Supplementary Material for "Relativistic short-range exchange energy functionals beyond the local-density approximation"

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I. EVEN-TEMPERED BASIS SETS CONSTRUCTED IN THIS WORK

TABLE I. Parameters ζ_1 and q for generating all the exponents $\zeta_\nu = \zeta_1\, q^{\nu-1}$ of our uncontracted even-tempered large-component basis functions for the Yb^{68+} and U^{90+} systems of the helium isoelectronic series. We use ten s basis functions, two sets of p basis functions, and one set of d basis functions. The small-component basis functions are generated from the unrestricted kinetic-balance scheme.

	Ten s basis functions		Two p basis functions		One d basis function
	ζ_1	q	ζ_1	q	ζ_1
Yb^{68+}	1.39601904E+07	0.30	3.39128349E+06	0.25	4.75587491E+03
U^{90+}	5.58567332E+07	0.295	2.64721605E+07	0.25	3.34172062E+04

TABLE II. Parameters ζ_1 and q for generating all the exponents $\zeta_\nu = \zeta_1\, q^{\nu-1}$ of our uncontracted even-tempered large-component basis functions for the beryllium isoelectronic series. We use ten s basis functions, six sets of p basis functions, and one set of d basis functions. The small-component basis functions are generated from the unrestricted kinetic-balance scheme.

	Ten s basis functions		Six p basis functions		One d basis function
	ζ_1	q	ζ_1	q	ζ_1
Be	6.40943779E+03	0.25	1.31800101E+01	0.25	2.71217265E-01
Ne^{6+}	2.63937466E+04	0.30	1.01356529E+02	0.25	2.16640868E+00
Ar^{14+}	2.16279421E+05	0.26	4.94782136E+02	0.25	1.13941141E+01
Kr^{32+}	4.14098736E+06	0.23	9.01590791E+03	0.25	2.25939509E+02
Xe^{50+}	9.04292743E+06	0.23	2.81773747E+05	0.25	1.95959651E+03
Yb^{66+}	1.39601904E+07	0.236	3.39128349E+06	0.25	4.75587491E+03
Rn^{82+}	1.46794059E+07	0.25	1.72824122E+07	0.25	1.25385658E+03
U^{88+}	1.46346866E+07	0.26	2.64721605E+07	0.25	3.34172062E+04

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TABLE III. Parameters ζ_1 and q for generating all the exponents $\zeta_\nu = \zeta_1\, q^{\nu-1}$ of our uncontracted even-tempered large-component basis functions for the neon isoelectronic series. We use ten s basis functions, six sets of p basis functions, and one set of d basis functions. The small-component basis functions are generated from the unrestricted kinetic-balance scheme.

	Ten s basis functions		Six p basis functions		One d basis function
	ζ_1	q	ζ_1	q	ζ_1
Ne	2.63937466E+04	0.30	1.01356529E+02	0.30	2.16640868E+00
Ar^{8+}	2.16279421E+05	0.29	4.94782136E+02	0.32	1.13941141E+01
Kr^{26+}	4.14098736E+06	0.25	9.01590791E+03	0.25	2.25939509E+02
Xe^{44+}	9.04292743E+06	0.255	9.36856349E+03	0.31	1.95959651E+03
Yb^{60+}	1.39601904E+07	0.235	2.61264417E+04	0.32	4.75587491E+03
Rn^{76+}	1.46794059E+07	0.25	5.70898829E+04	0.30	1.25385658E+03
U^{82+}	1.46346866E+07	0.26	1.22880210E+05	0.28	3.34172062E+04

TABLE IV. Parameters ζ_1 and q for generating all the exponents $\zeta_\nu = \zeta_1\, q^{\nu-1}$ of our uncontracted even-tempered large-component basis functions for the argon isoelectronic series. We use twelve s basis functions, eight sets of p basis functions, and three set of d basis functions. The small-component basis functions are generated from the unrestricted kinetic-balance scheme.

	Twelve s basis functions		Eight p basis functions		Three d basis functions	
	ζ_1	q	ζ_1	q	ζ_1	q
Ar	2.16279421E+05	0.30	4.94782136E+02	0.325	1.13941141E+01	0.25
Kr^{18+}	4.14098736E+06	0.25	9.01590791E+03	0.30	2.25939509E+02	0.25
Xe^{36+}	9.04292743E+06	0.25	9.36856349E+03	0.36	1.95959651E+03	0.25
Yb^{52+}	1.39601904E+07	0.26	2.61264417E+04	0.33	4.75587491E+03	0.25
Rn^{68+}	1.46794059E+07	0.30	1.92412503E+05	0.30	1.25385658E+03	0.25
U^{74+}	1.46346866E+07	0.29	1.22880210E+05	0.29	4.95593590E+02	0.25