Optimized complementary auxiliary basis sets for explicitly correlated methods: Valence and core-valence basis sets for the group 11 (Cu, Ag, Au) and 12 (Zn, Cd, Hg) elements

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Supplementary Information

Table SI. CCSD(T)-F12b spectroscopic constants (reference RI) and their RI errors (OptRI) for the $X\,^1\Sigma^+$ states of AgF and AuF. All Ag and Au electrons were correlated (except those replaced by the pseudopotential) and the cc-pVnZ-F12 orbital and RI basis sets were used on fluorine (n=4 was used in combination with the n=5 basis set on the transition metal).

Molecule	Basis set	RI basis	R_e (Å)	ω_e (cm^{-1})	D_e (kcal mol^{-1})
AgF	awCVDZ-PP	RefRI	1.9796	515.8	82.60
	awCVTZ-PP		1.9782	516.8	81.15
	awCVQZ-PP		1.9780	517.0	81.16
	awCV5Z-PP		1.9781	516.9	81.18
	awCVDZ-PP	OptRI	-0.0008	1.1	0.04
	awCVTZ-PP		-0.0001	0.1	-0.01
	awCVQZ-PP		0.0000	0.0	-0.01
	awCV5Z-PP		0.0000	0.0	0.00
AuF	awCVDZ-PP	RefRI	1.9265	553.7	70.53
	awCVTZ-PP		1.9257	556.4	69.20
	awCVQZ-PP		1.9258	556.8	69.14
	awCV5Z-PP		1.9257	556.7	69.19
	awCVDZ-PP	OptRI	-0.0004	1.2	0.08
	awCVTZ-PP		0.0000	0.2	0.00
	awCVQZ-PP		0.0000	-0.1	-0.01
	awCV5Z-PP		0.0000	0.0	0.00

Table SII. Effects of correlating the (n-1)s and (n-1)p electrons on the CCSD(T)-F12b equilibrium bond length (R_e), harmonic frequency (ω_e), and dissociation energy (D_e) of the coinage metal dimers and fluorides. The fluorine 1s electrons are treated with the frozen core approximation. The cc-pVnZ-F12 (n=4 in combination with the n=5 basis set on the transition metal) basis sets were used for fluorine.

Molecule	Basis set	R_e (Å)	ω_e (cm^{-1})	D_e (kcal mol^{-1})
Cu_2	awCVDZ-PP	-0.0016	1.8	0.12
	awCVTZ-PP	-0.0008	1.3	-0.07
	awCVQZ-PP	-0.0011	1.0	-0.07
	awCV5Z-PP	-0.0012	1.2	-0.06
Ag_2	awCVDZ-PP	-0.0128	4.9	1.07
	awCVTZ-PP	-0.0123	4.7	1.01
	awCVQZ-PP	-0.0130	5.2	1.04
	awCV5Z-PP	-0.0116	4.4	0.93
Au_2	awCVDZ-PP	-0.0124	3.9	1.72
	awCVTZ-PP	-0.0119	3.8	1.68
	awCVQZ-PP	-0.0108	3.5	1.51
	awCV5Z-PP	-0.0111	3.6	1.52
CuF	awCVDZ-PP	0.0026	-3.5	-1.06
	awCVTZ-PP	0.0031	-2.9	-0.96
	awCVQZ-PP	0.0029	-2.3	-0.90
	awCV5Z-PP	0.0029	-2.2	-0.88
AgF	awCVDZ-PP	-0.0076	5.2	-0.74
	awCVTZ-PP	-0.0075	5.1	-0.61
	awCVQZ-PP	-0.0076	5.3	-0.59
	awCV5Z-PP	-0.0075	5.2	-0.59
AuF	awCVDZ-PP	-0.0101	9.1	0.08
	awCVTZ-PP	-0.0094	8.9	0.26
	awCVQZ-PP	-0.0091	9.0	0.26
	awCV5Z-PP	-0.0091	8.9	0.27
ZnF	awCVDZ-PP	0.0019	-0.8	-0.81
	awCVTZ-PP	0.0019	-1.0	-0.75
	awCVQZ-PP	0.0018	-0.8	-0.74
	awCV5Z-PP	0.0017	-0.8	-0.73
CdF	awCVDZ-PP	-0.0025	1.1	-1.23
	awCVTZ-PP	-0.0024	1.4	-1.10
	awCVQZ-PP	-0.0025	1.3	-1.08

	awCV5Z-PP	-0.0025	1.2	-1.09
HgF	awCVDZ-PP	-0.0049	2.1	-1.00
	awCVTZ-PP	-0.0045	1.8	-0.80
	awCVQZ-PP	-0.0044	1.7	-0.78
	awCV5Z-PP	-0.0045	1.8	-0.77

Table SIII. Effect of correlating the (n-1)s and p transition metal electrons on the CCSD(T)-F12b equilibrium bond length (R_e) and dissociation energy (D_e) of the coinage metal difluorides. The fluorine 1s electrons are treated with the frozen core approximation. The cc-pVnZ-F12 (n=4 in combination with the n=5 basis set on the transition metal) basis sets were used for fluorine.

Molecule	Basis set	R_e (Å)	D_e (kcal mol^{-1})
CuF_2	awCVDZ-PP	0.0002	-1.95
	awCVTZ-PP	0.0004	-1.92
	awCVQZ-PP	0.0003	-1.94
	awCV5Z-PP	0.0003	-1.91
AgF_2	awCVDZ-PP	-0.0031	2.19
	awCVTZ-PP	-0.0028	2.28
	awCVQZ-PP	-0.0028	2.28
	awCV5Z-PP	-0.0027	2.27
AuF_2	awCVDZ-PP	-0.0027	1.88
	awCVTZ-PP	-0.0021	1.87
	awCVQZ-PP	-0.0020	1.77
	awCV5Z-PP	-0.0020	1.80

Table SIV. Calculated spectroscopic constants for the $X\,^1\Sigma_g^+$ states of Cu_2, Ag_2, and Au_2. Geminal exponents of 0.9, 1.0, 1.0, 1.0 were used for DZ, TZ, QZ, and 5Z.

System	Method	Basis set	R_e (Å)	ω_e (cm^{-1})	D_e (kcal mol^{-1})
Cu_2					
	CCSD(T)-F12b	aVDZ-PP	2.2271	262.8	45.79
		aVTZ-PP	2.2168	267.6	46.38
		aVQZ-PP	2.2146	267.8	46.55
		aV5Z-PP	2.2136	268.3	46.65
Ag_2					
	CCSD(T)-F12b	aVDZ-PP	2.5424	188.8	37.95
		aVTZ-PP	2.5355	191.5	38.36
		aVQZ-PP	2.5331	191.8	38.55
		aV5Z-PP	2.5323	192.0	38.60
Au_2					
	CCSD(T)-F12b	aVDZ-PP	2.4945	184.1	50.72
		aVTZ-PP	2.4903	186.3	51.06
		aVQZ-PP	2.4891	186.6	51.20
		aV5Z-PP	2.4881	186.9	51.32

Table SV. Calculated spectroscopic constants for the $X\,^1\Sigma^+$ states of CuF, AgF, and AuF. Geminal exponents of 0.9, 1.0, 1.0, 1.0 were used for DZ, TZ, QZ, and 5Z.

System	Method	Basis set	R_e (Å)	ω_e (cm^{-1})	D_e (kcal mol^{-1})
CuF					
	CCSD(T)-F12b	aVDZ-PP	1.7464	612.6	97.00
		aVTZ-PP	1.7436	617.8	98.50
		aVQZ-PP	1.7417	620.0	98.92
		aV5Z-PP	1.7414	620.1	98.95
AgF					
	CCSD(T)-F12b	aVDZ-PP	1.9886	510.6	79.89
		aVTZ-PP	1.9873	510.8	81.07
		aVQZ-PP	1.9861	511.7	81.52
		aV5Z-PP	1.9859	511.4	81.52
AuF					
	CCSD(T)-F12b	aVDZ-PP	1.9373	545.0	67.15
		aVTZ-PP	1.9363	546.4	68.18
		aVQZ-PP	1.9352	547.4	68.63
		aV5Z-PP	1.9350	547.5	68.68

Table SVI. Calculated equilibrium bond lengths and atomization energies for $X\,^2\Sigma_g^+$ CuF_2, AgF_2, and AuF_2. Geminal exponents of 0.9, 1.0, 1.0, 1.0 were used for DZ, TZ, QZ, and 5Z.

System	Method	Basis set	R_e (Å)	ΣD_e (kcal mol^{-1})
CuF_2				
	CCSD(T)-F12b	aVDZ-PP	1.7160	187.77
		aVTZ-PP	1.7131	187.65
		aVQZ-PP	1.7116	187.93
		aV5Z-PP	1.7113	187.80
AgF_2				
	CCSD(T)-F12b	aVDZ-PP	1.8905	122.39
		aVTZ-PP	1.8875	123.45
		aVQZ-PP	1.8862	124.10
		aV5Z-PP	1.8858	123.92
AuF_2				
	CCSD(T)-F12b	aVDZ-PP	1.9030	124.51
		aVTZ-PP	1.9021	125.54
		aVQZ-PP	1.9011	126.27
		aV5Z-PP	1.9008	126.29

Table SVII. Calculated spectroscopic constants for the $X\,^2\Sigma^+$ states of ZnF, CdF, and HgF. Geminal exponents of 0.9, 1.0, 1.0, 1.0 were used for DZ, TZ, QZ, and 5Z.

System	Method	Basis set	R_e (Å)	ω_e (cm^{-1})	D_e (kcal mol^{-1})
ZnF					
	CCSD(T)-F12b	aVDZ-PP	1.7658	632.5	69.15
		aVTZ-PP	1.7652	633.3	70.01
		aVQZ-PP	1.7637	634.3	70.37
		aV5Z-PP	1.7635	633.7	70.36
CdF					
	CCSD(T)-F12b	aVDZ-PP	1.9772	537.5	58.53
		aVTZ-PP	1.9793	535.8	59.11
		aVQZ-PP	1.9783	536.4	59.61
		aV5Z-PP	1.9783	535.9	59.57
HgF					
	CCSD(T)-F12b	aVDZ-PP	2.0262	482.5	30.89
		aVTZ-PP	2.0266	484.1	31.43
		aVQZ-PP	2.0256	484.9	31.79
		aV5Z-PP	2.0255	484.7	31.79

aug-cc-pVDZ-PP/OptRI ABS in MOLPRO format

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s,Cu,13.615148,7.443600,4.6986,2.374214,1.448319,0.346860
p,Cu,11.092379,7.350628,4.9315,2.027760,0.787881,0.431223
d,Cu,15.688531,6.460334,4.172327,2.792,1.068805,0.711447
f,Cu,21.890887,8.3307,5.569378,1.352344,0.397626
g,Cu,14.168307,5.368756,2.087487,0.755821
h,Cu,8.031276,2.628135
i,Cu,5.447213

s,Zn,13.700188,9.144466,5.0733,2.223742,1.485077,0.418160
p,Zn,23.262553,15.673667,5.3705,1.924780,0.846264,0.535715
d,Zn,18.613376,7.500930,4.982331,3.3188,1.615170,1.074883
f,Zn,25.132733,9.5199,6.371185,1.620494,0.451013
g,Zn,17.163671,6.446959,2.677679,1.018246
h,Zn,9.126286,3.097045
i,Zn,6.405320

s,Ag,12.639208,8.553992,2.3985,1.609317,0.891137,0.599502
p,Ag,11.469781,7.714739,5.179910,2.5852,1.749736,0.526969
d,Ag,21.001461,6.344167,4.240612,2.8365,0.830164,0.553665
f,Ag,11.659444,7.398598,3.9751,2.653284,0.663164
g,Ag,7.018740,3.088325,1.394563,0.583352
h,Ag,3.101564,1.319429
i,Ag,2.266770

s,Cd,12.869317,6.325854,2.6738,1.512305,0.694608,0.342760
p,Cd,12.571735,8.517452,5.746791,2.7157,1.856078,0.521311
d,Cd,21.832177,7.379851,4.941737,3.3125,2.046914,0.652840
f,Cd,15.377212,7.840530,4.5765,2.948192,0.773116
g,Cd,7.132087,3.452073,1.594405,0.688569
h,Cd,3.449903,1.515446
i,Cd,2.557535

s,Au,15.054592,10.041754,4.785404,2.0643,1.266123,0.845071
p,Au,27.283289,9.088068,6.052251,2.2606,1.509249,0.777021
d,Au,10.167352,6.801323,4.541946,2.0167,1.356432,0.509693
f,Au,7.399411,4.671651,3.125319,2.0995,0.566526
g,Au,4.474574,2.986018,1.399991,0.574471
h,Au,2.904463,1.282405
i,Au,1.722463

s,Hg,13.373935,8.923930,5.796751,2.3359,1.431409,0.427333
p,Hg,22.115298,11.483164,7.663051,2.3585,1.458042,0.748600
d,Hg,10.679549,7.133959,4.750467,2.2228,1.485468,0.394509
f,Hg,8.306281,5.553961,3.712129,2.2727,0.655914
g,Hg,4.892937,3.267930,1.576052,0.662148
h,Hg,2.981021,1.262406
i,Hg,1.880845
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aug-cc-pVTZ-PP/OptRI ABS in MOLPRO format

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s,Cu,15.772188,10.574469,4.1727,2.6091,1.754501,0.952406,0.359486
p,Cu,24.615719,8.4652,4.847573,2.1782,1.453721,0.286440
d,Cu,19.253621,10.697252,5.9415,3.3806,1.174655,0.459223
f,Cu,40.529898,12.223727,2.880473,1.922780,0.680482
g,Cu,19.543340,8.6183,5.231634,2.198382,0.620038
h,Cu,15.882772,6.762756,2.831186,1.130988
i,Cu,5.468239

s,Zn,18.015663,12.088070,4.5786,2.8641,1.928474,1.044178,0.421166
p,Zn,56.606056,14.681579,9.2192,5.222811,2.3491,1.116083
d,Zn,23.715730,11.317246,6.686,4.0411,2.694189,0.654023
f,Zn,35.281097,13.182172,8.797974,2.985906,0.809097
g,Zn,23.896822,9.7523,6.498175,2.566949,0.741572
h,Zn,20.723610,8.264814,3.633505,1.488507
i,Zn,6.423210

s,Ag,12.988006,8.666279,5.763862,2.2252,1.3969,0.933058,0.438789
p,Ag,13.307296,8.958439,3.5359,1.2402,0.836506,0.346601
d,Ag,56.086469,12.635014,8.399633,4.4524,1.5748,0.688713
f,Ag,18.400514,5.849233,3.894901,1.393457,0.431971
g,Ag,18.189227,12.128421,3.499,1.060203,0.448520
h,Ag,6.561213,3.765484,1.835194,0.768203
i,Ag,2.267719

s,Cd,14.003304,9.378160,6.281064,2.3847,1.4979,0.923058,0.447657
p,Cd,14.193694,9.635200,3.8946,1.311,0.890805,0.351955
d,Cd,53.113516,14.622010,8.567936,5.0344,1.8041,0.770792
f,Cd,12.501501,4.784750,1.914602,1.276152,0.507528
g,Cd,9.037991,6.012828,3.8914,1.224985,0.427850
h,Cd,7.359113,3.833540,1.835391,0.768524
i,Cd,2.558455

s,Au,15.864661,10.586349,7.067209,2.972435,1.9834,1.2448,0.831921
p,Au,11.788345,8.016150,2.6637,1.141,0.768002,0.182235
d,Au,11.546301,7.700194,3.4696,1.2171,0.590435,0.206321
f,Au,5.708764,3.805522,2.538991,0.802997,0.305853
g,Au,6.058611,4.064993,2.7283,0.821326,0.366808
h,Au,5.113380,3.408193,1.649750,0.704098
i,Au,1.723374

s,Hg,20.340321,13.589947,9.079807,3.175650,2.1304,1.3378,0.527257
p,Hg,11.805866,8.078510,2.8228,1.1949,0.801989,0.191385
d,Hg,11.809885,7.891999,3.7153,1.3573,0.672151,0.403747
f,Hg,7.277382,4.857194,3.242369,0.810052,0.327111
g,Hg,9.973051,6.648769,4.436766,2.9668,0.420024
h,Hg,7.155083,4.272495,1.960439,0.877876
i,Hg,1.881778
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aug-cc-pVQZ-PP/OptRI ABS in MOLPRO format

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s,Cu,15.659560,9.029141,5.0913,3.191,2.126129,0.396499
p,Cu,41.883727,9.898,6.606805,3.0653,1.215329,0.267938
d,Cu,18.901379,10.679323,7.1185,4.4632,2.974306,1.259012
f,Cu,27.811599,18.470412,12.327108,4.888539,1.624284
g,Cu,15.774896,3.990997,2.667199,1.057297
h,Cu,19.601209,8.9337,5.648684,2.382829,0.699566
i,Cu,8.919127,2.681940

s,Zn,16.806517,11.195794,5.8361,3.6596,2.441892,0.414289
p,Zn,56.314110,10.6413,6.044765,3.2895,2.199361,1.267423
d,Zn,29.676851,17.109170,8.1403,5.108,3.417191,0.948234
f,Zn,48.537283,19.996811,13.332583,4.593460,1.843904
g,Zn,17.841641,4.677746,3.123085,1.266507
h,Zn,23.057474,10.0727,6.688080,2.862004,0.848319
i,Zn,10.353342,3.245024

s,Ag,11.005431,7.411594,4.979457,2.5613,1.6037,0.410151
p,Ag,10.708050,7.162498,4.808487,3.2389,2.0247,0.650472
d,Ag,16.218238,5.088,3.090332,2.0554,1.331646,0.355574
f,Ag,22.606979,12.981227,6.703880,2.215544,0.952417
g,Ag,7.117436,3.866351,1.358450,0.599205
h,Ag,8.332970,5.557882,3.6986,1.196228,0.533939
i,Ag,3.212197,1.301610

s,Cd,12.605076,8.467612,5.682268,2.8823,1.8033,0.304075
p,Cd,18.327877,8.891973,5.817345,3.6161,2.0791,1.119693
d,Cd,13.539416,5.584,3.653520,2.252,1.514364,0.401073
f,Cd,20.970116,11.851443,7.676672,2.566429,1.083162
g,Cd,7.816151,5.151411,1.617392,0.695791
h,Cd,9.140353,6.108564,4.0892,1.375301,0.582183
i,Cd,3.619463,1.507041

s,Au,16.340262,10.881998,5.369200,3.095642,1.234,0.7723
p,Au,11.602799,7.769516,5.203444,2.6937,1.6857,0.929170
d,Au,11.516342,7.682605,3.7149,1.692,0.932730,0.280984
f,Au,8.611530,4.624714,3.082739,1.194189,0.529229
g,Au,5.510526,3.439681,1.265644,0.467596
h,Au,7.974885,4.203519,2.7477,0.861637,0.383965
i,Au,3.051497,1.187165

s,Hg,14.422509,9.624524,5.306559,2.936184,1.357,0.8492
p,Hg,12.287985,8.222334,5.504709,2.8456,1.7807,0.989905
d,Hg,11.838696,7.908146,3.977,1.8985,1.083248,0.307247
f,Hg,10.198599,6.805789,4.550244,3.054065,0.589957
g,Hg,5.861809,3.261856,1.402481,0.532453
h,Hg,7.310126,4.840528,2.94,0.954539,0.427287
i,Hg,3.316665,1.328657
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aug-cc-pV5Z-PP/OptRI ABS in MOLPRO format

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d,Cu,22.364827,14.722760,9.4711,5.9405,2.362743,0.982049
f,Cu,42.499660,19.156111,6.823665,2.271783,0.860824,0.270853
g,Cu,19.701957,5.007150,2.094867,0.624636
h,Cu,15.309592,3.738423,0.525565
i,Cu,23.172995,10.2939,3.407685,0.930645

s,Zn,18.914284,9.950917,6.6391,4.1605,1.886852,0.457764
p,Zn,27.222091,18.188312,12.1658,6.628000,4.4104,2.943188,1.070217
d,Zn,28.304446,16.032821,10.6203,6.6621,4.223721,1.310188
f,Zn,54.462517,22.940236,7.322918,2.766263,0.953681,0.313214
g,Zn,24.521706,5.473674,1.917828,0.739503
h,Zn,15.252873,4.733286,0.639418
i,Zn,21.724565,11.4367,1.869792,0.891341

s,Ag,13.609689,9.096707,6.081589,1.6649,1.0415,0.695188
p,Ag,35.254762,21.220247,12.894651,5.759698,3.8457,2.4086,0.555887
d,Ag,13.860367,9.236327,5.3756,3.650158,2.4802,1.502712
f,Ag,21.716749,10.672523,3.960392,1.650806,0.663244,0.225891
g,Ag,12.825187,5.121742,2.228789,0.933643
h,Ag,4.214113,1.611471,0.709563
i,Ag,9.468634,6.325471,4.2423,0.650527

s,Cd,14.906675,9.938904,4.765577,1.9234,1.2027,0.802950
p,Cd,43.960544,29.219285,13.097517,6.236902,4.1667,2.6094,0.670519
d,Cd,15.877271,10.590183,5.9557,3.988764,2.675,1.733364
f,Cd,29.998128,11.681173,5.035703,1.773103,0.751984,0.251902
g,Cd,14.106034,6.131847,2.519419,1.050849
h,Cd,4.750789,1.822244,0.812819
i,Cd,10.379539,6.931623,4.6428,0.756654

s,Au,14.806640,9.855079,6.3156,3.9472,1.224803,0.816165
p,Au,37.191119,24.754614,16.482404,8.971393,5.9859,3.7451,1.062814
d,Au,18.522641,12.359400,8.255771,5.5185,3.4524,1.046522
f,Au,17.487847,11.629073,7.742722,5.167079,3.450749,0.182493
g,Au,57.781498,5.719031,3.816393,0.755299
h,Au,6.865180,4.242552,1.215984
i,Au,7.081120,4.731164,3.1727,0.550374

s,Hg,14.422678,9.642560,6.451957,4.303317,1.8256,1.1414
p,Hg,31.482901,20.971311,13.978356,9.310675,6.2027,3.8825,1.046694
d,Hg,36.183564,8.550458,5.703356,3.7983,2.1417,1.120654
f,Hg,19.628275,13.060413,8.697925,5.798036,3.869293,0.206558
g,Hg,33.598859,6.331945,4.238134,0.845586
h,Hg,6.874971,4.096174,1.380405
i,Hg,7.538158,5.034666,3.3725,0.620177
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aug-cc-pwCVDZ-PP/OptRI ABS in MOLPRO format

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s,Cu,13.615148,7.443600,2.374214,1.448319,0.346860
p,Cu,11.092379,7.350628,2.027760,0.787881,0.431223
d,Cu,15.688531,6.460334,4.172327,1.068805,0.711447
f,Cu,21.890887,5.569378,1.352344,0.397626
g,Cu,14.168307,5.368756,2.087487,0.755821
h,Cu,8.031276,2.628135
i,Cu,5.447213

s,Zn,13.700188,9.144466,2.223742,1.485077,0.418160
p,Zn,23.262553,15.673667,1.924780,0.846264,0.535715
d,Zn,18.613376,7.500930,4.982331,1.615170,1.074883
f,Zn,25.132733,6.371185,1.620494,0.451013
g,Zn,17.163671,6.446959,2.677679,1.018246
h,Zn,9.126286,3.097045
i,Zn,6.405320

s,Ag,12.639208,8.553992,1.609317,0.891137,0.599502
p,Ag,11.469781,7.714739,5.179910,1.749736,0.526969
d,Ag,21.001461,6.344167,4.240612,0.830164,0.553665
f,Ag,11.659444,7.398598,2.653284,0.663164
g,Ag,7.018740,3.088325,1.394563,0.583352
h,Ag,3.101564,1.319429
i,Ag,2.266770

s,Cd,12.869317,6.325854,1.512305,0.694608,0.342760
p,Cd,12.571735,8.517452,5.746791,1.856078,0.521311
d,Cd,21.832177,7.379851,4.941737,2.046914,0.652840
f,Cd,15.377212,7.840530,2.948192,0.773116
g,Cd,7.132087,3.452073,1.594405,0.688569
h,Cd,3.449903,1.515446
i,Cd,2.557535

s,Au,15.054592,10.041754,4.785404,1.266123,0.845071
p,Au,27.283289,9.088068,6.052251,1.509249,0.777021
d,Au,10.167352,6.801323,4.541946,1.356432,0.509693
f,Au,7.399411,4.671651,3.125319,0.566526
g,Au,4.474574,2.986018,1.399991,0.574471
h,Au,2.904463,1.282405
i,Au,1.722463

s,Hg,13.373935,8.923930,5.796751,1.431409,0.427333
p,Hg,22.115298,11.483164,7.663051,1.458042,0.748600
d,Hg,10.679549,7.133959,4.750467,1.485468,0.394509
f,Hg,8.306281,5.553961,3.712129,0.655914
g,Hg,4.892937,3.267930,1.576052,0.662148
h,Hg,2.981021,1.262406
i,Hg,1.880845
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aug-cc-pwCVTZ-PP/OptRI ABS in MOLPRO format

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s,Cu,15.772188,10.574469,1.754501,0.952406,0.359486
p,Cu,24.615719,4.847573,1.453721,0.286440
d,Cu,19.253621,10.697252,1.174655,0.459223
f,Cu,24.873519,6.313110,2.327985,0.682437
g,Cu,19.543340,5.231634,2.198382,0.620038
h,Cu,15.882772,6.762756,2.831186,1.130988
i,Cu,5.468239

s,Zn,18.015663,12.088070,1.928474,1.044178,0.421166
p,Zn,56.606056,14.681579,5.222811,1.116083
d,Zn,23.715730,11.317246,2.694189,0.654023
f,Zn,28.083505,6.886404,2.728665,0.812320
g,Zn,23.896822,6.498175,2.566949,0.741572
h,Zn,20.723610,8.264814,3.633505,1.488507
i,Zn,6.423210

s,Ag,12.988006,8.666279,5.763862,0.933058,0.438789
p,Ag,13.307296,8.958439,0.836506,0.346601
d,Ag,56.086469,12.635014,8.399633,0.688713
f,Ag,13.794836,3.282507,1.261370,0.462578
g,Ag,18.189227,12.128421,1.060203,0.448520
h,Ag,6.561213,3.765484,1.835194,0.768203
i,Ag,2.267719

s,Cd,14.003304,9.378160,6.281064,0.923058,0.447657
p,Cd,14.193694,9.635200,0.890805,0.351955
d,Cd,53.113516,14.622010,8.567936,0.770792
f,Cd,13.872437,3.746691,1.429500,0.567276
g,Cd,9.037991,6.012828,1.224985,0.427850
h,Cd,7.359113,3.833540,1.835391,0.768524
i,Cd,2.558455

s,Au,15.864661,10.586349,7.067209,2.972435,0.831921
p,Au,11.788345,8.016150,0.768002,0.182235
d,Au,11.546301,7.700194,0.590435,0.206321
f,Au,11.777715,7.862358,0.846301,0.327529
g,Au,6.058611,4.064993,0.821326,0.366808
h,Au,5.113380,3.408193,1.649750,0.704098
i,Au,1.723374

s,Hg,20.340321,13.589947,9.079807,3.175650,0.527257
p,Hg,11.805866,8.078510,0.801989,0.191385
d,Hg,11.809885,7.891999,0.672151,0.403747
f,Hg,11.805499,7.895992,0.915076,0.363412
g,Hg,9.973051,6.648769,4.436766,0.420024
h,Hg,7.155083,4.272495,1.960439,0.877876
i,Hg,1.881778
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aug-cc-pwCVQZ-PP/OptRI ABS in MOLPRO format

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s,Cu,15.659560,9.029141,2.126129,0.396499
p,Cu,41.883727,6.606805,1.215329,0.267938
d,Cu,18.901379,10.679323,2.974306,1.259012
f,Cu,32.026859,7.417418,3.175571,1.416328
g,Cu,28.759448,6.685086,2.678734,1.055614
h,Cu,19.601209,5.648684,2.382829,0.699566
i,Cu,8.919127,2.681940

s,Zn,16.806517,11.195794,2.441892,0.414289
p,Zn,56.314110,6.044765,2.199361,1.267423
d,Zn,29.676851,17.109170,3.417191,0.948234
f,Zn,34.930719,8.376356,3.733233,1.611149
g,Zn,28.949762,7.626749,3.118398,1.260289
h,Zn,23.057474,6.688080,2.862004,0.848319
i,Zn,10.353342,3.245024

s,Ag,11.005431,7.411594,4.979457,0.410151
p,Ag,13.122121,8.757433,5.851749,1.085934
d,Ag,16.218238,3.090332,1.331646,0.355574
f,Ag,22.649641,4.597800,2.000245,0.874024
g,Ag,8.740823,5.823968,1.362649,0.599710
h,Ag,8.332970,5.557882,1.196228,0.533939
i,Ag,3.212197,1.301610

s,Cd,12.605076,8.467612,5.682268,0.304075
p,Cd,18.327877,8.891973,5.817345,1.119693
d,Cd,13.539416,3.653520,1.514364,0.401073
f,Cd,20.910246,5.148324,2.244110,0.983354
g,Cd,9.848688,6.454752,1.539698,0.696212
h,Cd,9.140353,6.108564,1.375301,0.582183
i,Cd,3.619463,1.507041

s,Au,16.340262,10.881998,5.369200,3.095642
p,Au,11.602799,7.769516,5.203444,0.929170
d,Au,11.516342,7.682605,0.932730,0.280984
f,Au,10.608926,7.068174,3.867171,0.577357
g,Au,7.931955,5.198920,1.052254,0.467955
h,Au,7.974885,4.203519,0.861637,0.383965
i,Au,3.051497,1.187165

s,Hg,14.422509,9.624524,5.306559,2.936184
p,Hg,12.287985,8.222334,5.504709,0.989905
d,Hg,11.838696,7.908146,1.083248,0.307247
f,Hg,11.388398,7.584190,4.148229,0.649929
g,Hg,10.422485,5.742827,1.165573,0.533318
h,Hg,7.310126,4.840528,0.954539,0.427287
i,Hg,3.316665,1.328657
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aug-cc-pwCV5Z-PP/OptRI ABS in MOLPRO format

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s,Cu,16.148770,9.764327,2.085724,0.428963
p,Cu,24.854938,16.581177,7.374131,2.777434,1.101004
d,Cu,22.364827,14.722760,2.362743,0.982049
f,Cu,41.476376,9.747061,2.057447,0.929563,0.331791
g,Cu,28.070724,18.747637,1.942620,0.624111
h,Cu,26.421002,3.364005,0.565560
i,Cu,23.172995,3.407685,0.930645

s,Zn,18.914284,9.950917,1.886852,0.457764
p,Zn,27.222091,18.188312,6.628000,2.943188,1.070217
d,Zn,28.304446,16.032821,4.223721,1.310188
f,Zn,44.623886,10.945003,2.331801,0.995723,0.382023
g,Zn,31.492775,21.019492,2.203531,0.737701
h,Zn,28.848044,3.793234,0.690355
i,Zn,21.724565,1.869792,0.891341

s,Ag,13.609689,9.096707,6.081589,0.695188
p,Ag,35.254762,21.220247,12.894651,5.759698,0.555887
d,Ag,13.860367,9.236327,3.650158,1.502712
f,Ag,45.705023,6.833300,3.155397,0.660342,0.252646
g,Ag,15.890467,9.960272,6.647781,0.998635
h,Ag,10.807996,1.652436,0.712921
i,Ag,9.468634,6.325471,0.650527

s,Cd,14.906675,9.938904,4.765577,0.802950
p,Cd,43.960544,29.219285,13.097517,6.236902,0.670519
d,Cd,15.877271,10.590183,3.988764,1.733364
f,Cd,58.627727,7.540236,3.505179,0.740884,0.287276
g,Cd,25.545937,11.032032,7.370119,1.110145
h,Cd,11.543387,1.828458,0.814020
i,Cd,10.379539,6.931623,0.756654

s,Au,14.806640,9.855079,1.224803,0.816165
p,Au,37.191119,24.754614,16.482404,8.971393,1.062814
d,Au,18.522641,12.359400,8.255771,1.046522
f,Au,17.846263,11.898690,7.946949,5.319007,0.183219
g,Au,11.763786,7.748489,5.164542,0.804246
h,Au,7.341440,4.848584,1.230939
i,Au,7.081120,4.731164,0.550374

s,Hg,14.422678,9.642560,6.451957,4.303317
p,Hg,31.482901,20.971311,13.978356,9.310675,1.046694
d,Hg,36.183564,8.550458,5.703356,1.120654
f,Hg,19.006688,12.674831,8.463221,5.659816,0.207084
g,Hg,12.925238,8.616696,5.678605,0.895039
h,Hg,7.804750,5.157946,1.339646
i,Hg,7.538158,5.034666,0.620177
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