0.4238796565E+03				
10	0.345	0.1867782626E+04	0.9687103210E+03				
11	0.068	0.6796825348E+03	0.1464433326E+04				
12	0.039	0.7272129435E+03	0.2213835158E+04				
13	0.047	0.1643766939E+04	0.3346732158E+04				
14	0.007	0.8378871871E+03	0.7648430241E+04				
15	0.005	0.1059460907E+04	0.1156239992E+05				
16	0.001	0.1121948635E+04	0.3994615809E+05				
17	0.000	0.7930673952E+01	0.6038800649E+05				
18	0.000	0.3502251551E+03	0.2086304635E+06				
19	0.000	0.3383617388E+03	0.3153939799E+06				

TABLE XXVI: Shell expansion for Fe atom density, Z= 26. Expansion fitted to HF/6-311G density, $N_s = 18$, $\Delta^2 = 0.17$.

i	n_i	q_i	ξ_i		ρ_{SCF}	ρ_{ASA}	%
1	0.460	0.1602157904E-02	0.7215282918E-01	$\langle\rho\|\rho\rangle$	4018.11	4017.95	-0.004
2	2.903	0.1205836221E+00	0.3768391984E+00	$\rho(0)$	11615.97	11629.33	0.115
3	0.542	0.4182958778E-01	0.5696810168E+00				
4	13.292	0.6590790311E+01	0.1968152643E+01				
5	3.132	0.6403295436E+02	0.2349161299E+02				
6	4.041	0.1535751648E+03	0.3551309425E+02				
7	0.194	0.1634049046E+03	0.2803928255E+03				
8	0.881	0.1381473837E+04	0.4238796565E+03				
9	0.343	0.1859427234E+04	0.9687103210E+03				
10	0.116	0.1169034976E+04	0.1464433326E+04				
11	0.019	0.3641345298E+03	0.2213835158E+04				
12	0.064	0.2227397786E+04	0.3346732158E+04				
13	0.006	0.7013145002E+03	0.7648430241E+04				
14	0.007	0.1465092847E+04	0.1156239992E+05				
15	0.001	0.1091705823E+04	0.3994615809E+05				
16	0.000	0.2395045346E+03	0.6038800649E+05				
17	0.000	0.2213889266E+03	0.2086304635E+06				
18	0.000	0.5210913019E+03	0.3153939799E+06				

TABLE XXVII: Shell expansion for Co atom density, Z= 27. Expansion fitted to HF/6-311G density, $N_s = 19$, $\Delta^2 = 0.19$.

i	n_i	q_i	ξ_i		ρ_{SCF}	ρ_{ASA}	%
1	0.390	0.1357831269E-02	0.7215282918E-01	$\langle\rho\|\rho\rangle$	4542.21	4542.03	-0.004
2	2.831	0.1176270144E+00	0.3768391984E+00	$\rho(0)$	13059.15	13068.30	0.070
3	0.613	0.4734738195E-01	0.5696810168E+00				
4	11.369	0.5637324288E+01	0.1968152643E+01				
5	3.110	0.2866612456E+01	0.2975325294E+01				
6	1.337	0.2733461942E+02	0.2349161299E+02				
7	5.711	0.2170541920E+03	0.3551309425E+02				
8	0.094	0.7897093741E+02	0.2803928255E+03				
9	0.920	0.1442326289E+04	0.4238796565E+03				
10	0.400	0.2165482051E+04	0.9687103210E+03				
11	0.098	0.9903258986E+03	0.1464433326E+04				
12	0.045	0.8350437497E+03	0.2213835158E+04				
13	0.065	0.2274500586E+04	0.3346732158E+04				
14	0.008	0.9862020423E+03	0.7648430241E+04				
15	0.007	0.1580332252E+04	0.1156239992E+05				
16	0.001	0.1316873910E+04	0.3994615809E+05				
17	0.000	0.2547378360E+03	0.6038800649E+05				
18	0.000	0.2275946163E+03	0.2086304635E+06				
19	0.000	0.6628474815E+03	0.3153939799E+06				

TABLE XXVIII: Shell expansion for Ni atom density, Z= 28. Expansion fitted to HF/6-311G density, $N_s = 21$, $\Delta^2 = 0.15$.

i	n_i	q_i	ξ_i		ρ_{SCF}	ρ_{ASA}	%
1	0.623	0.2167331719E-02	0.7215282918E-01	$\langle\rho\|\rho\rangle$	5111.73	5111.58	-0.003
2	0.918	0.3814558587E-01	0.3768391984E+00	$\rho(0)$	14596.36	14603.62	0.050
3	2.786	0.2151681984E+00	0.5696810168E+00				
4	7.789	0.3862160577E+01	0.1968152643E+01				
5	7.304	0.6732026068E+01	0.2975325294E+01				
6	6.569	0.2496642307E+03	0.3551309425E+02				
7	0.373	0.2631573831E+02	0.5368638860E+02				
8	0.007	0.5831914546E+01	0.2803928255E+03				
9	0.921	0.1442863090E+04	0.4238796565E+03				
10	0.022	0.6370310386E+02	0.6407937251E+03				
11	0.455	0.2460991934E+04	0.9687103210E+03				
12	0.067	0.6737431296E+03	0.1464433326E+04				
13	0.092	0.1713287766E+04	0.2213835158E+04				
14	0.047	0.1617108518E+04	0.3346732158E+04				
15	0.015	0.9975306120E+03	0.5059372238E+04				
16	0.003	0.3588428181E+03	0.7648430241E+04				
17	0.010	0.2173496085E+04	0.1156239992E+05				
18	0.001	0.1330784416E+04	0.3994615809E+05				
19	0.000	0.4779442135E+03	0.6038800649E+05				
20	0.000	0.1324895621E+03	0.2086304635E+06				
21	0.000	0.8681744122E+03	0.3153939799E+06				

TABLE XXIX: Shell expansion for Cu atom density, Z= 29. Expansion fitted to HF/6-311G density, $N_s = 18$, $\Delta^2 = 0.05$.

i	n_i	q_i	ξ_i		ρ_{SCF}	ρ_{ASA}	%
1	0.627	0.2182349659E-02	0.7215282918E-01	$\langle\rho\|\rho\rangle$	5727.37	5727.32	-0.001
2	3.866	0.2985489333E+00	0.5696810168E+00	$\rho(0)$	16263.32	16283.82	0.126
3	5.165	0.2561020079E+01	0.1968152643E+01				
4	10.695	0.9857219897E+01	0.2975325294E+01				
5	5.477	0.2081539148E+03	0.3551309425E+02				
6	1.550	0.1094620454E+03	0.5368638860E+02				
7	0.598	0.9366041324E+03	0.4238796565E+03				
8	0.531	0.1546734502E+04	0.6407937251E+03				
9	0.048	0.2624477056E+03	0.9687103210E+03				
10	0.338	0.3401430785E+04	0.1464433326E+04				
11	0.068	0.2368987810E+04	0.3346732158E+04				
12	0.026	0.1672100695E+04	0.5059372238E+04				
13	0.008	0.1887934333E+04	0.1156239992E+05				
14	0.002	0.1016721996E+04	0.1747928498E+05				
15	0.000	0.3586181998E+03	0.3994615809E+05				
16	0.001	0.1459757758E+04	0.6038800649E+05				
17	0.000	0.6553378053E+03	0.3153939799E+06				
18	0.000	0.3868047548E+03	0.4767921276E+06				

TABLE XXX: Shell expansion for Zn atom density, Z= 30. Expansion fitted to HF/6-311G density, $N_s = 18$, $\Delta^2 = 0.08$.

i	n_i	q_i	ξ_i		ρ_{SCF}	ρ_{ASA}	%
1	1.314	0.8502726932E-02	0.1090759594E+00	$\langle\rho\|\rho\rangle$	6399.35	6399.27	-0.001
2	3.154	0.2435787750E+00	0.5696810168E+00	$\rho(0)$	17993.91	18017.97	0.134
3	0.986	0.1415716013E+00	0.8612067488E+00				
4	15.873	0.1463000000E+02	0.2975325294E+01				
5	4.259	0.1618681904E+03	0.3551309425E+02				
6	2.801	0.1978952403E+03	0.5368638860E+02				
7	0.383	0.6001569957E+03	0.4238796565E+03				
8	0.749	0.2183322765E+04	0.6407937251E+03				
9	0.319	0.3206765189E+04	0.1464433326E+04				
10	0.070	0.1310009068E+04	0.2213835158E+04				
11	0.036	0.1263107931E+04	0.3346732158E+04				
12	0.042	0.2693449123E+04	0.5059372238E+04				
13	0.008	0.1767686002E+04	0.1156239992E+05				
14	0.003	0.1430058079E+04	0.1747928498E+05				
15	0.000	0.3406870071E+03	0.3994615809E+05				
16	0.001	0.1677093470E+04	0.6038800649E+05				
17	0.000	0.8577606680E+03	0.3153939799E+06				
18	0.000	0.3130859839E+03	0.4767921276E+06				

TABLE XXXI: Shell expansion for Ga atom density, Z= 31. Expansion fitted to HF/6-311G density, $N_s = 20$, $\Delta^2 = 0.11$.

i	n_i	q_i	ξ_i		ρ_{SCF}	ρ_{ASA}	%
1	0.734	0.2554696226E-02	0.7215282918E-01	$\langle\rho\|\rho\rangle$	7119.35	7119.24	-0.002
2	0.398	0.2575408806E-02	0.1090759594E+00	$\rho(0)$	19802.89	19837.55	0.175
3	2.957	0.1228588027E+00	0.3768391984E+00				
4	1.023	0.7897734452E-01	0.5696810168E+00				
5	14.551	0.1341100977E+02	0.2975325294E+01				
6	2.715	0.4650501364E+01	0.4497903472E+01				
7	2.897	0.1101177417E+03	0.3551309425E+02				
8	4.117	0.2908138054E+03	0.5368638860E+02				
9	0.239	0.3749984671E+03	0.4238796565E+03				
10	0.852	0.2481001166E+04	0.6407937251E+03				
11	0.324	0.3258065418E+04	0.1464433326E+04				
12	0.105	0.1957804559E+04	0.2213835158E+04				
13	0.023	0.8068060958E+03	0.3346732158E+04				
14	0.053	0.3438943659E+04	0.5059372238E+04				
15	0.007	0.1576647756E+04	0.1156239992E+05				
16	0.005	0.2007505448E+04	0.1747928498E+05				
17	0.000	0.6726935421E+02	0.3994615809E+05				
18	0.001	0.2100232385E+04	0.6038800649E+05				
19	0.000	0.7879917356E+03	0.3153939799E+06				
20	0.000	0.5610800209E+03	0.4767921276E+06				

TABLE XXXII: Shell expansion for Ge atom density, Z= 32. Expansion fitted to HF/6-311G density, $N_s = 20$, $\Delta^2 = 0.09$.

i	n_i	q_i	ξ_i		ρ_{SCF}	ρ_{ASA}	%
1	0.177	0.6156524454E-03	0.7215282918E-01	$\langle\rho\|\rho\rangle$	7898.56	7898.46	-0.001
2	1.029	0.6659342158E-02	0.1090759594E+00	$\rho(0)$	21844.59	21864.57	0.091
3	4.300	0.1786230973E+00	0.3768391984E+00				
4	0.143	0.1101164979E-01	0.5696810168E+00				
5	10.575	0.9746296056E+01	0.2975325294E+01				
6	7.289	0.1248699300E+02	0.4497903472E+01				
7	1.328	0.5048275422E+02	0.3551309425E+02				
8	5.548	0.3919394800E+03	0.5368638860E+02				
9	0.135	0.2114364899E+03	0.4238796565E+03				
10	0.910	0.2651527712E+04	0.6407937251E+03				
11	0.354	0.3558788389E+04	0.1464433326E+04				
12	0.110	0.2052842548E+04	0.2213835158E+04				
13	0.029	0.1024023018E+04	0.3346732158E+04				
14	0.059	0.3837269150E+04	0.5059372238E+04				
15	0.008	0.1697550817E+04	0.1156239992E+05				
16	0.006	0.2382207527E+04	0.1747928498E+05				
17	0.001	0.2437765261E+04	0.6038800649E+05				
18	0.000	0.5720786904E+01	0.9129066478E+05				
19	0.000	0.8758770250E+03	0.3153939799E+06				
20	0.000	0.6647061987E+03	0.4767921276E+06				

TABLE XXXIII: Shell expansion for As atom density, Z= 33. Expansion fitted to HF/6-311G density, $N_s = 20$, $\Delta^2 = 0.06$.

i	n_i	q_i	ξ_i		ρ_{SCF}	ρ_{ASA}	%
1	0.740	0.4789772065E-02	0.1090759594E+00	$\langle\rho\|\rho\rangle$	8735.86	8735.79	-0.001
2	0.574	0.6897478406E-02	0.1648939487E+00	$\rho(0)$	23982.86	23993.41	0.044
3	4.290	0.1782411339E+00	0.3768391984E+00				
4	1.059	0.8177995973E-01	0.5696810168E+00				
5	5.388	0.4966335424E+01	0.2975325294E+01				
6	12.572	0.2153734548E+02	0.4497903472E+01				
7	6.629	0.4682938656E+03	0.5368638860E+02				
8	0.124	0.1628746725E+02	0.8115959427E+02				
9	0.093	0.1463442892E+03	0.4238796565E+03				
10	0.890	0.2592273731E+04	0.6407937251E+03				
11	0.447	0.4496884993E+04	0.1464433326E+04				
12	0.046	0.8531140483E+03	0.2213835158E+04				
13	0.078	0.2696885225E+04	0.3346732158E+04				
14	0.053	0.3400438418E+04	0.5059372238E+04				
15	0.010	0.2306860090E+04	0.1156239992E+05				
16	0.006	0.2466935563E+04	0.1747928498E+05				
17	0.001	0.2764962063E+04	0.6038800649E+05				
18	0.000	0.3433056105E+02	0.9129066478E+05				
19	0.000	0.8724303623E+03	0.3153939799E+06				
20	0.000	0.8505947965E+03	0.4767921276E+06				

TABLE XXXIV: Shell expansion for Se atom density, Z= 34. Expansion fitted to HF/6-311G density, $N_s = 20$, $\Delta^2 = 0.13$.

i	n_i	q_i	ξ_i		ρ_{SCF}	ρ_{ASA}	%
1	0.159	0.1027002727E-02	0.1090759594E+00	$\langle\rho\|\rho\rangle$	9633.01	9632.88	-0.001
2	1.346	0.1618037297E-01	0.1648939487E+00	$\rho(0)$	26276.39	26300.54	0.092
3	3.298	0.1370143503E+00	0.3768391984E+00				
4	3.070	0.2370457220E+00	0.5696810168E+00				
5	0.293	0.2698427354E+00	0.2975325294E+01				
6	17.400	0.2980867467E+02	0.4497903472E+01				
7	5.689	0.4019218379E+03	0.5368638860E+02				
8	1.149	0.1508867446E+03	0.8115959427E+02				
9	0.777	0.2263173194E+04	0.6407937251E+03				
10	0.294	0.1589549556E+04	0.9687103210E+03				
11	0.182	0.1830480637E+04	0.1464433326E+04				
12	0.246	0.4606176584E+04	0.2213835158E+04				
13	0.077	0.4997774852E+04	0.5059372238E+04				
14	0.005	0.6482755896E+03	0.7648430241E+04				
15	0.005	0.1146385943E+04	0.1156239992E+05				
16	0.009	0.3665611762E+04	0.1747928498E+05				
17	0.001	0.2452202723E+04	0.6038800649E+05				
18	0.000	0.7100157602E+03	0.9129066478E+05				
19	0.000	0.4300480355E+03	0.3153939799E+06				
20	0.000	0.1377564858E+04	0.4767921276E+06				

TABLE XXXV: Shell expansion for Br atom density, Z= 35. Expansion fitted to HF/6-311G density, $N_s = 15$, $\Delta^2 = 0.29$.

i	n_i	q_i	ξ_i		ρ_{SCF}	ρ_{ASA}	%
1	8.173	0.3395567967E+00	0.3768391984E+00	$\langle\rho\|\rho\rangle$	10591.76	10591.45	-0.003
2	15.982	0.2737923377E+02	0.4497903472E+01	$\rho(0)$	28740.42	28754.60	0.049
3	2.400	0.7641950099E+01	0.6799638239E+01				
4	4.670	0.3298722008E+03	0.5368638860E+02				
5	2.189	0.2874639074E+03	0.8115959427E+02				
6	0.543	0.1582992393E+04	0.6407937251E+03				
7	0.606	0.3279145096E+04	0.9687103210E+03				
8	0.338	0.6321092878E+04	0.2213835158E+04				
9	0.065	0.4196071071E+04	0.5059372238E+04				
10	0.022	0.2673152478E+04	0.7648430241E+04				
11	0.010	0.4071229948E+04	0.1747928498E+05				
12	0.001	0.6894814312E+03	0.2642404740E+05				
13	0.001	0.1833326835E+04	0.6038800649E+05				
14	0.000	0.1603034800E+04	0.9129066478E+05				
15	0.000	0.1852381096E+04	0.4767921276E+06				

TABLE XXXVI: Shell expansion for Kr atom density, Z= 36. Expansion fitted to HF/6-311G density, $N_s = 18$, $\Delta^2 = 0.45$.

i	n_i	q_i	ξ_i		ρ_{SCF}	ρ_{ASA}	%
1	7.493	0.3112802737E+00	0.3768391984E+00	$\langle\rho\|\rho\rangle$	11618.03	11617.38	-0.006
2	1.549	0.1195777600E+00	0.5696810168E+00	$\rho(0)$	31266.03	31314.76	0.156
3	12.141	0.2079830623E+02	0.4497903472E+01				
4	6.444	0.2051938882E+02	0.6799638239E+01				
5	3.429	0.2422609615E+03	0.5368638860E+02				
6	3.370	0.4424870970E+03	0.8115959427E+02				
7	0.359	0.1046759713E+04	0.6407937251E+03				
8	0.779	0.4215905579E+04	0.9687103210E+03				
9	0.259	0.4851638699E+04	0.2213835158E+04				
10	0.117	0.4083115043E+04	0.3346732158E+04				
11	0.002	0.1233838084E+03	0.5059372238E+04				
12	0.048	0.5747045160E+04	0.7648430241E+04				
13	0.006	0.2558072881E+04	0.1747928498E+05				
14	0.003	0.2576692486E+04	0.2642404740E+05				
15	0.000	0.7169657919E+03	0.6038800649E+05				
16	0.001	0.2672647619E+04	0.9129066478E+05				
17	0.000	0.1544986330E+04	0.4767921276E+06				
18	0.000	0.4510491016E+03	0.7207833612E+06				