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REGULAR ARTICLE

Core correlating basis functions for elements 31–118

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Abstract Gaussian functions for correlation of all core shells of elements from $Z = 31$ to $Z = 118$ have been optimized in relativistic singles and doubles CI calculations, performed on the shell of highest angular momentum for each principal quantum number. The SCF functions were derived from the double-zeta, triple-zeta, and quadruple-zeta basis sets previously optimized by the author. Only those Gaussian functions that are not represented in the SCF basis sets were optimized. The functions are available from the Dirac program web site, http://dirac.chem.sdu.dk.

Keywords Gaussian basis sets · Relativistic basis sets · Core correlation

1 Introduction

In basis sets used for accurate molecular calculations, it is necessary to include basis functions for electron correlation. For moderate accuracy, it is often only necessary to correlate the valence shells, and the valence correlating functions serve also for polarization of the atomic valence shells. For higher accuracy, it is necessary to correlate at least part of the core, particularly for the heavy elements where the outer core becomes more polarizable as Z increases. Outer-core correlation is usually adequate for molecular energetics and valence properties, and outer-core correlating functions are provided with many basis sets [1–21]. The valence and outer core regions are not the only regions of interest. The higher the accuracy that is required, the deeper into the core one must correlate to obtain this accuracy. Moreover, nuclear properties can be sensitive to correlation of the inner shells. This paper addresses the correlation of all the core shells, for the elements from $Z = 31$ to $Z = 118$, which is the range of the relativistic basis sets developed by the author [22–33]. The core correlating functions are intended to be a supplement to these basis sets. The functions should be equally useful in one-component, two-component, and four-component all-electron calculations, as the optimizations are performed on atomic configuration averages.

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2 Methods

The atomic SCF functions were calculated at the Dirac–Coulomb level with the standard Gaussian nucleus [34] for the state average of the ground configuration, using the basis set adaption of GRASP [35, 36]. SCF calculations were performed in the double-zeta, triple-zeta, and quadruple-zeta basis sets of the author [22–33]. These SCF functions were used for the occupied spinors in the correlated calculations to generate the corresponding double-zeta, triple-zeta, and quadruple-zeta correlating sets.

The core correlating functions were optimized in Dirac–Coulomb singles and doubles CI (SDCI) calculations on the shell of highest angular momentum for each principal quantum number, using RAMCI [37]. All singles and doubles from the specified shell into the correlating space that couple with that shell to $J = 0$ were taken. The restriction to $J = 0$ limits the configuration space and ensures that only the specified shell is correlated.

Three sets of exponents were optimized, for double-zeta, triple-zeta, and quadruple-zeta basis sets. Because

flexibility is required in the SCF occupied spinors that are being correlated, the SCF basis sets are intended to be used uncontracted, and therefore it was not deemed necessary to optimize exponents where the SCF exponent set already provides functions of the right magnitude for correlation.

For shells (like the 1s) where some of the correlating functions are already represented in the basis, these correlating functions were represented by primitive functions from the SCF set, which were not optimized. The selection of primitives was made to approximately match the exponents that represent the outermost maximum of the selected shell. To obtain orthogonal spinors for the CI calculations, the spinors representing these functions were determined by adding the primitive functions to the SCF occupied functions and diagonalizing the Fock matrix in this basis. This ensures the proper representation of the large and small components.

For the remaining correlating functions, which were optimized, the spinors were derived from single Gaussians, with the large and small components determined in a Thomas-Fermi potential for the ground configuration.

For each subshell with principal quantum number n that was correlated, the correlating space consisted of the spinors that span a single subshell with $\ell = n$ for the double-zeta basis sets; two subshells with $\ell = n$ and one subshell with $\ell = n + 1$ for the triple-zeta basis sets; and three subshells with $\ell = n$, two subshells with $\ell = n + 1$, and one subshell with $\ell = n + 2$ for the quadruple-zeta basis

Table 1 Exponents of f functions for 3d and 4d correlation in the double-zeta basis sets

Shell	Element	Exponent	Element	Exponent	Element	Exponent
3d	Ga	3.93744E+00	Zr	1.05908E+01	In	2.00766E+01
	Ge	4.64271E+00	Nb	1.15101E+01	Sn	2.13030E+01
	As	5.34799E+00	Mo	1.24615E+01	Sb	2.25658E+01
	Se	6.05326E+00	Tc	1.34457E+01	Te	2.38650E+01
	Br	6.75853E+00	Ru	1.44648E+01	I	2.52007E+01
	Kr	7.46381E+00	Rh	1.55167E+01	Xe	2.65732E+01
	Rb	8.03966E+00	Pd	1.66108E+01	Cs	2.79834E+01
	Sr	8.81702E+00	Ag	1.77308E+01	Ba	2.94310E+01
	Y	9.70596E+00	Cd	1.88860E+01	La	3.09165E+01
4d	Cs	3.22076E+00	Ba	3.49335E+00	La	3.77622E+00

Table 2 Exponents of g functions for 4f and 5f correlation in the double-zeta basis sets

Shell	Element	Exponent	Element	Exponent	Element	Exponent
4f	Hf	7.14483E+00	Ra	1.79917E+01	Rf	3.22932E+01
	Ta	7.73013E+00	Ac	1.87863E+01	Db	3.33010E+01
	W	8.32738E+00	Th	1.95953E+01	Sg	3.43231E+01
	Re	8.93608E+00	Pa	2.04163E+01	Bh	3.53594E+01
	Os	9.55613E+00	U	2.12505E+01	Hs	3.64101E+01
	Ir	1.01876E+01	Np	2.20974E+01	Mt	3.74751E+01
	Pt	1.08306E+01	Pu	2.29573E+01	Ds	3.85544E+01
	Au	1.14853E+01	Am	2.38304E+01	Rg	3.96482E+01
	Hg	1.21519E+01	Cm	2.47161E+01	Cn	4.07562E+01
	Tl	1.28333E+01	Bk	2.56145E+01	Uut	4.18789E+01
	Pb	1.35278E+01	Cf	2.65264E+01	Uuq	4.30162E+01
	Bi	1.42364E+01	Es	2.74514E+01	Uup	4.41681E+01
	Po	1.49590E+01	Fm	2.83897E+01	Uuh	4.53346E+01
	At	1.56956E+01	Md	2.93413E+01	Uus	4.65156E+01
	Rn	1.64463E+01	No	3.03202E+01	Uuo	4.77114E+01
	Fr	1.72117E+01	Lr	3.12996E+01		
5f	Rf	3.44853E+00	Mt	4.67093E+00	Uuq	5.96241E+00
	Db	3.68890E+00	Ds	4.92260E+00	Uup	6.23224E+00
	Sg	3.93111E+00	Rg	5.17707E+00	Uuh	6.50599E+00
	Bh	4.17537E+00	Cn	5.43451E+00	Uus	6.78364E+00
	Hs	4.42191E+00	Uut	5.69651E+00	Uuo	7.06521E+00

Table 3 Exponents of f functions for 2p correlation in the triple-zeta basis sets

Element	Exponent	Element	Exponent	Element	Exponent
Ga	5.03818E+01	Zr	9.19818E+01	In	1.47488E+02
Ge	5.44566E+01	Nb	9.68640E+01	Sn	1.55321E+02
As	5.86810E+01	Mo	1.02668E+02	Sb	1.63246E+02
Se	6.29592E+01	Tc	1.09251E+02	Te	1.71139E+02
Br	6.73544E+01	Ru	1.14828E+02	I	1.79264E+02
Kr	7.18930E+01	Rh	1.21187E+02	Xe	1.87499E+02
Rb	7.66377E+01	Pd	1.26912E+02	Cs	1.95476E+02
Sr	8.16985E+01	Ag	1.34468E+02	Ba	2.04352E+02
Y	8.65930E+01	Cd	1.41767E+02	La	2.09280E+02

Table 4 Exponents of f and g functions for 3d and 4d correlation in the triple-zeta basis sets for $Z < 58$

Shell	Element	f	f	g
3d	Ga	7.53691E+00	2.10609E+00	4.73594E+00
	Ge	8.71519E+00	2.49719E+00	5.48492E+00
	As	9.94484E+00	2.90803E+00	6.27408E+00
	Se	1.12276E+01	3.33897E+00	7.10287E+00
	Br	1.25650E+01	3.79044E+00	7.97131E+00
	Kr	1.39583E+01	4.26276E+00	8.87951E+00
	Rb	1.54186E+01	4.76051E+00	9.83284E+00
	Sr	1.69434E+01	5.28252E+00	1.08302E+01
	Y	1.85359E+01	5.83038E+00	1.18725E+01
	Zr	2.01881E+01	6.40037E+00	1.29561E+01
	Nb	2.19031E+01	6.99390E+00	1.40819E+01
	Mo	2.36733E+01	7.60731E+00	1.52473E+01
	Tc	2.55000E+01	8.24099E+00	1.64527E+01
	Ru	2.73926E+01	8.89943E+00	1.77012E+01
	Rh	2.93422E+01	9.57826E+00	1.89899E+01
	Pd	3.13738E+01	1.02888E+01	2.03313E+01
	Ag	3.34446E+01	1.10117E+01	2.17033E+01
	Cd	3.55787E+01	1.17576E+01	2.31185E+01
	In	3.77772E+01	1.25271E+01	2.45774E+01
	Sn	4.00413E+01	1.33205E+01	2.60806E+01
	Sb	4.23710E+01	1.41378E+01	2.76281E+01
	Te	4.47671E+01	1.49793E+01	2.92204E+01
	I	4.72297E+01	1.58450E+01	3.08575E+01
	Xe	4.97594E+01	1.67351E+01	3.25395E+01
	Cs	5.23578E+01	1.76501E+01	3.42679E+01
	Ba	5.50258E+01	1.85905E+01	3.60424E+01
	La	5.77630E+01	1.95560E+01	3.78632E+01
4d	In	3.02134E+00	1.00488E+00	2.04007E+00
	Sn	3.39106E+00	1.15637E+00	2.29281E+00
	Sb	3.77151E+00	1.31218E+00	2.55221E+00
	Te	4.16446E+00	1.47294E+00	2.81869E+00
	I	4.57121E+00	1.63914E+00	3.09261E+00
	Xe	4.99357E+00	1.81160E+00	3.37429E+00
	Cs	5.43669E+00	1.99304E+00	3.66666E+00
	Ba	5.90064E+00	2.18317E+00	3.96825E+00
	La	6.38586E+00	2.38265E+00	4.28068E+00

Table 5 Exponents of g functions for 3d correlation in the triple-zeta basis sets

Element	Exponent	Element	Exponent	Element	Exponent
Ce	3.97251E+01	Au	8.99628E+01	Fm	1.62048E+02
Pr	4.17453E+01	Hg	9.28244E+01	Md	1.66091E+02
Nd	4.36947E+01	Tl	9.57334E+01	No	1.70192E+02
Pm	4.56949E+01	Pb	9.86994E+01	Lr	1.74296E+02
Sm	4.77442E+01	Bi	1.01721E+02	Rf	1.78373E+02
Eu	4.98418E+01	Po	1.04795E+02	Db	1.82538E+02
Gd	5.19368E+01	At	1.07926E+02	Sg	1.86807E+02
Tb	5.41803E+01	Rn	1.11111E+02	Bh	1.91154E+02
Dy	5.64206E+01	Fr	1.14359E+02	Hs	1.95572E+02
Ho	5.87081E+01	Ra	1.17654E+02	Mt	2.00059E+02
Er	6.10431E+01	Ac	1.20934E+02	Ds	2.04612E+02
Tm	6.34256E+01	Th	1.24702E+02	Rg	2.09231E+02
Yb	6.58559E+01	Pa	1.28175E+02	Cn	2.13916E+02
Lu	6.82631E+01	U	1.31710E+02	Uut	2.18502E+02
Hf	7.10997E+01	Np	1.35299E+02	Uuq	2.23308E+02
Ta	7.37012E+01	Pu	1.39003E+02	Uup	2.28177E+02
W	7.63142E+01	Am	1.42700E+02	Uuh	2.33110E+02
Re	7.89568E+01	Cm	1.46398E+02	Uus	2.38107E+02
Os	8.16387E+01	Bk	1.50267E+02	Uuo	2.43170E+02
Ir	8.43658E+01	Cf	1.54138E+02		
Pt	8.71388E+01	Es	1.58064E+02		

Table 6 Exponents of g and h functions for 4f correlation in the triple-zeta basis sets

Element	g	g	h	Element	g	g	h
Hf	1.30857E+01	3.90470E+00	8.39548E+00	Cm	4.43206E+01	1.54736E+01	2.91183E+01
Ta	1.41594E+01	4.29051E+00	9.08425E+00	Bk	4.59022E+01	1.60690E+01	3.01792E+01
W	1.52462E+01	4.68266E+00	9.78740E+00	Cf	4.75057E+01	1.66727E+01	3.12558E+01
Re	1.63472E+01	5.08131E+00	1.05043E+01	Es	4.91318E+01	1.72852E+01	3.23480E+01
Os	1.74636E+01	5.48682E+00	1.12347E+01	Fm	5.07803E+01	1.79064E+01	3.34558E+01
Ir	1.85963E+01	5.89938E+00	1.19788E+01	Md	5.24516E+01	1.85365E+01	3.45791E+01
Pt	1.97462E+01	6.31925E+00	1.27365E+01	No	5.41772E+01	1.91907E+01	3.57358E+01
Au	2.09140E+01	6.74667E+00	1.35082E+01	Lr	5.58945E+01	1.98386E+01	3.68920E+01
Hg	2.21004E+01	7.18177E+00	1.42940E+01	Rf	5.76360E+01	2.04959E+01	3.80652E+01
Tl	2.33125E+01	7.62762E+00	1.50966E+01	Db	5.94024E+01	2.11628E+01	3.92551E+01
Pb	2.45476E+01	8.08312E+00	1.59156E+01	Sg	6.11936E+01	2.18394E+01	4.04621E+01
Bi	2.58062E+01	8.54831E+00	1.67513E+01	Bh	6.30098E+01	2.25258E+01	4.16858E+01
Po	2.70882E+01	9.02315E+00	1.76035E+01	Hs	6.48509E+01	2.32219E+01	4.29266E+01
At	2.83939E+01	9.50772E+00	1.84724E+01	Mt	6.67167E+01	2.39276E+01	4.41842E+01
Rn	2.97232E+01	1.00019E+01	1.93580E+01	Ds	6.86078E+01	2.46430E+01	4.54588E+01
Fr	3.10772E+01	1.05064E+01	2.02610E+01	Rg	7.05237E+01	2.53681E+01	4.67505E+01
Ra	3.24564E+01	1.10210E+01	2.11813E+01	Cn	7.24656E+01	2.61033E+01	4.80595E+01
Ac	3.38601E+01	1.15458E+01	2.21189E+01	Uut	7.15618E+01	2.51417E+01	4.85201E+01
Th	3.52884E+01	1.20805E+01	2.30735E+01	Uuq	7.35479E+01	2.58887E+01	4.98572E+01
Pa	3.67416E+01	1.26258E+01	2.40429E+01	Uup	7.55597E+01	2.66456E+01	5.12117E+01
U	3.82147E+01	1.31787E+01	2.50277E+01	Uuh	7.75966E+01	2.74122E+01	5.25834E+01
Np	3.97084E+01	1.37396E+01	2.60274E+01	Uus	7.96589E+01	2.81886E+01	5.39722E+01
Pu	4.12244E+01	1.43094E+01	2.70425E+01	Uuo	8.17466E+01	2.89749E+01	5.53783E+01
Am	4.27629E+01	1.48879E+01	2.80729E+01				

Table 7 Exponents of g and h functions for 5f correlation in the triple-zeta basis sets

Element	g	g	h
Rf	5.59311E+00	1.91995E+00	3.90272E+00
Db	5.96675E+00	2.08478E+00	4.16995E+00
Sg	6.34031E+00	2.24974E+00	4.43876E+00
Bh	6.71508E+00	2.41537E+00	4.70939E+00
Hs	7.09207E+00	2.58209E+00	4.98210E+00
Mt	7.47200E+00	2.75020E+00	5.25710E+00
Ds	7.85554E+00	2.91998E+00	5.53465E+00
Rg	8.24309E+00	3.09158E+00	5.81488E+00
Cn	8.63513E+00	3.26521E+00	6.09798E+00
Uut	9.03872E+00	3.44541E+00	6.38587E+00
Uuq	9.44934E+00	3.62919E+00	6.67782E+00
Uup	9.86695E+00	3.81644E+00	6.97373E+00
Uuh	1.02914E+01	4.00702E+00	7.27359E+00
Uus	1.07228E+01	4.20088E+00	7.57737E+00
Uuo	1.11610E+01	4.39800E+00	7.88513E+00

sets, following the style of the correlation-consistent basis sets [1–4]. For example, for 3d correlation, the dz correlating set was 1f, the tz correlating set was 2f1g, and the qz correlating set was 3f2g1h.

3 Results

The exponents for each basis set size are described in the sections below.

3.1 Double-zeta basis sets

The p exponents required for 1s correlation are already represented in the SCF basis set, and so are the d exponents for 2p correlation. For 3d correlation, an f exponent is required for $Z < 58$, and an f exponent for 4d correlation for Cs, Ba, and La. For 4f correlation, a g exponent is required for $Z > 80$ (beyond what is already published). The exponents, including those previously published for outer-core correlation, are given in Tables 1 and 2.

3.2 Triple-zeta basis sets

The p and d exponents required in a 2p1d set for 1s correlation are already represented in the SCF basis set, and so are the d exponents in a 2d1f set for 2p correlation. The f exponents for 2p correlation are required for $Z < 58$. For 3d and 4d correlation, a 2f1g exponent set is required for $Z < 58$. For 3d correlation for higher Z, the f exponents are

Table 8 Exponents of f functions for 1s correlation in the quadruple-zeta basis sets

Element	Exponent	Element	Exponent	Element	Exponent	Element	Exponent
Ga	8.20620E+02	I	2.71721E+03	Re	6.99077E+03	Bk	1.68645E+04
Ge	8.77822E+02	Xe	2.84420E+03	Os	7.27821E+03	Cf	1.75692E+04
As	9.36340E+02	Cs	2.97690E+03	Ir	7.57658E+03	Es	1.83060E+04
Se	9.97655E+02	Ba	3.11283E+03	Pt	7.88720E+03	Fm	1.90732E+04
Br	1.06130E+03	La	3.25662E+03	Au	8.21017E+03	Md	1.98750E+04
Kr	1.12743E+03	Ce	3.40392E+03	Hg	8.54561E+03	No	2.07290E+04
Rb	1.19649E+03	Pr	3.56125E+03	Tl	8.88158E+03	Lr	2.16316E+04
Sr	1.26769E+03	Nd	3.71818E+03	Pb	9.24230E+03	Rf	2.25493E+04
Y	1.33970E+03	Pm	3.88227E+03	Bi	9.62260E+03	Db	2.35700E+04
Zr	1.41657E+03	Sm	4.05322E+03	Po	1.00170E+04	Sg	2.45555E+04
Nb	1.49642E+03	Eu	4.23020E+03	At	1.04268E+04	Bh	2.56415E+04
Mo	1.57925E+03	Gd	4.41881E+03	Rn	1.08533E+04	Hs	2.67823E+04
Tc	1.66428E+03	Tb	4.61285E+03	Fr	1.13055E+04	Mt	2.79820E+04
Ru	1.75415E+03	Dy	4.80406E+03	Ra	1.17392E+04	Ds	2.92544E+04
Rh	1.84666E+03	Ho	5.00962E+03	Ac	1.22388E+04	Rg	3.05839E+04
Pd	1.94258E+03	Er	5.22361E+03	Th	1.27389E+04	Cn	3.19992E+04
Ag	2.04192E+03	Tm	5.44487E+03	Pa	1.32232E+04	Uut	3.35019E+04
Cd	2.14468E+03	Yb	5.67507E+03	U	1.37768E+04	Uuq	3.50808E+04
In	2.25110E+03	Lu	5.94276E+03	Np	1.43430E+04	Uup	3.67755E+04
Sn	2.36144E+03	Hf	6.19003E+03	Pu	1.49329E+04	Uuh	3.85782E+04
Sb	2.47590E+03	Ta	6.44753E+03	Am	1.55471E+04	Uus	4.05295E+04
Te	2.59413E+03	W	6.71341E+03	Cm	1.61904E+04	Uuo	4.24800E+04

Table 9 Exponents of 2f1g set for 2p correlation in the quadruple-zeta basis sets for $Z < 58$

Element	f	f	g
Ga	9.26669E+01	3.65812E+01	6.48465E+01
Ge	1.01323E+02	3.99880E+01	6.99907E+01
As	1.09941E+02	4.33981E+01	7.53214E+01
Se	1.18539E+02	4.68155E+01	8.08601E+01
Br	1.27142E+02	5.02503E+01	8.66224E+01
Kr	1.35748E+02	5.36973E+01	9.26014E+01
Rb	1.46452E+02	5.83462E+01	9.94756E+01
Sr	1.55519E+02	6.20103E+01	1.06015E+02
Y	1.56117E+02	6.02854E+01	1.07022E+02
Zr	1.65721E+02	6.40421E+01	1.13518E+02
Nb	1.75165E+02	6.77406E+01	1.20324E+02
Mo	1.84617E+02	7.15060E+01	1.27349E+02
Tc	1.96247E+02	7.60008E+01	1.34293E+02
Ru	2.07471E+02	8.02997E+01	1.41651E+02
Rh	2.18780E+02	8.46938E+01	1.49233E+02
Pd	2.30035E+02	8.90769E+01	1.57097E+02
Ag	2.42007E+02	9.37902E+01	1.65067E+02
Cd	2.52692E+02	9.81859E+01	1.73480E+02
In	2.57430E+02	1.00778E+02	1.82463E+02
Sn	2.71754E+02	1.06204E+02	1.91321E+02
Sb	2.86844E+02	1.11879E+02	2.00363E+02
Te	3.02342E+02	1.17705E+02	2.09591E+02
I	3.17103E+02	1.23355E+02	2.19105E+02
Xe	3.33347E+02	1.29458E+02	2.28785E+02
Cs	3.49937E+02	1.35699E+02	2.38700E+02
Ba	3.66713E+02	1.42032E+02	2.48871E+02
La	3.78503E+02	1.47256E+02	2.59720E+02

Table 10 Exponents of g functions for 2p correlation in the quadruple-zeta basis sets for $Z > 57$

Element	Exponent	Element	Exponent	Element	Exponent
Ce	2.68947E+02	Au	5.80726E+02	Fm	1.08533E+03
Pr	2.82307E+02	Hg	6.00035E+02	Md	1.11710E+03
Nd	2.92859E+02	Tl	6.15479E+02	No	1.15037E+03
Pm	3.03933E+02	Pb	6.39018E+02	Lr	1.19658E+03
Sm	3.15469E+02	Bi	6.54755E+02	Rf	1.24239E+03
Eu	3.27413E+02	Po	6.74645E+02	Db	1.28803E+03
Gd	3.39289E+02	At	6.94963E+02	Sg	1.33382E+03
Tb	3.52460E+02	Rn	7.16108E+02	Bh	1.38025E+03
Dy	3.65522E+02	Fr	7.38634E+02	Hs	1.42860E+03
Ho	3.78941E+02	Ra	7.62898E+02	Mt	1.47812E+03
Er	3.92714E+02	Ac	7.85609E+02	Ds	1.52987E+03
Tm	4.06841E+02	Th	8.17018E+02	Rg	1.58017E+03
Yb	4.21320E+02	Pa	8.38165E+02	Cn	1.63409E+03
Lu	4.29791E+02	U	8.63466E+02	Uut	1.78266E+03
Hf	4.50859E+02	Np	8.89992E+02	Uuq	1.84196E+03
Ta	4.69843E+02	Pu	9.06484E+02	Uup	1.90063E+03
W	4.88285E+02	Am	9.35072E+02	Uuh	1.96152E+03
Re	5.06462E+02	Cm	9.74477E+02	Uus	2.01991E+03
Os	5.24739E+02	Bk	9.92834E+02	Uuo	2.08399E+03
Ir	5.43128E+02	Cf	1.02265E+03		
Pt	5.61770E+02	Es	1.05336E+03		

Table 11 Exponents of f, g, and h functions for 3d and 4d correlation in the quadruple-zeta basis sets for $Z < 58$

Shell	Element	f	f	f	g	g	h
3d	Ga	1.22480E+01	4.13113E+00	1.39235E+00	8.49733E+00	2.70975E+00	5.42526E+00
	Ge	1.41607E+01	4.85873E+00	1.68461E+00	9.82558E+00	3.20854E+00	6.29850E+00
	As	1.61450E+01	5.61650E+00	1.99098E+00	1.12147E+01	3.73317E+00	7.21665E+00
	Se	1.82069E+01	6.40664E+00	2.31219E+00	1.26662E+01	4.28396E+00	8.17986E+00
	Br	2.03504E+01	7.23060E+00	2.64874E+00	1.41813E+01	4.86136E+00	9.18848E+00
	Kr	2.25786E+01	8.08954E+00	3.00103E+00	1.57614E+01	5.46573E+00	1.02429E+01
	Rb	2.49173E+01	8.99500E+00	3.37518E+00	1.74177E+01	6.10246E+00	1.13499E+01
	Sr	2.73579E+01	9.94296E+00	3.76892E+00	1.91478E+01	6.77029E+00	1.25081E+01
	Y	2.99053E+01	1.09352E+01	4.18367E+00	2.09549E+01	7.47091E+00	1.37185E+01
	Zr	3.25444E+01	1.19650E+01	4.61522E+00	2.28307E+01	8.20006E+00	1.49767E+01
	Nb	3.52802E+01	1.30342E+01	5.06485E+00	2.47784E+01	8.95930E+00	1.62839E+01
	Mo	3.81006E+01	1.41376E+01	5.52887E+00	2.67906E+01	9.74444E+00	1.76369E+01
	Tc	4.10085E+01	1.52764E+01	6.00782E+00	2.88686E+01	1.05560E+01	1.90361E+01
	Ru	4.40186E+01	1.64564E+01	6.50591E+00	3.10213E+01	1.13991E+01	2.04856E+01
	Rh	4.71174E+01	1.76722E+01	7.01904E+00	3.32405E+01	1.22687E+01	2.19816E+01
	Pd	5.03547E+01	1.89460E+01	7.56047E+00	3.55527E+01	1.31790E+01	2.35394E+01
	Ag	5.36413E+01	2.02368E+01	8.10660E+00	3.79104E+01	1.41052E+01	2.51320E+01
	Cd	5.70365E+01	2.15731E+01	8.67190E+00	4.03439E+01	1.50618E+01	2.67751E+01
	In	6.05304E+01	2.29485E+01	9.25482E+00	4.28502E+01	1.60484E+01	2.84688E+01
	Sn	6.41284E+01	2.43660E+01	9.85630E+00	4.54312E+01	1.70655E+01	3.02139E+01
	Sb	6.78320E+01	2.58263E+01	1.04766E+01	4.80875E+01	1.81133E+01	3.20108E+01
	Te	7.16409E+01	2.73289E+01	1.11157E+01	5.08203E+01	1.91923E+01	3.38595E+01
	I	7.55573E+01	2.88747E+01	1.17737E+01	5.36292E+01	2.03022E+01	3.57604E+01
	Xe	7.95809E+01	3.04638E+01	1.24509E+01	5.65148E+01	2.14433E+01	3.77138E+01
	Cs	7.51514E+01	2.94822E+01	1.09443E+01	5.94595E+01	2.26067E+01	3.95832E+01
	Ba	8.16273E+01	3.25893E+01	1.28761E+01	6.25159E+01	2.38184E+01	4.17244E+01
	La	8.71316E+01	3.58243E+01	1.50709E+01	6.56404E+01	2.50571E+01	4.38958E+01
4d	In	4.56172E+00	1.83190E+00	7.22085E-01	3.03282E+00	1.20819E+00	2.34037E+00
	Sn	5.25231E+00	2.12818E+00	8.55202E-01	3.37233E+00	1.38465E+00	2.63459E+00
	Sb	6.03497E+00	2.44816E+00	9.95627E-01	3.71690E+00	1.56501E+00	2.93676E+00
	Te	6.94341E+00	2.79719E+00	1.14495E+00	4.06794E+00	1.74990E+00	3.24762E+00
	I	8.02111E+00	3.18008E+00	1.30447E+00	4.42632E+00	1.93971E+00	3.56761E+00
	Xe	9.31683E+00	3.59949E+00	1.47483E+00	4.79266E+00	2.13467E+00	3.89682E+00
	Cs	1.09443E+01	4.07128E+00	1.66355E+00	5.17129E+00	2.33914E+00	4.23798E+00
	Ba	1.28761E+01	4.57563E+00	1.86323E+00	5.56026E+00	2.55101E+00	4.58858E+00
	La	1.50709E+01	5.10166E+00	2.07185E+00	5.96061E+00	2.77155E+00	4.94917E+00

covered by the SCF basis set, but a g function is required. Correlation of the 4d and 5d is covered by the 4f and 5f correlating sets, respectively. For 4f correlation and 5f correlation, a 2g1h set is required where these shells become core shells at $Z = 72$ and $Z = 104$. The exponents, including those previously published for outer-core correlation, are given in Tables 3, 4, 5, 6, and 7.

For 5d correlation, a g exponent is required for Fr, Ra, and Ac, which have not been previously published. They are Fr: 2.47115, Ra: 2.63972, and Ac: 2.81301.

3.3 Quadruple-zeta basis sets

For 1s correlation, a 3p2d1f correlating set is required. The p and d exponents are already represented in the SCF basis set, but the f function is not, even for elements where the 4f is occupied.

For 2p correlation, a 3d2f1g correlating set is required. The d exponents are already represented in the SCF basis set, and the f exponents are represented for $Z > 57$. A 2f1g set is therefore required for $Z < 58$, and a g function thereafter.

Table 12 Exponents of 2g1h set for 3d correlation in the quadruple-zeta basis sets for $Z > 57$

Element	g	g	h	Element	g	g	h
Ce	6.89658E+01	2.62450E+01	4.58026E+01	Ac	2.08195E+02	8.10097E+01	1.46165E+02
Pr	7.22137E+01	2.75357E+01	4.70934E+01	Th	2.14073E+02	8.33044E+01	1.50643E+02
Nd	7.56058E+01	2.88674E+01	4.96430E+01	Pa	2.20098E+02	8.56545E+01	1.55370E+02
Pm	7.90697E+01	3.02291E+01	5.21835E+01	U	2.26220E+02	8.80417E+01	1.59836E+02
Sm	8.26075E+01	3.16205E+01	5.47334E+01	Np	2.32441E+02	9.04653E+01	1.64380E+02
Eu	8.62205E+01	3.30421E+01	5.73099E+01	Pu	2.38795E+02	9.29421E+01	1.68731E+02
Gd	8.99325E+01	3.45056E+01	6.08574E+01	Am	2.45217E+02	9.54404E+01	1.73437E+02
Tb	9.36775E+01	3.59756E+01	6.25546E+01	Cm	2.51713E+02	9.79621E+01	1.78429E+02
Dy	9.75232E+01	3.74880E+01	6.52381E+01	Bk	2.58373E+02	1.00551E+02	1.83038E+02
Ho	1.01448E+02	3.90308E+01	6.79612E+01	Cf	2.65103E+02	1.03165E+02	1.87937E+02
Er	1.05452E+02	4.06046E+01	7.07268E+01	Es	2.71941E+02	1.05815E+02	1.92917E+02
Tm	1.09537E+02	4.22097E+01	7.35366E+01	Fm	2.78879E+02	1.08504E+02	1.97960E+02
Yb	1.13703E+02	4.38459E+01	7.63918E+01	Md	2.85937E+02	1.11235E+02	2.03071E+02
Lu	1.17646E+02	4.55729E+01	7.24164E+01	No	2.93095E+02	1.14003E+02	2.08266E+02
Hf	1.22255E+02	4.72242E+01	8.39484E+01	Lr	3.00335E+02	1.16796E+02	2.13698E+02
Ta	1.26609E+02	4.89456E+01	8.72700E+01	Rf	3.07690E+02	1.19630E+02	2.19088E+02
W	1.31041E+02	5.06959E+01	9.05463E+01	Db	3.15164E+02	1.22508E+02	2.24502E+02
Re	1.35561E+02	5.24785E+01	9.38378E+01	Sg	3.22743E+02	1.25425E+02	2.29970E+02
Os	1.40169E+02	5.42941E+01	9.71698E+01	Bh	3.30438E+02	1.28383E+02	2.35511E+02
Ir	1.44867E+02	5.61432E+01	1.00554E+02	Hs	3.38250E+02	1.31383E+02	2.41134E+02
Pt	1.49655E+02	5.80266E+01	1.03994E+02	Mt	3.46179E+02	1.34426E+02	2.46848E+02
Au	1.54534E+02	5.99440E+01	1.07495E+02	Ds	3.54225E+02	1.37510E+02	2.52657E+02
Hg	1.59499E+02	6.18955E+01	1.11058E+02	Rg	3.62392E+02	1.40638E+02	2.58566E+02
Tl	1.64325E+02	6.38334E+01	1.14529E+02	Cn	3.70675E+02	1.43807E+02	2.64577E+02
Pb	1.69593E+02	6.58835E+01	1.18224E+02	Uut	3.79147E+02	1.47095E+02	2.70493E+02
Bi	1.74723E+02	6.79103E+01	1.22044E+02	Uuq	3.87652E+02	1.50345E+02	2.76703E+02
Po	1.80050E+02	6.99980E+01	1.25925E+02	Uup	3.96277E+02	1.53638E+02	2.82992E+02
At	1.85470E+02	7.21202E+01	1.29881E+02	Uuh	4.05027E+02	1.56974E+02	2.89346E+02
Rn	1.90986E+02	7.42782E+01	1.33904E+02	Uus	4.13893E+02	1.60353E+02	2.95785E+02
Fr	1.96607E+02	7.64765E+01	1.37970E+02	Uuo	4.22884E+02	1.63773E+02	3.02297E+02
Ra	2.02306E+02	7.87016E+01	1.42144E+02				

For 3d correlation, a 3f2g1h correlating set is required. Optimization of f exponents is only needed for $Z < 58$, as they are represented in the SCF functions for higher Z. Likewise, for 4d correlation, a 3f2g1h exponent set is required. As the 4d contracts into the core, the innermost f exponent for 4d correlation approaches the outermost f exponent for 3d correlation, creating a linear dependence problem. The outermost f exponent of the 3d set was therefore replaced with the innermost f exponent of the 4d set for Cs, Ba, and La and held fixed, while the other two f exponents of the 3d set were reoptimized. For $Z > 57$, where the f exponents in the correlating sets are represented in the SCF basis set, a 2g1h set is required. These sets are covered by the 4f and 5f correlating sets, for 4d and 5d correlation, and the 2g1h set needed for 5d correlation up to $Z = 90$ has already been published.

For 4f and 5f correlation, a 3g2h1i set is required for each shell where they become core shells, at $Z = 72$ and $Z = 104$. As the 4f and 5f shells contract with increasing Z, the g sets begin to overlap, and on the inner side, the g functions for the 4f shell overlap with the g functions for the 3d shell, creating linear dependence problems. The g set for 4f correlation was therefore reoptimized with the inner g function replaced by the outer g function for 3d correlation, and the remaining two g functions were reoptimized, from $Z = 91$ on. This starting point was chosen to keep consistency across the 5f block, because the linear dependence is severe at the end of the block, even though it is not at the beginning. The loss of correlation energy is about 2 millihartrees for $Z = 91$ and declines to about 0.6 millihartrees for $Z = 118$. The exponent set for 4f correlation is tighter as a consequence of the reoptimization,

Table 13 Exponents of g, h, and i functions for 4f correlation in the quadruple-zeta basis sets

Element	g	g	g	h	h	i
Hf	2.03269E+01	7.22416E+00	2.51514E+00	1.43052E+01	4.81135E+00	9.35318E+00
Ta	2.20235E+01	7.91607E+00	2.80885E+00	1.54761E+01	5.28350E+00	1.01409E+01
W	2.37296E+01	8.61304E+00	3.10577E+00	1.66630E+01	5.76386E+00	1.09425E+01
Re	2.54501E+01	9.31698E+00	3.40667E+00	1.78668E+01	6.25254E+00	1.17582E+01
Os	2.71884E+01	1.00292E+01	3.71210E+00	1.90885E+01	6.74984E+00	1.25880E+01
Ir	2.89475E+01	1.07510E+01	4.02249E+00	2.03290E+01	7.25602E+00	1.34325E+01
Pt	3.07294E+01	1.14830E+01	4.33814E+00	2.15890E+01	7.77136E+00	1.42918E+01
Au	3.25363E+01	1.22262E+01	4.65934E+00	2.28693E+01	8.29603E+00	1.51665E+01
Hg	3.43683E+01	1.29806E+01	4.98622E+00	2.41709E+01	8.83042E+00	1.60568E+01
Tl	3.62574E+01	1.37610E+01	5.32559E+00	2.55057E+01	9.37430E+00	1.70388E+01
Pb	3.81737E+01	1.45536E+01	5.67218E+00	2.68607E+01	9.93343E+00	1.79695E+01
Bi	4.01257E+01	1.53621E+01	6.02678E+00	2.82416E+01	1.05045E+01	1.89190E+01
Po	4.21133E+01	1.61865E+01	6.38919E+00	2.96485E+01	1.10874E+01	1.98872E+01
At	4.41360E+01	1.70266E+01	6.75950E+00	3.10818E+01	1.16823E+01	2.08741E+01
Rn	4.61949E+01	1.78826E+01	7.13755E+00	3.25411E+01	1.22890E+01	2.18800E+01
Fr	4.82915E+01	1.87553E+01	7.52394E+00	3.40281E+01	1.29084E+01	2.29054E+01
Ra	5.04254E+01	1.96448E+01	7.91861E+00	3.55431E+01	1.35403E+01	2.39506E+01
Ac	5.25963E+01	2.05504E+01	8.32113E+00	3.70849E+01	1.41846E+01	2.50153E+01
Th	5.48043E+01	2.14724E+01	8.73160E+00	3.86539E+01	1.48410E+01	2.60993E+01
Pa	8.56545E+01	2.81191E+01	1.06915E+01	4.02962E+01	1.55964E+01	2.72089E+01
U	8.80417E+01	2.91328E+01	1.11363E+01	4.18679E+01	1.61891E+01	2.83180E+01
Np	9.04653E+01	3.01589E+01	1.15869E+01	4.35098E+01	1.68779E+01	2.94528E+01
Pu	9.29421E+01	3.12002E+01	1.20445E+01	4.51771E+01	1.75783E+01	3.06050E+01
Am	9.54404E+01	3.22539E+01	1.25081E+01	4.68681E+01	1.82886E+01	3.17747E+01
Cm	9.79621E+01	3.33184E+01	1.29765E+01	4.85814E+01	1.90081E+01	3.29611E+01
Bk	1.00551E+02	3.44002E+01	1.34527E+01	5.03220E+01	1.97401E+01	3.41654E+01
Cf	1.03165E+02	3.54952E+01	1.39350E+01	5.20863E+01	2.04820E+01	3.53872E+01
Es	1.05815E+02	3.66037E+01	1.44236E+01	5.38757E+01	2.12348E+01	3.66266E+01
Fm	1.08504E+02	3.77267E+01	1.49188E+01	5.56901E+01	2.19983E+01	3.78837E+01
Md	1.11235E+02	3.88646E+01	1.54207E+01	5.75297E+01	2.27726E+01	3.91586E+01
No	1.14003E+02	4.00351E+01	1.59432E+01	5.94286E+01	2.35771E+01	4.04722E+01
Lr	1.16796E+02	4.12010E+01	1.64583E+01	6.13205E+01	2.43740E+01	4.17844E+01
Rf	1.19630E+02	4.23830E+01	1.69808E+01	6.32395E+01	2.51827E+01	4.31157E+01
Db	1.22508E+02	4.35815E+01	1.75108E+01	6.51860E+01	2.60032E+01	4.44661E+01
Sg	1.25425E+02	4.47959E+01	1.80481E+01	6.71596E+01	2.68355E+01	4.58359E+01
Bh	1.28383E+02	4.60265E+01	1.85930E+01	6.91608E+01	2.76797E+01	4.72248E+01
Hs	1.31383E+02	4.72737E+01	1.91455E+01	7.11897E+01	2.85359E+01	4.86331E+01
Mt	1.34426E+02	4.85375E+01	1.97055E+01	7.32462E+01	2.94041E+01	5.00608E+01
Ds	1.37510E+02	4.98178E+01	2.02732E+01	7.53304E+01	3.02841E+01	5.15076E+01
Rg	1.40638E+02	5.11151E+01	2.08488E+01	7.74428E+01	3.11764E+01	5.29741E+01
Cn	1.43807E+02	5.24288E+01	2.14318E+01	7.95827E+01	3.20805E+01	5.44597E+01
Uut	1.47095E+02	5.37733E+01	2.20262E+01	8.17512E+01	3.29968E+01	5.59649E+01
Uuq	1.50345E+02	5.51201E+01	2.26245E+01	8.39477E+01	3.39251E+01	5.74898E+01
Uup	1.53638E+02	5.64843E+01	2.32311E+01	8.61733E+01	3.48661E+01	5.90348E+01
Uuh	1.56974E+02	5.78661E+01	2.38457E+01	8.84274E+01	3.58194E+01	6.05996E+01
Uus	1.60353E+02	5.92647E+01	2.44682E+01	9.07100E+01	3.67849E+01	6.21839E+01
Uuo	1.63773E+02	6.06804E+01	2.50986E+01	9.30214E+01	3.77627E+01	6.37882E+01

Table 14 Exponents of g, h, and i functions for 5f correlation in the quadruple-zeta basis sets

Element	g	g	g	h	h	i
Rf	7.74062E+00	3.24551E+00	1.28230E+00	5.65125E+00	2.25566E+00	4.35805E+00
Db	8.27934E+00	3.51985E+00	1.41803E+00	6.00520E+00	2.44502E+00	4.66140E+00
Sg	8.82446E+00	3.79606E+00	1.55397E+00	6.35737E+00	2.63411E+00	4.96615E+00
Bh	9.37971E+00	4.07582E+00	1.69097E+00	6.70896E+00	2.82354E+00	5.27274E+00
Hs	9.94806E+00	4.36037E+00	1.82963E+00	7.06090E+00	3.01378E+00	5.58155E+00
Mt	1.05320E+01	4.65067E+00	1.97038E+00	7.41388E+00	3.20518E+00	5.89295E+00
Ds	1.11339E+01	4.94754E+00	2.11356E+00	7.76845E+00	3.39794E+00	6.20718E+00
Rg	1.17560E+01	5.25166E+00	2.25945E+00	8.12505E+00	3.59234E+00	6.52453E+00
Cn	1.24006E+01	5.56373E+00	2.40830E+00	8.48406E+00	3.78853E+00	6.84523E+00
Uut	1.30923E+01	5.89751E+00	2.56924E+00	8.85217E+00	3.98923E+00	7.18976E+00
Uuq	1.38187E+01	6.24313E+00	2.73549E+00	9.22196E+00	4.19500E+00	7.52088E+00
Uup	1.45915E+01	6.60495E+00	2.90867E+00	9.59643E+00	4.40471E+00	7.85726E+00
Uuh	1.54092E+01	6.98094E+00	3.08742E+00	9.97502E+00	4.61765E+00	8.19839E+00
Uus	1.62770E+01	7.37177E+00	3.27176E+00	1.03577E+01	4.83375E+00	8.54424E+00
Uuo	1.72015E+01	7.77832E+00	3.46183E+00	1.07446E+01	5.05298E+00	8.89487E+00

Table 15 Krypton atom 2p binding energies and 2p spin-orbit splitting, in eV, from DHF and SDCI calculations with the Coulomb and Breit interactions, correlating the 2s and 2p shells

	Basis	Hamiltonian	DHF	CI	Corr.
$2p_{3/2}$	tz	Coulomb	1681.26	1682.11	0.85
	qz	Coulomb	1681.26	1682.36	1.10
	tz	Coulomb–Breit	1679.34	1680.23	0.89
	qz	Coulomb–Breit	1679.33	1680.49	1.16
	tz	Breit	−1.92	−1.88	0.04
	qz	Breit	−1.93	−1.87	0.06
$2p_{1/2}$	tz	Coulomb	1735.09	1735.96	0.86
	qz	Coulomb	1735.09	1736.20	1.11
	tz	Coulomb–Breit	1732.14	1733.05	0.92
	qz	Coulomb–Breit	1732.14	1733.31	1.17
	tz	Breit	−2.95	−2.91	0.04
	qz	Breit	−2.95	−2.89	0.06
SO	tz	Coulomb	53.83	53.84	0.01
	qz	Coulomb	53.83	53.84	0.01
	tz	Coulomb–Breit	52.80	52.82	0.02
	qz	Coulomb–Breit	52.80	52.83	0.03
	tz	Breit	−1.03	−1.02	0.01
	qz	Breit	−1.03	−1.01	0.02

but this alleviates the linear dependence with the 5f correlating set for high Z somewhat. No overlap problems occur for the h and i functions.

The exponents, including those previously published for outer-core correlation, are given in Tables 8, 9, 10, 11, 12, 13, and 14.

4 Application

As an example of the use of these core correlating functions, the Kr 2p binding energies were calculated, with the tz and qz basis sets. Singles and doubles CI calculations were performed on the neutral atom and the 2p hole state in which the 2s and 2p shells were correlated. Both the Dirac–Coulomb and the Dirac–Coulomb–Breit Hamiltonian were used, the latter with frequency dependence. As for the exponent optimization, the calculations were performed using the basis set adaption of GRASP [35, 36] and RAMCI [37].

The correlating set for the tz basis was 2s2p2d1f, which comprised the 8th and 9th s, 8th and 9th p, and the 7th and 8th d primitives from the SCF set, counting from the smallest exponents, and the correlating f function given in Table 3. Likewise the correlating set for the qz basis was 3s3p3d2f1g, which comprised the 9th through 11th s, 9th through 11th p, and 8th through 10th d from the SCF set, counting from the smallest exponents, and the correlating 2f1g set given in Table 9. The Fock matrix in the basis of the occupied spinors plus the primitive correlating set was diagonalized to obtain the spinors that were used in the CI calculations. The eigenvalues of the correlating spinors are required in the evaluation of the frequency-dependent Breit (transverse) interaction.

The results at both the DHF and the CI level are given in Table 15. The effect of the Breit interaction on the binding energies, at about 2 eV for the $2p_{3/2}$ and 3 eV for the $2p_{1/2}$, is larger than the correlation effect, which is about 1 eV for both binding energies. The contribution to correlation from the Breit interaction is about 5 % of the total correlation

contribution to the binding energies. Correlation makes very little difference to the spin-orbit splitting. The experimental ionization thresholds are 1678.4 eV ($2p_{3/2}$) and 1730.9 eV ($2p_{1/2}$) [38]. The current results are about 2 eV larger, with correlation and the Breit interaction. However, it should be remembered that these states are resonances in a continuum, and correlation of the $n = 2$ shell alone in a relatively small CI calculation is unlikely to recover all the difference.

5 Summary

Exponents of correlating functions for the core shells of all elements from $Z = 31$ to $Z = 118$ have been optimized in MR–SDCI calculations. The exponents cover the ranges that are not covered in the SCF exponent set. The functions should be equally useful in one-component, two-component, and four-component calculations. These core correlating functions have been added to the archives on the Dirac web site, http://dirac.chem.sdu.dk.

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