Well-tempered Gaussian basis sets for the calculation of matrix Hartree–Fock wavefunctions

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Gaussian basis sets leading to wavefunctions with atomic total energies within 1 mE_h of the Hartree–Fock values were prepared using the well-tempered formula for atoms Ga through Rn.

Recently, Huzinaga and Miguel [1], improving upon the earlier work [2], reported results of matrix Hartree–Fock calculations for atoms from helium to cadmium using a new recursive well-tempered formula (WTF) for the generation of the exponential parameters in Gaussian basis sets,

$$\zeta_N = \alpha\,, \tag{1a}$$

$$\zeta_{N-k+1} = \zeta_{N-k+2}\beta\left[1+\gamma\left(\frac{k}{N}\right)^{\delta}\right], \quad k=2,...,N\,. \tag{1b}$$

The well-tempered formula is a modification of the even-tempered formula, originally recommended by Reeves [3] and explored by Ruendenberg and coworkers [4]. In the well-tempered formula there are only four parameters (which need to be optimized) for each atom in the periodic table. The values of exponential parameters are shared between the angular symmetries, thus reducing the effort required in the optimization of basis sets. Usually, the higher angular subspaces use only a subset of the complete pool of exponential parameters defined by N; in consequence, the well-tempered basis sets contain a hidden parameter, the pattern of sharing the exponents between the s, p, d, and f symmetries.

The total energies obtained with the well-tempered formula [1] were lower than the ones calculated by Clementi and Corongiu who used the geometrical formula (GF) [5] in the context of the universal basis sets [6],

$$\zeta_k = \alpha\beta^{k-1}, \quad k=1,2,...,N\,. \tag{2}$$

In the present Letter, we report results for the atoms from gallium to radon. The total atomic energies are compared in table 1 with the numerical Hartree–Fock results [7,8] and with the extensive set of results available with the extra large geometrical basis sets prepared by Clementi [9]. The present WT total energies differ from the Hartree–Fock values by about 1 mE_h; this represents a reduction of the errors in our previous compilation of the well-tempered basis sets [10] by a factor of 2 to 10, with a more constant error as a function of the atomic number. (The large error for palladium indicates that the s space requires two to three additional functions.)

The use of the well-tempered formula leads to consistently more accurate energies which may be obtained with expansions shorter than the ones afforded by the geometrical formula. The gains in total energy are particularly large for the heavier elements, reaching over 2 mE_h. Given the shorter expansions, the present basis sets offer not only more accurate wavefunctions, but also shorter integral evaluation times. Further savings in the computing time may be achieved especially in the evaluation of energy derivatives with the integral codes which utilize the sharing of the exponents between the atomic angular symmetries (e.g. GAMESS [11], HONDO [12], or GAUSSIAN 90 [13]). The universal basis sets, with the same basis set for each atom in the

Table 1
Results for atoms gallium through radon

Z	Atom	WTF basis [a]	E(WTF) [b]	ΔE_{WT-HF} [c]	GF basis [d]	ΔE_{GF-WT} [c]
31	Ga ^{2}P	(26.20.14)	−1923.260947	0.1	(30.23.17)	0.019
32	Ge ^{3}P	(26.20.14)	−2075.359681	0.0	(30.24.17)	0.008
33	As ^{4}S	(26.20.14)	−2234.238607	0.0	(30.23.17)	0.026
34	Se ^{3}P	(26.20.14)	−2399.867562	0.0	(30.24.17)	0.031
35	Br ^{2}P	(26.20.14)	−2572.441282	0.0	(30.24.17)	0.066
36	Kr ^{1}S	(26.20.14)	−2752.054927	0.1	(30.24.17)	0.097
37	Rb ^{2}S	(28.20.14)	−2938.357357	0.0	(32.25.17)	0.266
38	Sr ^{1}S	(27.20.14)	−3131.545580	0.1	(33.24.17)	0.661
39	Y ^{2}D	(27.20.17)	−3331.684053	0.1	(33.24.20)	1.046
40	Zr ^{5}F	(27.20.17)	−3539.009463	1.3	n/a [f]	
41	Nb ^{6}D	(27.20.17)	−3753.597595	1.2	(33.24.20)	0.159
42	Mo ^{7}S	(27.20.17)	−3975.549367	1.2	(32.24.20)	0.090
43	Tc ^{6}S	(27.20.17)	−4204.788619	0.1	(32.24.20)	0.103
44	Ru ^{5}F	(28.20.17)	−4441.539362	1.6	(32.24.20)	0.195
45	Rh ^{4}F	(28.20.17)	−4685.881574	1.7	(32.24.20)	0.141
45	Rh ^{4}F	(28.20.17)	−4685.881602	1.7	(32.24.20)	0.169
46	Pd ^{1}S	(25.20.17)	−4937.920897	9.0	(30.24.20)	0.116
47	Ag ^{2}S	(28.20.17)	−5197.698318	1.8	(32.24.20)	0.124
48	Cd ^{1}S	(28.20.17)	−5465.132996	1.0	(33.24.20)	0.296
49	In ^{2}P	(28.23.17)	−5740.169018	0.1	(33.27.20)	1.205
50	Sn ^{3}P	(28.23.17)	−6022.931572	0.1	(33.27.20)	0.676
51	Sb ^{4}S	(28.23.17)	−6313.485205	0.1	(33.26.20)	0.546
52	Te ^{3}P	(28.23.17)	−6611.783948	0.1	(33.26.20)	0.456
53	I ^{2}P	(28.23.17)	−6917.980787	0.1	(33.26.20)	0.858
54	Xe ^{1}S	(28.23.17)	−7232.138256	0.1	(33.26.20)	0.600
55	Cs ^{2}S	(30.23.17)	−7553.933406	0.2	(32.25.17)	0.920
55	Cs ^{2}S	(30.22.16)	−7553.933344	0.3	(32.25.17)	0.858
56	Ba ^{1}S	(30.23.17)	−7883.543648	0.2	(32.25.17)	0.815
56	Ba ^{1}S	(30.22.16)	−7883.543542	0.3	(32.25.17)	0.710
57	La ^{2}F	(30.23.17.14)	−8221.063631	0.2	n/a [f]	
57	La ^{2}F	(29.22.16.13)	−8221.063495	0.3	n/a [f]	
58	Ce ^{3}H	(30.23.17.14)	−8566.919396	0.2	n/a [f]	
58	Ce ^{3}H	(29.22.16.13)	−8566.919256	0.2	n/a [f]	
59	Pr ^{4}I	(30.23.17.14)	−8921.180837	0.2	(32.25.17.16)	0.657
59	Pr ^{4}I	(29.22.16.13)	−8921.180691	0.3	(32.25.17.16)	0.511
60	Nd ^{5}I	(30.23.17.14)	−9283.882750	0.2	(32.25.17.16)	1.020
60	Nd ^{5}I	(29.22.16.13)	−9283.882591	0.3	(32.25.17.16)	0.861
61	Pm ^{6}H	(30.23.17.14)	−9655.098768	0.2	(32.25.17.16)	1.109
61	Pm ^{6}H	(29.22.16.13)	−9655.098597	0.4	(32.25.16.16)	0.938
62	Sm ^{7}F	(30.23.17.14)	−10034.95234	1	(32.25.17.16)	1.080
62	Sm ^{7}F	(29.22.16.13)	−10034.95216	1	(32.25.17.16)	0.900
63	Eu ^{8}S	(30.23.17.14)	−10423.54280	0	(32.25.17.16)	1.099
63	Eu ^{8}S	(29.22.16.13)	−10423.54261	0	(32.25.17.16)	0.910
64	Gd ^{7}F	(30.23.17.14)	−10820.61709	0	n/a [f]	
65	Tb ^{6}H	(30.23.17.14)	−11226.56814	0	(33.26.18.16)	0.819
66	Dy ^{5}I	(29.22.16.13)	−11641.45209	1	(33.26.18.16)	1.190
67	Ho ^{4}I	(29.22.16.13)	−12065.28927	1	(32.24.17.14)	1.029
68	Er ^{3}H	(29.22.16.13)	−12498.15221	1	(32.24.17.14)	1.089
69	Tm ^{2}F	(29.22.16.13)	−12940.17380	0	(32.24.17.14)	1.239
70	Yb ^{1}S	(29.22.16.13)	−13391.45555	1	(32.24.17.14)	1.320
71	Lu ^{2}D	(28.21.18.12)	−13851.80635	2	(31.24.20.14)	0.380
72	Hf ^{3}F	(28.21.18.12)	−14321.24839	2	(31.24.20.14)	0.830
73	Ta ^{4}F	(28.21.18.12)	−14799.81137	2	(31.24.20.14)	0.790

Table 1
Continued

Z	Atom	WTF basis [a]	E(WTF) [b]	ΔE_{WT-HF} [c]	GF basis [d]	ΔE_{GF-WT} [e]
74	W ^{5}D	(28.21.18.12)	−15287.54525	1	(31.24.20.14)	1.239
75	Re ^{6}S	(28.21.18.12)	−15784.53216	1	(31.24.20.14)	1.330
76	Os ^{5}D	(28.21.18.12)	−16290.64760	1	(32.24.20.15)	1.449
77	Ir ^{4}F	(28.21.18.12)	−16806.11218	1	(32.24.20.15)	1.870
78	Pt ^{3}F	(28.21.18.12)	−17330.94853	1	n/a [f]	
79	Au ^{2}D	(28.21.18.12)	−17865.21057	1	n/a [f]	
80	Hg ^{1}S	(29.21.19.13)	−18408.99066	0	(32.24.20.15)	2.949
81	Tl ^{2}P	(28.24.18.12)	−18961.82286	2	(31.25.18.13)	1.260
82	Pb ^{3}P	(28.24.18.12)	−19524.00666	1	(31.27.18.13)	2.079
83	Bi ^{4}S	(28.24.18.12)	−20095.58511	1	(32.27.17.13)	1.690
84	Po ^{3}P	(28.24.18.12)	−20676.49965	1	(31.27.17.13)	2.250
85	At ^{2}P	(28.24.18.12)	−21266.88050	2	(32.27.19.13)	1.799
86	Rn ^{1}S	(28.24.18.12)	−21866.77108	1	(32.27.19.13)	1.969

[a] Basis set composition, in the form $(N_sN_pN_dN_f)$, where N_s, N_p, N_d, and N_f denote the number of primitive Gaussian functions in s, p, d, and f symmetries, respectively.

[b] In E_h.

[c] $\Delta E_{WT-HF} = E(WTF) - E(Hartree-Fock)$, in m$E_h$. The Hartree–Fock energies for Zr, Nb, Mo, Ru, Rh, Pd, and Ag were taken from ref. [7]; for the remaining atoms, the values from ref. [8] were used.

[d] Composition of the geometrical basis set of Clementi et al. [9].

[e] $\Delta E_{GF-WT} = E_T(GF) - E_T(WTF)$, in m$E_h$.

[f] The total energy value with geometrical basis set was not available.

Table 2
Well-tempered basis set parameters for atoms gallium through radon

Z	Atom	Basis [a]	N [b]	n_s [c]	n_p [c]	n_d [c]	n_f [c]	α	β	γ	δ
31	Ga ^{2}P	(26.20.14)	26	1–26	7–26	11–24		0.033478856	1.9656669	1.5539089	6.2772092
32	Ge ^{3}P	(26.20.14)	26	1–26	7–26	11–24		0.043801291	1.9442305	1.5511544	6.0342177
33	As ^{4}S	(26.19.14)	26	1–26	7–26	11–24		0.054008662	1.9302825	1.5370025	5.8571955
34	Se ^{3}P	(26.20.14)	26	1–26	7–26	11–24		0.058044499	1.9309896	1.5034554	5.7796177
35	Br ^{2}P	(26.20.14)	26	1–26	7–26	11–24		0.065368677	1.9242003	1.4932524	5.6770996
36	Kr ^{1}S	(26.20.14)	26	1–26	7–26	11–24		0.074140048	1.9161479	1.4790484	5.5537223
37	Rb ^{2}S	(28.20.14)	28	1–28	5–24	9–22		0.006994845	1.9333439	1.6727633	7.9251256
39	Y ^{2}D	(27.20.17)	27	1–27	5–24	9–25		0.013399914	1.9341040	1.6577129	7.5300706
40	Zr ^{5}F	(27.20.17)	27	1–27	5–24	9–25		0.012729382	1.9391086	1.6537103	7.5657467
41	Nb ^{6}D	(27.20.17)	27	1–27	5–24	9–25		0.014967864	1.9275700	1.6470356	7.3842378
42	Mo ^{7}S	(27.20.17)	27	1–27	5–24	9–25		0.017093309	1.9229625	1.6523403	7.3546046
43	Tc ^{6}S	(27.20.17)	27	1–27	5–24	9–25		0.025190452	1.9051284	1.6556004	7.1700089
44	Ru ^{5}F	(28.20.17)	28	1–28	5–24	10–26		0.016814835	1.9041149	1.5960644	7.0931386
45	Rh ^{4}F	(28.20.17)	28	1–28	5–24	10–26		0.018454915	1.8994527	1.5911554	7.0072394
46	Pd ^{1}S	(25.20.17)	27	1–25	6–25	11–27		0.064111928	1.9008769	1.4989843	6.1172938
47	Ag ^{2}S	(28.20.17)	28	1–28	5–24	9–25		0.014309780	1.8964432	1.6329277	7.2130815
48	Cd ^{1}S	(28.20.17)	28	1–28	5–24	9–25		0.018295851	1.8841030	1.6382719	7.0970719
49	In ^{2}P	(28.23.17)	28	1–28	6–28	9–25		0.026831215	1.8828322	1.5800531	6.5791409
50	Sn ^{3}P	(28.23.17)	28	1–28	6–28	9–25		0.032105564	1.8667463	1.5696267	6.3472325
51	Sb ^{4}S	(28.23.17)	28	1–28	6–28	9–25		0.036980271	1.8575179	1.5615381	6.2163092
52	Te ^{3}P	(28.23.17)	28	1–28	6–28	9–25		0.041574137	1.8504398	1.5546086	6.1152297
53	I ^{2}P	(28.23.17)	28	1–28	6–28	9–25		0.046805988	1.8410014	1.5219766	5.8949277

Table 2
Continued

Z	Atom	Basis [a]	N [b]	n_s [c]	n_p [c]	n_d [c]	n_f [c]	α	β	γ	δ
54	Xe ^{1}S	(28.23.17)	28	1–28	6–28	9–25		0.051768411	1.8356669	1.5306431	5.8707155
55	Cs ^{2}S	(30.23.17)	30	1–30	6–28	9–25		0.006205750	1.8965736	1.6339200	7.3981445
55	Cs ^{2}S	(30.22.16)	30	1–30	5–26	8–23		0.005647588	1.8732380	1.6436412	7.5401384
56	Ba ^{1}S	(30.23.17)	30	1–30	5–27	8–24		0.008193867	1.8635741	1.6554853	7.4850042
56	Ba ^{1}S	(30.22.16)	30	1–30	5–26	8–23		0.006882942	1.8601334	1.6197031	7.2510350
57	La ^{2}F	(30.23.17.14)	30	1–30	5–27	8–24	13–26	0.009424034	1.8524563	1.6417791	7.2711946
57	La ^{2}F	(29.22.16.13)	29	1–29	5–26	8–23	13–25	0.012167500	1.8786395	1.6490068	7.3681762
58	Ce ^{3}H	(30.23.17.14)	30	1–30	5–27	8–24	13–26	0.009886241	1.8525013	1.6440774	7.2834906
58	Ce ^{3}H	(29.22.16.13)	29	1–29	5–26	8–23	13–25	0.012749486	1.8794185	1.6560415	7.4132006
59	Pr ^{4}I	(30.23.17.14)	30	1–30	5–27	8–24	13–26	0.010603989	1.8498369	1.6429707	7.2434941
59	Pr ^{4}I	(29.22.16.13)	29	1–29	5–26	8–23	13–25	0.013756969	1.8733229	1.6427874	7.2683088
60	Nd ^{5}I	(30.23.17.14)	30	1–30	5–27	8–24	13–26	0.011769041	1.8432048	1.6367820	7.1284981
60	Nd ^{5}I	(29.22.16.13)	29	1–29	5–26	8–23	13–25	0.014446770	1.8721559	1.6420637	7.2493023
61	Pm ^{6}H	(30.23.17.14)	30	1–30	5–27	8–24	13–26	0.012594447	1.8405081	1.6349346	7.0847864
61	Pm ^{6}H	(29.22.16.13)	29	1–29	5–26	8–23	13–25	0.015062335	1.8719857	1.6433392	7.2527774
62	Sm ^{7}F	(30.23.17.14)	30	1–30	5–27	8–24	13–26	0.013110674	1.8408554	1.6358087	7.0931771
62	Sm ^{7}F	(29.22.16.13)	29	1–29	5–26	8–23	13–25	0.015655533	1.8718921	1.6508714	7.2854057
63	Eu ^{8}S	(30.23.17.14)	30	1–30	5–27	8–24	13–26	0.013634696	1.8412842	1.6368254	7.1032381
63	Eu ^{8}S	(29.22.16.13)	29	1–29	5–26	8–23	13–25	0.016323905	1.8726612	1.6316624	7.2103133
64	Gd ^{7}F	(30.23.17.14)	30	1–30	5–27	8–24	13–26	0.014880098	1.8357112	1.6297028	6.9969975
65	Tb ^{6}H	(30.23.17.14)	30	1–30	5–27	8–24	13–26	0.015719028	1.8355373	1.6418157	7.0506604
66	Dy ^{5}I	(29.22.16.13)	29	1–29	5–26	8–23	13–25	0.017356543	1.8776945	1.6545193	7.3802779
67	Ho ^{4}I	(29.22.16.13)	29	1–29	5–26	8–23	13–25	0.018299088	1.8751135	1.6537262	7.3375433
68	Er ^{3}H	(29.22.16.13)	29	1–29	5–26	8–23	13–25	0.018331714	1.8777085	1.6427217	7.3213070
69	Tm ^{2}F	(29.22.16.13)	29	1–29	5–26	8–23	13–25	0.018816196	1.8835579	1.6561962	7.4705881
70	Yb ^{1}S	(29.22.16.13)	29	1–29	5–26	8–23	13–25	0.019609755	1.8769006	1.6336652	7.2633387
71	Lu ^{2}D	(28.21.18.12)	28	1–28	5–25	9–26	12–23	0.014709150	1.9108988	1.5499378	6.8465126
72	Hf ^{3}F	(28.21.18.12)	28	1–28	5–25	9–26	12–23	0.018835349	1.9046337	1.5920657	6.9968492
73	Ta ^{4}F	(28.21.18.12)	28	1–28	5–25	9–26	12–23	0.021258913	1.9049112	1.6107335	7.1094981
74	W ^{5}D	(28.21.18.12)	28	1–28	5–25	9–26	12–23	0.024350157	1.8956066	1.6070043	6.9773212
75	Re ^{6}S	(28.21.18.12)	28	1–28	5–25	9–26	12–23	0.026726780	1.8917422	1.6086724	6.9437078
76	Os ^{5}D	(28.21.18.12)	28	1–28	5–25	9–26	12–23	0.028440892	1.8910588	1.6137351	6.9651962
77	Ir ^{4}F	(28.21.18.12)	28	1–28	5–25	9–26	12–23	0.030886535	1.8846474	1.6015049	6.8305667
78	Pt ^{3}F	(28.21.18.12)	28	1–28	5–25	9–26	12–23	0.034846613	1.8725279	1.5507198	6.4723861
79	Au ^{2}D	(28.21.18.12)	28	1–28	5–25	9–26	12–23	0.035988705	1.8768550	1.6055441	6.7570415
80	Hg ^{1}S	(29.21.19.13)	29	1–29	5–25	8–26	11–23	0.019734899	1.8709082	1.6319225	7.1792006
81	Tl ^{2}P	(28.24.18.12)	29	1–28	6–29	8–25	11–22	0.014716794	1.8785862	1.6189210	6.5660739
82	Pb ^{3}P	(28.24.18.12)	28	1–28	5–28	8–25	11–22	0.028780466	1.8662415	1.6426297	6.8426661
83	Bi ^{4}S	(28.24.18.12)	28	1–28	5–28	8–25	11–22	0.033493819	1.8605779	1.6351168	6.7566267
84	Po ^{3}P	(28.24.18.12)	28	1–28	5–28	8–25	11–22	0.037976823	1.8564612	1.6270079	6.6811922
85	At ^{2}P	(28.24.18.12)	28	1–28	5–28	8–25	11–22	0.042684207	1.8464375	1.5695743	6.3280601
86	Rn ^{1}S	(28.24.18.12)	28	1–28	5–28	8–25	11–22	0.047179407	1.8420977	1.5402892	6.1641823

[a] Basis set composition, see table 1.
[b] The number of exponential parameters, see eq. (1).
[c] The range of exponents taken from the exponent pool generated by eq. (1) to span the s, p, d, and f spaces.

molecule, may nevertheless outperform the well-tempered basis sets in the studies of the potential energy surfaces for related families of molecules, when the integrals from one molecule may be re-used for another provided the geometry remains unchanged [14].

The present well-tempered basis sets may appear too large for the calculations of the structure and

properties of large molecules. However, the computer technology is quickly catching up with our dreams, and, assisted by the development of direct methods for molecular structure calculations, will allow us to use basis sets which are free of the basis set superposition error affecting the computed geometries and properties, and ubiquitous in the results obtained with smaller, unbalanced basis sets.

The optimized values of the well-tempered parameters used in the generation of the present basis sets are collected in table 2 together with the description of the composition of the basis set. The atomic expansion coefficients and orbital energies may be obtained by an anonymous ftp from kamuy.chem.ualberta.ca (or 129.128.2.22). Complete information about retrieval is contained in the file README. Also available are tables of our best well-tempered basis sets for atoms helium through radon.

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