Correlation consistent basis sets for explicitly correlated wavefunctions: Valence and core-valence basis sets for Li, Be, Na, and Mg

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Supplementary Information

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Table SI. DF error in select orbital and auxiliary basis combinations for Na_2 and Mg.

System	Orbital basis	DF basis	E_{MP2}^{corr} (mE_h)	E_{DF-MP2}^{corr} (mE_h)	DF error (μE_h)
Na_2	cc-pVDZ	cc-pVDZ	-17.240	-17.196	-44.1
	cc-pV(D+d)Z	cc-pVDZ	-17.343	-17.297	-45.8
	aug-cc-pVDZ	aug-cc-pVDZ	-17.435	-17.419	-15.5
	aug-cc-pV(D+d)Z	aug-cc-pVDZ	-17.510	-17.495	-15.3
	cc-pVTZ	cc-pVTZ	-19.149	-19.122	-26.8
	cc-pV(T+d)Z	cc-pVTZ	-19.155	-19.128	-27.2
	aug-cc-pVTZ	aug-cc-pVTZ	-19.308	-19.298	-9.7
	aug-cc-pV(T+d)Z	aug-cc-pVTZ	-19.314	-19.304	-9.8
	cc-pVQZ	cc-pVQZ	-19.801	-19.756	-44.5
	cc-pV(Q+d)Z	cc-pVQZ	-19.798	-19.760	-37.8
	aug-cc-pVQZ	aug-cc-pVQZ	-19.901	-19.884	-17.1
	aug-cc-pV(Q+d)Z	aug-cc-pVQZ	-19.903	-19.887	-15.6
	cc-pV5Z	cc-pV5Z	-20.125	-20.118	-7.4
	cc-pV(5+d)Z	cc-pV5Z	-20.125	-20.118	-7.5
	aug-cc-pV5Z	aug-cc-pV5Z	-20.197	-20.194	-3.1
	aug-cc-pV(5+d)Z	aug-cc-pV5Z	-20.197	-20.194	-3.1
Mg	cc-pVDZ	cc-pVDZ	-21.343	-21.343	-0.8
	cc-pV(D+d)Z	cc-pVDZ	-21.421	-21.419	-2.0
	aug-cc-pVDZ	aug-cc-pVDZ	-21.691	-21.691	-0.7
	aug-cc-pV(D+d)Z	aug-cc-pVDZ	-21.773	-21.771	-1.6
	cc-pVTZ	cc-pVTZ	-23.535	-23.534	-0.2
	cc-pV(T+d)Z	cc-pVTZ	-23.549	-23.548	-0.3
	aug-cc-pVTZ	aug-cc-pVTZ	-23.713	-23.712	-0.2
	aug-cc-pV(T+d)Z	aug-cc-pVTZ	-23.726	-23.726	-0.2
	cc-pVQZ	cc-pVQZ	-24.320	-24.320	-0.2
	cc-pV(Q+d)Z	cc-pVQZ	-24.315	-24.314	-1.3
	aug-cc-pVQZ	aug-cc-pVQZ	-24.444	-24.444	-0.2
	aug-cc-pV(Q+d)Z	aug-cc-pVQZ	-24.435	-24.434	-0.4
	cc-pV5Z	cc-pV5Z	-24.684	-24.684	-0.2
	cc-pV(5+d)Z	cc-pV5Z	-24.683	-24.682	-0.3
	aug-cc-pV5Z	aug-cc-pV5Z	-24.775	-24.775	-0.1
	aug-cc-pV(5+d)Z	aug-cc-pV5Z	-24.768	-24.768	-0.2

TABLE SII. CCSD(T)-F12b optimized geometries and harmonic frequencies with the cc-pV*n*Z-F12 (denoted V*n*Z-F12) and cc-pCV*n*Z-F12 (denoted CV*n*Z-F12) families of basis sets.

Molecule	Basis set	Bond Length (Å)	Frequency (cm^{-1})	Basis set	Bond Length (Å)	Frequency (cm^{-1})
Li_2 ($^1\Sigma_g^+$)	VDZ-F12	2.7001	348.3	CVDZ-F12	2.6751	354.0
	VTZ-F12	2.6991	348.4	CVTZ-F12	2.6729	360.5
	VQZ-F12	2.6990	348.4	CVQZ-F12	2.6734	353.6
LiF ($^1\Sigma^+$)	VDZ-F12	1.5799	901.1	CVDZ-F12	1.5638	916.3
	VTZ-F12	1.5802	900.6	CVTZ-F12	1.5643	914.3
	VQZ-F12	1.5801	900.4	CVQZ-F12	1.5642	914.3
BeO ($^1\Sigma^+$)	VDZ-F12	1.3376	1476.4	CVDZ-F12†	1.3311	1488.4
	VTZ-F12	1.3373	1475.3	CVTZ-F12	1.3306	1489.4
	VQZ-F12	1.3365	1478.7	CVQZ-F12	1.3299	1493.2
BeF ($^2\Sigma^+$)	VDZ-F12	1.3684	1255.6	CVDZ-F12	1.3619	1266.1
	VTZ-F12	1.3679	1255.5	CVTZ-F12	1.3614	1266.4
	VQZ-F12	1.3673	1256.7	CVQZ-F12	1.3610	1267.3
Na_2 ($^1\Sigma_g^+$)	VDZ-F12	3.1780	152.6	CVDZ-F12†	3.0902	159.0
	VTZ-F12	3.1791	152.5	CVTZ-F12	3.0811	159.3
	VQZ-F12	3.1793	152.5	CVQZ-F12	3.0770	150.3
NaF ($^1\Sigma^+$)	VDZ-F12	1.9853	540.6	CVDZ-F12	1.9270	535.7
	VTZ-F12	1.9876	540.7	CVTZ-F12	1.9273	535.3
	VQZ-F12	1.9888	540.4	CVQZ-F12	1.9266	535.4
MgO ($^1\Sigma^+$)	VDZ-F12	1.7558	786.4	CVDZ-F12	1.7382	811.8
	VTZ-F12	1.7530	796.2	CVTZ-F12	1.7370	816.7
	VQZ-F12	1.7530	797.7	CVQZ-F12	1.7372	816.7
MgF ($^2\Sigma^+$)	VDZ-F12	1.7641	710.8	CVDZ-F12	1.7500	719.9
	VTZ-F12	1.7646	710.1	CVTZ-F12	1.7508	718.4
	VQZ-F12	1.7643	710.4	CVQZ-F12	1.7505	718.5

† Harmonic frequencies obtained from a Dunham analysis based on near-equilibrium potential energy functions. See text for further details.

TABLE SIII. CCSD(T)-F12b optimized geometries (Å) and harmonic frequencies (ω_n, in cm^{-1}) with the cc-pV*n*Z-F12 (denoted V*n*Z-F12) and cc-pCV*n*Z-F12 (denoted CV*n*Z-F12, calculated with all-electrons correlated) families of basis sets.

Molecule	Basis	Bond 1	Bond 2	ω_1	ω_2	ω_3	Basis	Bond 1	Bond 2	ω_1	ω_2	ω_3
BeH_2 ($^1\Sigma_g^+$)	VDZ-F12	1.3312		715.5	2040.1	2247.4	CVDZ-F12	1.3263[†]		718.4	2050.0	2262.3
	VTZ-F12	1.3310		714.1	2040.8	2249.0	CVTZ-F12	1.3264		716.8	2050.2	2259.6
	VQZ-F12	1.3307		713.7	2041.6	2249.7	CVQZ-F12	1.3260		717.1	2051.0	2260.3
BeF_2 ($^1\Sigma_g^+$)	VDZ-F12	1.3801		341.4	726.0	1573.2	CVDZ-F12*	1.3739[†]		339.1	731.5	1585.5
	VTZ-F12	1.3792		339.9	726.1	1576.6	CVTZ-F12	1.3734		341.6	731.9	1586.2
	VQZ-F12	1.3787		339.3	726.5	1577.1	CVQZ-F12	1.3731		341.9	732.2	1586.7
MgH_2 ($^1\Sigma_g^+$)	VDZ-F12	1.7097		432.5	1600.4	1623.3	CVDZ-F12	1.6964		437.9	1614.0	1637.1
	VTZ-F12	1.7101		433.9	1599.4	1622.8	CVTZ-F12	1.6970		435.8	1615.8	1639.3
	VQZ-F12	1.7098		433.1	1600.2	1623.7	CVQZ-F12	1.6965		436.8	1617.7	1640.9
MgF_2 ($^1\Sigma_g^+$)	VDZ-F12	1.7522		149.6	565.2	875.9	CVDZ-F12	1.7378		150.5	573.3	888.4
	VTZ-F12	1.7529		150.0	564.0	875.2	CVTZ-F12	1.7383		149.9	572.0	888.0
	VQZ-F12	1.7525		150.2	564.1	875.8	CVQZ-F12	1.7380		151.5	572.1	887.8
Li_2O ($^1\Sigma_g^+$)	VDZ-F12	1.6287		91.5	783.1	1028.1	CVDZ-F12	1.6132[†]		87.3	792.1	1040.2
	VTZ-F12	1.6287		109.7	782.6	1027.7	CVTZ-F12	1.6138		109.7	794.4	1040.8
	VQZ-F12	1.6285		113.5	782.7	1028.6	CVQZ-F12	1.6134		113.6	794.9	1042.8
Na_2O ($^1\Sigma_g^+$)	VDZ-F12	2.0140		18.3	348.8	668.5	CVDZ-F12	1.9813[†]		29.5	359.5	680.5
	VTZ-F12	2.0137		29.6	348.9	668.8	CVTZ-F12	1.9809		29.2	357.7	684.2
	VQZ-F12	2.0140		39.8	348.8	669.0	CVQZ-F12	1.9802		38.4	358.6	686.6

LiOH ($^1\Sigma_g^+$)	VDZ-F12	1.5946	0.9486	331.7	940.0	4023.7	CVDZ-F12	1.5787	0.9473	338.6	956.6	4035.8
	VTZ-F12	1.5942	0.9487	327.5	940.6	4019.3	CVTZ-F12	1.5783	0.9478	340.1	956.7	4025.7
	VQZ-F12	1.5942	0.9485	331.7	940.0	4020.7	CVQZ-F12	1.5783	0.9477	345.9	956.5	4026.8
NaOH ($^1\Sigma_g^+$)	VDZ-F12	1.9714	0.9516	247.5	554.4	3972.9	CVDZ-F12	1.9380	0.9500	253.6	567.8	3988.2
	VTZ-F12	1.9712	0.9517	233.3	554.7	3968.3	CVTZ-F12	1.9372	0.9507	239.1	568.4	3976.4
	VQZ-F12	1.9715	0.9515	234.4	554.2	3969.8	CVQZ-F12	1.9364	0.9505	238.4	568.7	3977.5

† Harmonic frequencies calculated *via* second order perturbation theory with the SURFIT program. See text for further details.

* Slight symmetry breaking required for a true minimum.

TABLE SIV. CCSD(T)-F12b atomization energies calculated with the cc-pV*n*Z-F12 (shortened below to V*n*Z-F12) and cc-pCV*n*Z-F12 (CV*n*Z-F12) families of basis sets. V(T,Q)Z-F12 and CV(T,Q)Z-F12 estimates of the CBS limits obtained by extrapolation with a Schwenke-type formula, see text for further details. All calculations with the cc-pCV*n*Z-F12 basis sets were performed "all-electron".

	Atomization energy (kcal mol^{-1})							
Molecule	VDZ-F12	VTZ-F12	VQZ-F12	V(T,Q)Z-F12	CVDZ-F12	CVTZ-F12	CVQZ-F12	CV(T,Q)Z-F12
Li_2	23.881	24.041	24.052	24.055	24.087	24.325	24.312	24.314
LiF	136.408	137.724	138.180	138.399	137.914	138.916	139.392	139.622
BeO	102.783	104.976	105.690	106.004	104.589	106.722	107.439	107.759
BeF	134.746	135.983	136.431	136.621	136.192	137.212	137.640	137.832
Na_2	16.670	16.777	16.786	16.787	17.079	17.248	17.334	17.394
NaF	112.714	114.093	114.588	114.828	113.510	114.553	115.112	115.381
MgO	58.502	61.089	61.707	62.000	58.894	61.269	61.815	62.092
MgF	106.390	107.917	108.471	108.710	105.869	107.039	107.540	107.756
BeH_2	146.232	146.904	147.066	147.121	146.906	147.881	148.025	148.073
BeF_2	303.732	306.065	306.886	307.249	306.579	308.208	308.983	309.344
MgH_2	105.206	105.883	106.049	106.093	103.786	104.817	104.975	105.031
MgF_2	247.094	249.834	250.830	251.266	246.937	248.935	249.872	250.297
Li_2O	168.762	171.476	172.270	172.663	171.655	174.400	175.259	175.686
Na_2O	112.071	115.075	115.914	116.323	113.334	116.358	117.318	117.804
LiOH	208.753	210.941	211.741	212.112	210.578	212.536	213.328	213.700
NaOH	184.906	187.127	187.989	188.383	185.246	187.203	188.054	188.458

cc-pVDZ-F12 orbital basis sets in MOLPRO format

```
s,Li,0.59880000E+04,0.89890000E+03,0.20590000E+03,0.59240000E+02,0.19870000E+02,0.74060000E+01,
0.29300000E+01,0.11890000E+01,0.47980000E+00,0.75090000E-01,0.28320000E-01,0.0076
c,1.11,0.13300000E-03,0.10250000E-02,0.52720000E-02,0.20929000E-01,0.66340000E-01,
0.16577500E+00,0.31503800E+00,0.39352300E+00,0.19087000E+00,0.5414000E-02,-0.13280000E-02
c,1.11,-0.21000000E-04,-0.16100000E-03,-0.82000000E-03,-0.33260000E-02,-0.10519000E-01,-0.28097000E-01,
-0.55936000E-01,-0.99237000E-01,-0.11218900E+00,0.56788900E+00,0.53038200E+00
c,10.10,1
c,11.11,1
c,12.12,1
p,Li,0.32660000E+01,0.65110000E+00,0.16960000E+00,0.55780000E-01,0.20500000E-01,0.0091
c,1.5,0.86300000E-02,0.47538000E-01,0.20977200E+00,0.52852200E+00,0.38274400E+00
c,3.3,1
c,4.4,1
c,5.5,1
c,6.6,1
d,Li,0.148438,0.068473

s,Be,6863,1030,234.7,66.56,21.69,7.734,2.916,1.13,.2577,.1101,.04409,0.0147
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c,1.11,-.000043,-.000333,-.001736,-.007012,-.023126,-.058138,-.114556,-.135908,.228026,.577441,.317873
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c,11.11,1
c,12.12,1
p,Be,7.436,1.577,.4352,.1438,.04994,0.0093
c,1.5,.010736,.062854,.24818,.523699,.353425
c,3.3,1
c,4.4,1
c,5.5,1
c,6.6,1
d,Be,0.299284,0.125050

s,Na,.42300000E+06,.63340000E+05,.14410000E+05,.40770000E+04,.13280000E+04,.47860000E+03,.18620000E+03,.769
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.60150000E-01,.23820000E-01,0.0067
c,1.16,.18061800E-04,.14043000E-03,.73843800E-03,.31118200E-02,.11208100E-01,.35282800E-01,
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.95989700E-01,.21373500E+00,.34868800E+00,.32456600E+00,.11263300E+00,.70679700E-02,.59801000E-03,
.20413000E-03,-.53087000E-05,.18260500E-05
c,1.16,-.44065300E-05,-.34344300E-04,-.18011400E-03,-.76390000E-03,-.27524800E-02,-.88601600E-02,
-.24793900E-01,-.60599500E-01,-.11644600E+00,-.16243700E+00,-.43889100E-01,
.33791700E+00,.56134700E+00,.24524000E+00,.40675400E-02,-.12674600E-02
c,1.16,.66301900E-06,.51576900E-05,.27125000E-04,.11463500E-03,.41511800E-03,.13297800E-02,
.37559500E-02,.91402500E-02,.17985900E-01,.25147700E-01,.76352200E-02,-.61458900E-01,-.11572100E+00,
-.15890600E+00,.62640600E+00,.47540200E+00
c,14.14,1
c,16.16,1
c,17.17,1
p,Na,.24330000E+03,.57390000E+02,.18100000E+02,.65750000E+01,.25210000E+01,.96070000E+00,.35120000E+00,
.98270000E-01,.37340000E-01,.15000000E-01,0.0060
c,1.10,.22439200E-02,.17399700E-01,.77412500E-01,
.21910200E+00,.37852200E+00,.39490200E+00,.16042400E+00,.23331100E-02,.19953600E-02,-.77734400E-03
c,1.10,-.22240100E-03,-.17427700E-02,-.77545600E-02,-.22518700E-01,-.38433000E-01,-.45017700E-01,
-.19213200E-01,.18269700E+00,.55789700E+00,.37302200E+00
c,10.10,1
c,11.11,1
p,Na,3.33428581,0.08836183
d,Na,0.896311,0.110745,0.056176

s,Mg,.16490000E+06,.24710000E+05,.56280000E+04,.15960000E+04,.52100000E+03,.18800000E+03,.73010000E+02,
.29900000E+02,.12540000E+02,.43060000E+01,.18260000E+01,.74170000E+00,.14570000E+00,
.76120000E-01,.33100000E-01,0.0120
c,1.15,.72992852E-04,.56665208E-03,.29626934E-02,.12296244E-01,.42732390E-01, .12301339E+00,
.27483212E+00,.40181847E+00,.26469734E+00,.33261243E-01,-.44133529E-02,.20602406E-02,
-.83847033E-03,.70819497E-03,-.20060176E-03
c,1.15,-.18424833E-04,-.14350020E-03,-.74871024E-03,-.31440747E-02,-.11048121E-01,-.33605846E-01,
-.82594554E-01,-.15931351E+00,-.15288784E+00,.19084949E+00,.57996406E+00,.37202938E+00,.21169123E-01,
-.11934365E-01,.27732867E-02
c,1.15,.35517561E-05,.27642017E-04,.14440388E-03,.60574423E-03,.21352674E-02,.64993445E-02,
.16144594E-01,.31576557E-01,.31637441E-01,-.43914029E-01,-.15109333E+00,-.21766839E+00,
.25980682E+00,.54724537E+00,.32590951E+00
c,13.13,1
c,15.15,1
c,16.16,1
p,Mg,.31690000E+03,.74860000E+02,.23720000E+02,.86690000E+01,.33630000E+01,.13100000E+01,.49110000E+00,
.23640000E+00,.87330000E-01,.32370000E-01,0.0090
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-.43753955E-02,.62958244E-02,-.15676869E-02
c,1.10,-.32972687E-03,-.25875416E-02,-.11912032E-01,-.35022673E-01,-.63996825E-01,-.70443568E-01,
-.37583553E-01,.17704345E+00,.56670743E+00,.39614295E+00
c,10.10,1
c,11.11,1
p,Mg,3.182039,0.171848
d,Mg,1.431308,0.199432,0.090937
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cc-pVTZ-F12 orbital basis sets in MOLPRO format

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s,Li,0.66010000E+04,0.98970000E+03,0.22570000E+03,0.64290000E+02,0.21180000E+02,0.77240000E+01,
0.30030000E+01,0.12120000E+01,0.49300000E+00,0.95150000E-01,0.47910000E-01,0.22200000E-01,0.0064
c,1.12,0.11700000E-03,0.91100000E-03,0.47280000E-02,0.19197000E-01,0.63047000E-01,
0.16320800E+00,0.31482700E+00,0.39393600E+00,0.19691800E+00,0.99970000E-02,-0.54020000E-02,0.17040000E-02
c,1.12,-0.18000000E-04,-0.14200000E-03,-0.74100000E-03,-0.30200000E-02,-0.10123000E-01,-0.27094000E-01,
-0.57359000E-01,-0.93895000E-01,-0.12109100E+00,0.27660800E+00,0.54954800E+00,0.27738500E+00
c,10.10,1
c,11.11,1
c,12.12,1
c,13.13,1
p,Li,0.62500000E+01,0.13700000E+01,0.36720000E+00,0.11920000E+00,0.44740000E-01,0.17950000E-01,0.0075
c,1.6,0.33880000E-02,0.19316000E-01,0.79104000E-01,0.27409500E+00,0.51948800E+00,0.28442300E+00
c,3.3,1
c,4.4,1
c,5.5,1
c,6.6,1
c,7.7,1
d,Li,0.235118,0.119404,0.060639
f,Li,0.163775,0.075910

s,Be,.14630000E+05,.21910000E+04,.49820000E+03,.14090000E+03,.45860000E+02,.16470000E+02,.63190000E+01,
.25350000E+01,.10350000E+01,.25280000E+00,.10520000E+00,.42610000E-01,0.0141
c,1.12,.91806606E-04,.71342800E-03,.37346072E-02,.15468005E-01,.52873737E-01,
.14569439E+00,.30268071E+00,.40493577E+00,.22238740E+00,.12912029E-01,-.46478855E-02,.12281708E-02
c,1.12,-.16701238E-04,-.13045864E-03,-.67947283E-03,-.28571410E-02,-.98127014E-02,-.28609231E-01,
-.63760000E-01,-.11723138E+00,-.12120227E+00,.25322864E+00,.58183718E+00,.29195422E+00
c,10.10,1
c,11.11,1
c,12.12,1
c,13.13,1
p,Be,.14030000E+02,.31680000E+01,.90240000E+00,.30360000E+00,.11300000E+00,.42860000E-01,0.0084
c,1.6,.40993290E-02,.25626424E-01,.10376777E+00,.31154736E+00,.49812835E+00,.25887570E+00
c,3.3,1
c,4.4,1
c,5.5,1
c,6.6,1
```

```
c,7.7,1
d,Be,0.467046,0.220597,0.104194
f,Be,0.316640,0.145788

s,Na,.12240000E+07,.18320000E+06,.41700000E+05,.11810000E+05,.38530000E+04,.13910000E+04,.54250000E+03,
.22490000E+03,.97930000E+02,.44310000E+02,.20650000E+02,.97290000E+01,.42280000E+01,.19690000E+01,
.88900000E+00,.39640000E+00,.69930000E-01,.32890000E-01,.16120000E-01,0.0050
c,1.19,.47889400E-05,.37239500E-04,.19583100E-03,.82669800E-03,.30025100E-02,.97031000E-02,
.28233700E-01,.73205800E-01,.16289700E+00,.28870800E+00,.34682900E+00,.20686500E+00,.32800900E-01,
-.64773600E-03,.14587800E-02,-.17834600E-03,.91478900E-04,-.82518200E-04,.29225200E-04
c,1.19,-.11695800E-05,-.90911000E-05,-.47849900E-04,-.20196200E-03,-.73583700E-03,-.23874600E-02,
-.70496900E-02,-.18785600E-01,-.44615300E-01,-.89774100E-01,-.14294000E+00,-.12431500E+00,
.99964800E-01,.41708000E+00,.47512300E+00,.16326800E+00,.30954300E-02,-.15526300E-02,.55776300E-03
c,1.19,.17587100E-06,.13659400E-05,.71979500E-05,.30334900E-04,.11075200E-03,.35859600E-03,
.10627200E-02,.28268700E-02,.67674200E-02,.13648000E-01,.22281400E-01,.19601100E-01,-.16770800E-01,
-.77373400E-01,-.11350100E+00,-.13913000E+00,.44008300E+00,.53895200E+00,.13388900E+00
c,17.17,1
c,18.18,1
c,19.19,1
c,20.20,1
p,Na,.41340000E+03,.97980000E+02,.31370000E+02,.11620000E+02,.46710000E+01,.19180000E+01,.77750000E+00,
.30130000E+00,.22750000E+00,.75270000E-01,.31260000E-01,.13420000E-01,0.0072
c,1.12,.90819600E-03,.74177300E-02,.35746400E-01,.11852000E+00,.26140300E+00,.37839500E+00,
.33463200E+00,.12684400E+00,-.14711700E-01,.56865000E-02,-.17097400E-02,.54714200E-03
c,1.12,-.90174100E-04,-.73934200E-03,-.35730900E-02,-.12014200E-01,-.26717800E-01,-.39275300E-01,
-.37608300E-01,-.43322800E-01,.51800300E-01,.26019400E+00,.54968100E+00,.28187200E+00
c,10.10,1
c,11.11,1
c,12.12,1
c,13.13,1
p,Na,0.796814
d,Na,1.145665
d,Na,0.051789,0.091634,0.162136
f,Na,0.134197,0.069524

s,Mg,.32760000E+06,.49050000E+05,.11150000E+05,.31520000E+04,.10250000E+04,.36880000E+03,.14320000E+03,
.58960000E+02,.25400000E+02,.11150000E+02,.40040000E+01,.17010000E+01,.70600000E+00,.14100000E+00,
.68080000E-01,.30630000E-01,0.0109
```

```
c,1.16,.30960809E-04,.24095411E-03,.12666017E-02,.53335908E-02,.19077024E-01,.58805754E-01,
.15145366E+00,.30071600E+00,.38114885E+00,.21358376E+00,.23121033E-01,-.23075697E-02,.12889998E-02,
-.42638745E-03,.35432021E-03,-.11258778E-03
c,1.16,-.78317328E-05,-.60793506E-04,-.32119671E-03,-.13495523E-02,-.49057028E-02,-.15356145E-01,
-.42340895E-01,-.94060347E-01,-.16342527E+00,-.12475430E+00,.23562334E+00,.57756255E+00,
.33523236E+00,.15633813E-01,-.83779924E-02,.22305631E-02
c,1.16,.15090770E-05,.11713361E-04,.61898027E-04,.26008758E-03,.94621789E-03,.29659518E-02,
.82124464E-02,.18397739E-01,.32665723E-01,.25731486E-01,-.53535071E-01,-.15689492E+00,-.20665872E+00,
.32429847E+00,.55261115E+00,.26035173E+00
c,14.14,1
c,15.15,1
c,16.16,1
c,17.17,1
p,Mg,.53960000E+03,.12790000E+03,.41020000E+02,.15250000E+02,.61660000E+01,.25610000E+01,.10600000E+01,
.41760000E+00,.26900000E+00,.12230000E+00,.54760000E-01,.23880000E-01,0.0081
c,1.12,.83396886E-03,.68921519E-02,.33787368E-01,.11440056E+00,.25951391E+00,.38509477E+00,
.33537254E+00,.11064124E+00,-.12131497E-01,.70056199E-02,-.15133527E-02,.44892460E-03
c,1.12,-.13207580E-03,-.10953792E-02,-.53949542E-02,-.18557230E-01,-.42737490E-01,-.64768429E-01,
-.62781782E-01,-.24491228E-01,.10476111E+00,.35890875E+00,.49250052E+00,.18528024E+00
c,10.10,1
c,11.11,1
c,12.12,1
c,13.13,1
p,Mg,2.812615
d,Mg,1.837506,0.288307,0.151085,0.077449
f,Mg,0.225791,0.109140
```

cc-pVQZ-F12 orbital basis sets in MOLPRO format

```
s,Li,29493.0,4417.10,1005.22,284.701,92.8654,33.5118,13.0418,5.35754,2.27934,0.993990,0.433471,0.095566,
0.044657,0.020633,0.0061
c,1.14,0.000018,0.000141,0.000739,0.003107,0.011135,0.034670,0.092171,0.199576,0.328836,0.345976,0.142761,
0.005319,-0.002101,0.000815
c,1.14,-0.000003,-0.000022,-0.000115,-0.000487,-0.001746,-0.005520,-0.014928,-0.034207,-0.062156,-0.095904,
-0.103974,0.307166,0.579033,0.223211
c,11.11,1
c,12.12,1
c,13.13,1
c,14.14,1
c,15.15,1
p,Li,19.6635,4.62311,1.41378,0.473721,0.176151,0.072675,0.032141,0.014556,0.0065
c,1.8,0.000540,0.003865,0.015171,0.049204,0.154661,0.360095,0.441852,0.156000
c,4.4,1
c,5.5,1
c,6.6,1
c,7.7,1
c,8.8,1
c,9.9,1
d,Li,0.326357,0.177836,0.096905,0.052804
f,Li,0.207628,0.121194,0.070742
g,Li,0.196134,0.108733

s,Be,.54620000E+05,.81800000E+04,.18620000E+04,.52730000E+03,.17200000E+03,.62100000E+02,.24210000E+02,
.99930000E+01,.43050000E+01,.19210000E+01,.86630000E+00,.24750000E+00,.10090000E+00,.41290000E-01,0.0128
c,1.14,.17710340E-04,.13760197E-03,.72299900E-03,.30388057E-02,.10908403E-01,.34035077E-01,
.91192587E-01,.19926775E+00,.32935508E+00,.34048879E+00,.14373990E+00,.65168111E-02,-.18647716E-02,
.47991942E-03
c,1.14,-.32215111E-05,-.25153448E-04,-.13130846E-03,-.55790538E-03,-.19884660E-02,-.63703189E-02,
-.17217416E-01,-.40858269E-01,-.74237431E-01,-.11923373E+00,-.87776953E-01,.27878824E+00,
.58349869E+00,.26900674E+00
c,11.11,1
c,12.12,1
c,13.13,1
c,14.14,1
c,15.15,1
```

```
p,Be,.43750000E+02,.10330000E+02,.32260000E+01,.11270000E+01,.43340000E+00,.18080000E+00,.78270000E-01,
.33720000E-01,0.0076
c,1.8,.63343171E-03,.48081655E-02,.20527371E-01,.67816498E-01,.19286754E+00,.37869226E+00,.40057389E+00,
.13806744E+00
c,4.4,1
c,5.5,1
c,6.6,1
c,7.7,1
c,8.8,1
c,9.9,1
d,Be,1.026822,0.483892,0.228035,0.107462
f,Be,0.438694,0.230223,0.120820
g,Be,0.343616,0.167359

s,Na,2185572,327228.4,74466.84,21093.15,6881.898,2484.696,969.2232,402.0643,175.3545,79.65199,37.38672,
18.00194,8.724371,3.857715,1.815686,0.838254,0.381935,0.071679,0.033916,0.016525,0.0051
c,1.20,0.000002,0.000018,0.000095,0.000401,0.001459,0.004746,0.014031,0.037733,0.090702,0.186466,0.301837,
0.323830,0.168700,0.023083,-0.000147,0.001099,-0.000101,0.000061,-0.000053,0.000018
c,1.20,-0.000001,-0.000004,-0.000023,-0.000098,-0.000357,-0.001165,-0.003464,-0.009495,-0.023587,-0.052394,
-0.098028,-0.143673,-0.102298,0.138029,0.429006,0.447813,0.144543,0.002617,-0.001192,0.000440
c,1.20,0.000000,0.000001,0.000003,0.000015,0.000054,0.000175,0.000520,0.001431,0.003554,0.007954,0.014955,
0.022472,0.016205,-0.023550,-0.080120,-0.112921,-0.132989,0.417516,0.549443,0.148110
c,17.17,1
c,18.18,1
c,19.19,1
c,20.20,1
c,21.21,1
p,Na,1119.578,265.3239,85.99553,32.53759,13.51565,5.966856,2.700045,1.218512,0.542187,0.227413,0.133040,
0.057577,0.025971,0.011901,0.0055
c,1.14,0.000162,0.001408,0.007586,0.029615,0.088477,0.195519,0.306621,0.341242,0.229690,0.054921,-0.003441,
0.002340,-0.000662,0.000199
c,1.14,-0.000016,-0.000140,-0.000754,-0.002968,-0.008919,-0.020029,-0.031380,-0.036489,-0.029625,-0.010146,
0.082128,0.334553,0.508142,0.196636
c,10.10,1
c,11.11,1
c,12.12,1
c,13.13,1
c,14.14,1
c,15.15,1
```

```
d,Na,1.522314
d,Na,0.235314,0.136141,0.078764,0.045569
f,Na,0.181127,0.109200,0.065836
g,Na,0.157858,0.091607

s,Mg,.29680000E+07,.44430000E+06,.10110000E+06,.28640000E+05,.93430000E+04,.33730000E+04,.13160000E+04,
.54580000E+03,.23810000E+03,.10820000E+03,.50800000E+02,.24480000E+02,.11930000E+02,.55430000E+01,
.26750000E+01,.12630000E+01,.58830000E+00,.14960000E+00,.67000000E-01,.29520000E-01,0.0108
c,1.20,.19717729E-05,.15336187E-04,.80685186E-04,.34077130E-03,.12419366E-02,.40412371E-02,
.11979690E-01,.32425251E-01,.78933243E-01,.16657542E+00,.28287101E+00,.33188993E+00,
.20328704E+00,.38289740E-01,.30891571E-03,.13890739E-02,-.13615909E-03,.85532166E-04,-.56910200E-04,
.17725931E-04
c,1.20,-.49816008E-06,-.38756303E-05,-.20385410E-04,-.86165921E-04,-.31417603E-03,-.10257663E-02,
-.30581568E-02,-.84106280E-02,-.21120161E-01,-.47688198E-01,-.92411942E-01,-.14254794E+00,
-.12616761E+00,.71528228E-01,.38303878E+00,.49013333E+00,.20438050E+00,.70223118E-02,
-.26787413E-02,.69368983E-03
c,1.20,.96017472E-07,.74616390E-06,.39311860E-05,.16581175E-04,.60625713E-04,.19732216E-03,.59088089E-03,
.16190379E-02,.40975627E-02,.92298919E-02,.18216806E-01,.28288360E-01,.26505867E-01,-.17205272E-01,
-.88591709E-01,-.16387148E+00,-.15950640E+00,.32171495E+00,.59137316E+00,.23686576E+00
c,17.17,1
c,18.18,1
c,19.19,1
c,20.20,1
c,21.21,1
p,Mg,.14410000E+04,.34140000E+03,.11070000E+03,.41970000E+02,.17490000E+02,.77530000E+01,.35340000E+01,
.16140000E+01,.72990000E+00,.30290000E+00,.15830000E+00,.81900000E-01,.41230000E-01,.19880000E-01,0.0071
c,1.14,.15240713E-03,.13276371E-02,.72193728E-02,.28520477E-01,.86534603E-01,.19494957E+00,
.31205125E+00,.34847626E+00,.21888589E+00,.43557946E-01,-.37374701E-02,.30512299E-02,-.86692173E-03,
.23051656E-03
c,1.14,-.24103074E-04,-.21080852E-03,-.11452963E-02,-.45641674E-02,-.13960337E-01,-.32110509E-01,
-.51621713E-01,-.61371346E-01,-.44246480E-01,.52319091E-01,.22169161E+00,.39525503E+00,
.36407820E+00,.97795238E-01
c,10.10,1
c,11.11,1
c,12.12,1
c,13.13,1
c,14.14,1
c,15.15,1
d,Mg,2.043044,0.356152,0.204072,0.116932,0.067001
```

```
f,Mg,0.332321,0.178223,0.094316
g,Mg,0.267541,0.134147
```

cc-pCVDZ-F12 orbital basis sets in MOLPRO format

```
spd,Li,cc-pVDZ-F12;c
s,Li,1.442737
p,Li,0.703963

spd,Be,cc-pVDZ-F12;c
s,Be,1.868915
p,Be,1.577635

spd,Na,cc-pVDZ-F12;c
s,Na,3.798746
p,Na,0.744795
d,Na,4.715702

spd,Mg,cc-pVDZ-F12;c
s,Mg,3.721568
p,Mg,0.927962
d,Mg,6.571650
```

cc-pCVTZ-F12 orbital basis sets in MOLPRO format

```
spdf,Li,cc-pVTZ-F12;c
s,Li,0.406129
p,Li,1.375260
d,Li,4.518674

spdf,Be,cc-pVTZ-F12;c
s,Be,1.165772
p,Be,3.102503
d,Be,5.991579

spdf,Na,cc-pVTZ-F12;c
s,Na,3.764945
p,Na,3.051100
d,Na,5.420585
f,Na,4.557524

spdf,Mg,cc-pVTZ-F12;c
s,Mg,5.425948
p,Mg,0.937022
d,Mg,7.668928
f,Mg,5.520473
```

cc-pCVQZ-F12 orbital basis sets in MOLPRO format

```
spdfg,Li,cc-pVQZ-F12;c
s,Li,1.080878
p,Li,1.578306
d,Li,5.188378

spdfg,Be,cc-pVQZ-F12;c
s,Be,2.105181
p,Be,3.460177
d,Be,7.629658

spdfg,Na,cc-pVQZ-F12;c
s,Na,4.713446
p,Na,2.910439
d,Na,6.466863
f,Na,4.635851

spdfg,Mg,cc-pVQZ-F12;c
s,Mg,6.628966
p,Mg,4.013581
d,Mg,8.402766
f,Mg,5.703089
```

cc-pVDZ-F12/OptRI ABS in MOLPRO format

```
s,He,6.186444,2.105197,0.444703,0.139255
p,He,15.6885,3.55190,1.73889,0.593703
d,He,3.70761,0.810428

s,Li,0.35371261,0.21258866,0.05747471,0.02102723
p,Li,0.39971706,0.10751005,0.03793473,0.01409188
d,Li,0.56424368,0.21190397,0.09176883,0.03499148
f,Li,0.55389765,0.29557321,0.08517342
g,Li,0.26901921

s,Be,0.87797,0.45954,0.11436,0.02915
p,Be,0.97459,0.29016,0.09412,0.0323
d,Be,0.87952,0.47411,0.19898,0.08909738
f,Be,1.19524565,0.35010419,0.08898933
g,Be,0.56096384

s,Na,2.93474100,0.348607,0.092676,0.011855
p,Na,10.891993,1.200796,0.333449,0.068619,0.011507
d,Na,5.53154400,0.315764,0.144577,0.084987
f,Na,0.71103335,0.26536755,0.04613484
g,Na,2.38269605

s,Mg,3.503953,0.22886,0.058604,0.025465
p,Mg,7.221093,1.504399,0.47977,0.12880066,0.047697
d,Mg,5.746645,0.887913,0.59714,0.133535
f,Mg,0.93180207,0.59297896,0.23387784
g,Mg,0.26609700
```

cc-pVTZ-F12/OptRI ABS in MOLPRO format

```
s,He,6.46673,1.07625,0.358309,0.122283
p,He,11.9956,2.42546,0.734471
d,He,3.17199,1.10760,0.354700
f,He,1.92985,1.11619

s,Li,0.28448946,0.06519006,0.0305793,0.00996085
p,Li,0.79841894,0.24203593,0.06768423,0.02963571
d,Li,0.73694207,0.16729184,0.08472805,0.03983372
f,Li,0.79255996,0.22195881,0.12565437
g,Li,0.62433431,0.29648783

s,Be,1.03892532,0.19312791,0.07216840,0.05547194
p,Be,3.84589935,0.53985952,0.14717917,0.05582622
d,Be,2.46453001,0.35877444,0.13998339,0.07443736
f,Be,1.06630670,0.44277460,0.18965962
g,Be,0.62933243,0.28068029

s,Na,0.30232914,0.22602908,0.04964697,0.01142339
p,Na,3.94497270,0.25779989,0.04569074,0.01977456
d,Na,5.67482245,0.43983751,0.31588449,0.06740995
f,Na,0.49936339,0.31530505,0.09688784
g,Na,0.77760598,0.47393510

s,Mg,0.48655988,0.10847663,0.05235468,0.02354632
p,Mg,6.31735570,0.42386468,0.0939448,0.03107846
d,Mg,3.00269477,0.60919319,0.37947308,0.10102759
f,Mg,1.25890086,0.29360684,0.14189589
g,Mg,0.38133207,0.19731969
```

cc-pVQZ-F12/OptRI ABS in MOLPRO format

```
s,He,12.5145,1.85801,0.670937,0.268516
p,He,30.2470,4.34894,1.84113
d,He,5.21187,1.93819,0.639057
f,He,3.06375,1.67869
g,He,2.94822

s,Li,0.84519851,0.24887901,0.06464998,0.03016188
p,Li,1.08575419,0.22978344,0.10959524,0.04437389
d,Li,2.50692559,1.21899641,0.63754339,0.06943147
f,Li,0.68218478,0.26987366,0.05436959
g,Li,0.78957590,0.25481984
h,Li,0.21463543

s,Be,1.15384757,0.67898278,0.14646294,0.07596445
p,Be,2.67896661,0.86635933,0.33204328,0.13711404
d,Be,3.38315011,0.63133869,0.35848633,0.15290382
f,Be,1.56610939,0.85807551,0.31250307
g,Be,0.44687380,0.21803548
h,Be,0.47374815

s,Na,0.97079353,0.26422634,0.05450489,0.02601365
p,Na,0.97883998,0.40017231,0.17458329,0.07713661
d,Na,6.81892927,1.16461100,0.74720294,0.17791867
f,Na,0.76563613,0.23631495,0.14063583
g,Na,0.26806985,0.20567749
h,Na,0.09191597

s,Mg,1.3130881,0.26079421,0.10029064,0.04875049
p,Mg,1.02459291,0.23225820,0.12188311,0.06297149
d,Mg,3.99886625,1.19738080,0.27279992,0.15272362
f,Mg,1.63724142,0.69313136,0.23268902
g,Mg,0.66770449,0.51247490
h,Mg,0.11896904
```

cc-pCVDZ-F12/OptRI ABS in MOLPRO format

```
s,Li,15.17509777,2.27629359,0.36122030,0.21258866,0.05747471,0.02102723
p,Li,18.83282215,3.16937973,1.62567022,0.32022453,0.10751005,0.03793473,0.01409188
d,Li,1.42956539,0.56424368,0.21190397,0.09176883,0.03499148
f,Li,0.55389765,0.29557321,0.08517342
g,Li,0.26901921

s,Be,12.72683786,3.00400402,0.74518076,0.45954,0.11436,0.02915
p,Be,33.48724006,7.42180522,4.63790195,0.86568855,0.29016,0.09412,0.0323
d,Be,1.99027344,0.87952,0.47411,0.19898,0.08909738
f,Be,1.19524565,0.35010419,0.08898933
g,Be,0.56096384

s,Na,34.30210547,12.82336807,4.97588207,1.04024312,0.76453926,0.348607,0.092676,0.011855
p,Na,15.20670292,11.58758513,8.41498519,1.51726751,0.30447611,0.068619,0.011507
d,Na,35.97947856,10.80171902,2.12444147,0.63777087,0.32037310,0.084987
f,Na,35.74001867,7.51248426,3.03871525,1.18202346,0.26536755,0.04613484
g,Na,6.30941629,2.38269605

s,Mg,54.86887548,17.09236737,6.40692437,1.34457192,0.57504981,0.22886,0.058604,0.025465
p,Mg,38.20161635,13.65211573,7.05255652,1.42906790,0.37710262,0.12880066,0.047697
d,Mg,44.43808838,15.16838205,3.06126512,0.53136456,0.40033273,0.133535
f,Mg,17.14057121,6.91802228,2.52889276,0.89946896,0.59297896,0.23387784
g,Mg,4.52380786,0.26609700
```

cc-pCVTZ-F12/OptRI ABS in MOLPRO format

```
s,Li,5.32014174,3.96841097,1.15425036,0.31568586,0.06519006,0.0305793
p,Li,65.17647685,2.36876713,0.58798837,0.24203593,0.06768423,0.02963571
d,Li,5.86681409,0.72347264,0.16729184,0.08472805,0.03983372
f,Li,3.49747761,2.57794849,0.22195881,0.12565437
g,Li,0.62433431,0.29648783

s,Be,31.35437071,8.37636961,0.81749892,0.19312791,0.07216840,0.05547194
p,Be,71.68891568,10.03357832,1.76491449,0.53985952,0.14717917,0.05582622
d,Be,9.61013957,1.75138118,0.35877444,0.13998339,0.07443736
f,Be,2.09951868,1.53193277,0.44277460,0.18965962
g,Be,0.62933243,0.28068029

s,Na,10.34651204,1.09208073,0.82293668,0.60005545,0.22602908,0.04964697,0.01142339
p,Na,8.19971,1.11017610,0.61342526,0.15729554,0.04569074,0.01977456
d,Na,16.32108597,2.47106841,0.88096037,0.67720946,0.31588449,0.06740995
f,Na,11.87934669,1.88789559,0.85836930,0.31530505,0.09688784
g,Na,3.72805218,0.77760598,0.47393510

s,Mg,12.23975120,4.05859139,1.42346407,0.46634904,0.10847663,0.05235468,0.02354632
p,Mg,17.00676947,6.47534381,1.40743655,0.72059461,0.0939448,0.03107846
d,Mg,28.95152928,5.92033595,4.56563664,1.32762278,0.37947308,0.10102759
f,Mg,16.97918436,4.31399963,2.12534930,0.29360684,0.14189589
g,Mg,5.66143987,0.38133207,0.19731969
```

cc-pCVQZ-F12/OptRI ABS in MOLPRO format

```
s,Li,13.99818948,2.55610184,0.82807401,0.24887901,0.06464998,0.03016188
p,Li,12.27756279,3.30764088,0.61803345,0.22978344,0.10959524,0.04437389
d,Li,4.02331426,1.21899641,0.63754339,0.06943147
f,Li,0.94543889,0.26987366,0.05436959
g,Li,1.51089334,0.25481984
h,Li,0.21463543

s,Be,35.58861903,3.52952138,1.13475333,0.67898278,0.14646294,0.07596445
p,Be,38.75661649,6.47779650,1.46297636,0.86635933,0.33204328,0.13711404
d,Be,3.48665882,0.63133869,0.35848633,0.15290382
f,Be,1.55648295,0.85807551,0.31250307
g,Be,3.83096273,0.44505326
h,Be,0.47374815

s,Na,21.89139508,8.62918230,2.29687162,1.51907687,0.26422634,0.05450489,0.02601365
p,Na,19.19965756,8.77309033,4.66171400,1.43686896,0.40017231,0.17458329,0.07713661
d,Na,23.74159152,11.21798805,2.86290934,1.16826853,0.74720294,0.17791867
f,Na,12.35435289,1.93342144,0.82925753,0.23631495,0.14063583
g,Na,12.26457305,4.43840145,1.64733518,0.20567749
h,Na,0.09191597

s,Mg,17.75246670,9.59932340,2.66522137,1.17902263,0.26079421,0.10029064,0.04875049
p,Mg,21.51156564,8.70805433,2.41851317,0.62259234,0.23225820,0.12188311,0.06297149
d,Mg,34.10600982,18.51880403,3.91486070,1.00574575,0.27279992,0.15272362
f,Mg,12.62735470,7.34923153,1.76411397,0.69313136,0.23268902
g,Mg,13.98315355,1.01056986,0.66657587,0.51247490
h,Mg,0.11896904
```

cc-pV5Z/MP2FIT ABS in MOLPRO format

```
s,Na,400.873,74.4967,36.4625,10.7936,5.29936,1.93777,1.01712,0.414619,0.22435,0.136222,0.0806265,0.0473961
p,Na,93.4239,25.3469,8.52195,3.87851,2.13627,1.02399,0.437132,0.223328,0.140095,0.0951487,0.0559091
d,Na,32.4304,9.71975,3.46822,1.55938,0.540694,0.288717,0.170367,0.115665,0.0740876
f,Na,5.41015,1.87207,0.920046,0.457874,0.285729,0.176785,0.105124
g,Na,2.00507,0.833273,0.446755,0.245535,0.122323
h,Na,1.09862,0.513689,0.260977
i,Na,0.682035
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aug-cc-pVDZ/MP2FIT ABS in MOLPRO format

```
s,Li,30.4075,7.58805,2.5668,0.787336,0.345354,0.160474,0.0923455,0.0130916
p,Li,6.71598,2.33264,0.772809,0.183739,0.0783946,0.0200254
d,Li,1.49284,0.575267,0.241521,0.142015,0.0888708
f,Li,1.61775,0.361631,0.200382

s,Be,41.8746,8.51217,3.10685,1.0695,0.43143,0.213349,0.124175,0.060234
p,Be,9.76007,2.64058,0.788905,0.316492,0.126019,0.0556308
d,Be,2.31369,0.700086,0.353642,0.170008,0.114965
f,Be,2.02219,0.452039,0.363516

s,Na,159.646,35.0886,9.68068,5.65459,1.83236,0.640241,0.329007,0.130603,0.0504624,0.0125190
p,Na,51.3091,5.34079,1.72797,0.908608,0.410309,0.102451,0.0616833,0.0141438
d,Na,16.944,4.70522,1.08925,0.528614,0.155416,0.0585937
f,Na,2.31497,0.682956,0.27357,0.149747

s,Mg,200.427,44.0693,11.9447,6.90059,2.30732,0.79142,0.442013,0.194707,0.0832303,0.0400543
p,Mg,59.6825,9.00677,3.761,1.17635,0.594066,0.210529,0.0895356,0.0367681
d,Mg,22.3994,6.43683,1.18113,0.749498,0.259159,0.108646
f,Mg,2.891,0.928774,0.326783,0.180059
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aug-cc-pVTZ/MP2FIT ABS in MOLPRO format

```
s,Li,98.0209,20.4906,6.23005,1.97995,0.81248,0.302821,0.132817,0.0687151,0.0133628
p,Li,9.98153,2.74212,0.995132,0.455449,0.190615,0.0859203,0.0232973
d,Li,3.90895,0.950364,0.273703,0.148839,0.0746477,0.0641678
f,Li,0.979494,0.362171,0.182526,0.0942062
g,Li,0.300000,0.160856

s,Be,115.41,27.4201,8.95789,3.30036,1.07939,0.450645,0.186293,0.102049,0.0591756
p,Be,12.9585,3.56324,1.15263,0.550086,0.2445,0.107562,0.0555035
d,Be,5.02291,1.698,0.488912,0.265357,0.100698,0.072884
f,Be,1.67053,0.452696,0.254672,0.150785
g,Be,0.500000,0.339542

s,Na,262.945,59.3272,24.4106,10.3153,3.82467,1.21138,0.626025,0.231136,0.099616,0.0608538,0.0116721
p,Na,45.9602,5.92673,2.44801,1.25173,0.555056,0.323653,0.131738,0.0679466,0.0192736
d,Na,23.7262,7.20337,2.54853,0.965966,0.423426,0.250862,0.102838,0.0314073
f,Na,3.71955,1.16754,0.529388,0.265125,0.146659,0.0877992
g,Na,1.44688,0.514372,0.248868

s,Mg,247.482,82.3065,31.8882,12.3628,4.99341,1.70781,0.790449,0.275153,0.123443,0.0771233,0.0349975
p,Mg,58.6402,7.1768,3.49873,1.51822,0.806848,0.326559,0.15472,0.0724774,0.0347277
d,Mg,29.9212,9.11394,3.17149,1.48838,0.572001,0.392816,0.18472,0.0841238
f,Mg,4.60912,1.54347,0.64499,0.334225,0.174575,0.110939
g,Mg,1.76455,0.717219,0.291521
```

aug-cc-pVQZ/MP2FIT ABS in MOLPRO format

```
s,Li,109.055,20.8783,6.48699,1.9545,1.04023,0.429079,0.161718,0.0829282,0.0170155
p,Li,17.5494,5.44422,1.87561,0.775204,0.371484,0.163201,0.076565,0.022329
d,Li,6.80179,2.21726,1.0076,0.497801,0.202532,0.11806,0.0350788
f,Li,2.78579,1.03442,0.532421,0.277415,0.11709,0.0724729
g,Li,0.973573,0.413563,0.203462,0.137078
h,Li,0.428565,0.167003

s,Be,136.646,28.3921,8.68918,3.7802,1.16278,0.430644,0.18601,0.0973907,0.0453197
p,Be,22.2394,6.38157,2.5546,1.01598,0.444495,0.201832,0.0948127,0.0445393
d,Be,8.49613,3.04272,1.18451,0.584073,0.278041,0.162619,0.0814135
f,Be,3.40182,1.48135,0.623318,0.344031,0.140547,0.0727809
g,Be,1.86007,0.53622,0.272843,0.148535
h,Be,0.535704,0.3825

s,Na,214.738,48.6437,16.3062,9.60658,3.49236,1.31021,0.608485,0.352171,0.185033,0.0882043,0.0506201,
0.0106701
p,Na,67.8947,25.5016,6.26963,2.29751,1.32529,0.534763,0.280666,0.139646,0.0670942,0.0184038
d,Na,29.3304,8.491,3.17181,1.40043,0.717681,0.407893,0.269587,0.121099,0.0316729
f,Na,4.8028,2.1908,0.838895,0.358626,0.215661,0.117546,0.0600729
g,Na,1.36508,0.578782,0.297583,0.0983548
h,Na,0.648943,0.298253

s,Mg,265.858,65.1123,23.5047,11.5247,4.82385,1.95043,0.74041,0.429062,0.228177,0.126216,0.066462,0.0349955
p,Mg,72.0405,45.366,6.73673,2.25791,1.14991,0.348795,0.208905,0.106035,0.0588464,0.0265578
d,Mg,35.2442,10.9473,3.99744,2.10185,1.00886,0.467248,0.268153,0.155964,0.0685515
f,Mg,5.8836,2.84658,1.31819,0.439446,0.25776,0.129503,0.0646084
g,Mg,2.67583,1.09711,0.384743,0.18191
h,Mg,1.0598,0.649696
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aug-cc-pV5Z/MP2FIT ABS in MOLPRO format

```
s,Li,115.553,24.2286,7.79537,2.89136,1.42394,0.705917,0.380123,0.246901,0.123532,0.0642881,0.0122985
p,Li,20.0939,6.08149,2.34726,1.02995,0.52019,0.223276,0.121261,0.0727775,0.0187707
d,Li,6.96358,2.68153,1.35163,0.771893,0.339644,0.173452,0.101078,0.0296694
f,Li,3.22949,1.34929,0.76464,0.415519,0.25928,0.156013,0.0497839
g,Li,1.81964,0.856517,0.43491,0.196188,0.0843501
h,Li,1.18528,0.598672,0.427119,0.146929
i,Li,0.598672,0.253741

s,Be,155.476,33.6165,9.86575,5.18723,2.04825,0.941824,0.494373,0.304521,0.168188,0.0908364,0.0490966
p,Be,29.2263,8.19087,3.2447,1.27464,0.594885,0.289372,0.148487,0.0785465,0.0425786
d,Be,9.7761,3.81802,1.73383,0.897386,0.453927,0.238389,0.136955,0.0725133
f,Be,4.09104,1.76139,0.874992,0.497082,0.330842,0.205294,0.138098
g,Be,2.35614,0.727039,0.51533,0.380351,0.160344
h,Be,1.50462,0.672211,0.511708,0.275472
i,Be,0.672211,0.357670

s,Na,400.873,74.4967,36.4625,10.7936,5.29936,1.93777,1.01712,0.414619,0.22435,0.136222,0.0806265,0.0473961,
0.00920948
p,Na,93.4239,25.3469,8.52195,3.87851,2.13627,1.02399,0.437132,0.223328,0.140095,0.0951487,0.0559091,
0.0148607
d,Na,32.4304,9.71975,3.46822,1.55938,0.540694,0.288717,0.170367,0.115665,0.0740876,0.031284
f,Na,5.41015,1.87207,0.920046,0.457874,0.285729,0.176785,0.105124,0.0490626
g,Na,2.00507,0.833273,0.446755,0.245535,0.122323,0.100353
h,Na,1.09862,0.513689,0.260977,0.125079
i,Na,0.682035,0.248199

s,Mg,540.416,102.127,43.1114,13.4767,7.37556,2.6068,1.29897,0.584075,0.330108,0.180505,0.119148,0.0691447,
0.0401233
p,Mg,123.479,33.4832,12.3366,5.61338,2.42395,1.15789,0.531815,0.293408,0.194135,0.130156,0.0845925,0.054956
d,Mg,28.3542,8.2488,2.95615,1.2873,0.58346,0.344419,0.22243,0.151929,0.09125,0.0548064
f,Mg,6.95067,2.76214,1.25072,0.575997,0.334257,0.216355,0.12609,0.0734838
g,Mg,2.5501,1.0726,0.552581,0.30805,0.146581,0.0697491
h,Mg,1.51258,0.45792,0.292537,0.196604
i,Mg,1.07457,0.769869
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aug-cc-pwCVDZ/MP2FIT ABS in MOLPRO format

```
s,Li,99.9253,30.4075,14.9763,7.58805,3.98647,2.5668,0.787336,0.345354,0.160474,0.0923455,0.0130916
p,Li,24.0101,6.71598,3.99706,2.33264,0.772809,0.183739,0.0783946,0.0200254
d,Li,3.87398,1.49284,0.575267,0.241521,0.142015,0.0888708
f,Li,1.61775,0.361631,0.200382

s,Be,142.716,41.8746,21.4043,8.51217,4.30354,3.10685,1.0695,0.43143,0.213349,0.124175,0.060234
p,Be,35.6755,9.76007,4.21747,2.64058,0.788905,0.316492,0.126019,0.0556308
d,Be,4.2173,2.31369,0.700086,0.353642,0.170008,0.114965
f,Be,2.02219,0.452039,0.363516

s,Na,294.906,159.646,55.518,35.0886,15.3653,9.68068,5.65459,1.83236,0.640241,0.329007,0.130603,0.0504624,
0.0125190
p,Na,109.933,51.3091,18.6641,5.34079,3.13814,1.72797,0.908608,0.410309,0.102451,0.0616833,0.0141438
d,Na,28.5633,16.944,8.94061,4.70522,2.08557,1.08925,0.528614,0.155416,0.0585937
f,Na,6.12765,2.31497,1.17888,0.682956,0.27357,0.149747

s,Mg,406.591,200.427,100.478,44.0693,22.107,11.9447,6.90059,2.30732,0.79142,0.442013,0.194707,0.0832303,
0.0400543
p,Mg,127.033,59.6825,19.5551,9.00677,5.11369,3.761,1.17635,0.594066,0.210529,0.0895356,0.0367681
d,Mg,31.8814,22.3994,10.2021,6.43683,2.43961,1.18113,0.749498,0.259159,0.108646
f,Mg,7.40658,2.891,0.928774,0.601439,0.326783,0.180059
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aug-cc-pwCVTZ/MP2FIT ABS in MOLPRO format

```
s,Li,224.500,98.0209,42.7996,20.4906,9.80609,6.23005,1.97995,1.32156,0.81248,0.302821,0.132817,0.0687151,
0.0133628
p,Li,28.4029,9.98153,5.34928,2.74212,1.4928,0.995132,0.455449,0.190615,0.0859203,0.0232973
d,Li,8.86060,3.90895,1.71086,0.950364,0.273703,0.148839,0.0746477,0.0641678
f,Li,2.64905,0.979494,0.362171,0.182526,0.0942062
g,Li,0.300000,0.160856

s,Be,249.463,115.41,46.1748,27.4201,12.0268,8.95789,3.30036,1.74388,1.07939,0.450645,0.186293,0.102049,
0.0591756
p,Be,33.2632,12.9585,6.65163,3.56324,2.10073,1.15263,0.550086,0.2445,0.107562,0.0555035
d,Be,11.6407,5.02291,2.88642,1.698,0.488912,0.265357,0.100698,0.072884
f,Be,3.32571,1.67053,0.452696,0.254672,0.150785
g,Be,0.500000,0.339542

s,Na,486.432,262.945,149.620,59.3272,24.4106,13.8553,10.3153,3.82467,2.02943,1.21138,0.626025,0.231136,
0.099616,0.0608538,0.0116721
p,Na,121.060,45.9602,24.3319,11.7584,5.92673,3.16342,2.44801,1.25173,0.555056,0.323653,0.131738,0.0679466,
0.0192736
d,Na,38.8902,23.7262,13.9795,7.20337,4.87595,2.54853,0.965966,0.423426,0.250862,0.102838,0.0314073
f,Na,8.74658,3.71955,2.443545,1.16754,0.529388,0.265125,0.146659,0.0877992
g,Na,5.48634,1.44688,0.514372,0.248868

s,Mg,515.399,247.482,138.454,82.3065,47.6771,31.8882,17.9990,12.3628,4.99341,1.70781,0.790449,0.275153,
0.123443,0.0771233,0.0349975
p,Mg,145.327,58.6402,30.6960,16.3965,7.1768,3.49873,2.11780,1.51822,0.806848,0.326559,0.15472,0.0724774,
0.0347277
d,Mg,61.9729,29.9212,16.2135,9.11394,5.57856,3.17149,1.48838,0.572001,0.392816,0.18472,0.0841238
f,Mg,11.0847,4.60912,3.30483,1.54347,0.64499,0.334225,0.174575,0.110939
g,Mg,3.84017,1.76455,0.717219,0.291521
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aug-cc-pwCVQZ/MP2FIT ABS in MOLPRO format

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s,Li,353.892,109.055,64.9667,20.8783,13.6826,6.48699,4.22075,1.9545,1.04023,0.429079,0.161718,0.0829282,
0.0170155
p,Li,69.5061,25.7524,17.5494,7.76894,5.44422,3.65992,1.87561,0.775204,0.371484,0.163201,0.076565,0.022329
d,Li,22.2298,10.4756,6.80179,4.50953,2.21726,1.0076,0.497801,0.202532,0.11806,0.0350788
f,Li,4.41399,2.78579,1.81962,1.03442,0.532421,0.277415,0.11709,0.0724729
g,Li,4.36658,0.973573,0.413563,0.203462,0.137078
h,Li,0.428565,0.167003

s,Be,479.978,136.646,58.3449,28.3921,15.5143,8.68918,4.21824,3.7802,1.16278,0.430644,0.18601,0.0973907,
0.0453197
p,Be,106.326,48.6208,22.2394,13.2640,6.38157,4.19726,2.5546,1.01598,0.444495,0.201832,0.0948127,0.0445393
d,Be,53.8212,20.6066,8.49613,5.36850,3.04272,1.18451,0.584073,0.278041,0.162619,0.0814135
f,Be,12.0828,4.52273,3.40182,1.48135,0.623318,0.344031,0.140547,0.0727809
g,Be,6.45232,1.86007,0.53622,0.272843,0.148535
h,Be,0.535704,0.3825

s,Na,609.215,214.738,98.3291,48.6437,28.3770,16.3062,9.60658,2.58893,3.49236,1.31021,0.608485,0.352171,
0.185033,0.0882043,0.0506201,0.0106701
p,Na,200.293,67.8947,25.5016,16.2568,9.43552,6.26963,2.87851,2.29751,1.32529,0.534763,0.280666,0.139646,
0.0670942,0.0184038
d,Na,57.8740,29.3304,12.6688,8.491,3.54451,3.17181,1.40043,0.717681,0.407893,0.269587,0.121099,0.0316729
f,Na,17.0121,7.89065,4.8028,2.1908,1.51538,0.838895,0.358626,0.215661,0.117546,0.0600729
g,Na,11.2370,5.74341,2.31628,1.36508,0.578782,0.297583,0.0983548
h,Na,9.86624,5.61323,0.648943,0.298253

s,Mg,703.635,265.858,74.0329,65.1123,44.3085,23.5047,11.5247,8.174275,4.82385,1.95043,0.74041,0.429062,
0.228177,0.126216,0.066462,0.0349955
p,Mg,223.939,72.0405,45.366,21.3035,10.9998,6.73673,2.99693,2.25791,1.14991,0.348795,0.208905,0.106035,
0.0588464,0.0265578
d,Mg,69.3680,35.2442,19.4010,10.9473,5.97030,3.99744,2.10185,1.00886,0.467248,0.268153,0.155964,0.0685515
f,Mg,21.9202,11.1046,5.8836,2.84658,2.28141,1.31819,0.439446,0.25776,0.129503,0.0646084
g,Mg,13.4222,7.31963,2.67583,1.46206,1.09711,0.384743,0.18191
h,Mg,5.10463,2.44242,1.0598,0.649696
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aug-cc-pwCV5Z/MP2FIT ABS in MOLPRO format

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s,Li,499.975,115.553,49.8112,24.2286,14.4799,7.79537,4.74962,2.89136,1.42394,0.705917,0.380123,0.246901,
0.123532,0.0642881,0.0122985
p,Li,40.3767,20.0939,12.0087,6.08149,4.19963,2.34726,1.59978,1.02995,0.52019,0.223276,0.121261,0.0727775,
0.0187707
d,Li,44.9679,24.3192,14.3724,6.96358,4.16211,2.68153,1.35163,0.771893,0.339644,0.173452,0.101078,0.0296694
f,Li,22.9007,10.5581,5.31933,3.22949,1.34929,0.76464,0.415519,0.25928,0.156013,0.0497839
g,Li,6.46499,3.53875,1.81964,0.856517,0.43491,0.196188,0.0843501
h,Li,2.60102,1.18528,0.598672,0.427119,0.146929
i,Li,0.598672,0.253741

s,Be,692.470,155.476,64.8482,33.6165,24.6783,9.86575,6.20800,5.18723,2.04825,0.941824,0.494373,0.304521,
0.168188,0.0908364,0.0490966
p,Be,66.2143,29.2263,19.7040,8.19087,6.13730,3.2447,2.11521,1.27464,0.594885,0.289372,0.148487,0.0785465,
0.0425786
d,Be,55.2100,30.8319,17.3608,9.7761,6.18372,3.81802,1.73383,0.897386,0.453927,0.238389,0.136955,0.0725133
f,Be,30.7915,19.2209,6.44691,4.09104,1.76139,0.874992,0.497082,0.330842,0.205294,0.138098
g,Be,8.01931,3.92822,2.35614,0.727039,0.51533,0.380351,0.160344
h,Be,3.36781,1.50462,0.672211,0.511708,0.275472
i,Be,0.672211,0.357670

s,Na,955.488,400.873,166.641,74.4967,36.4625,14.9579,10.7936,5.29936,2.71610,1.93777,1.01712,0.414619,
0.224350,0.136222,0.0806265,0.0473961,0.00920948
p,Na,406.554,93.4239,42.8202,25.3469,13.2957,8.52195,3.87851,2.91225,2.13627,1.02399,0.437132,0.223328,
0.140095,0.0951487,0.0559091,0.0148607
d,Na,106.059,32.4304,14.9817,9.71975,4.81039,3.46822,1.55938,1.02764,0.540694,0.288717,0.170367,0.115665,
0.0740876,0.031284
f,Na,22.9370,8.68901,5.41015,3.58510,1.87207,0.920046,0.457874,0.285729,0.176785,0.105124,0.0490626
g,Na,12.3596,6.52564,3.44004,2.00507,0.833273,0.446755,0.245535,0.122323,0.100353
h,Na,7.54404,2.50072,1.09862,0.513689,0.260977,0.125079
i,Na,9.71738,6.35811,0.682035,0.248199

s,Mg,1204.16,540.416,221.088,102.127,43.1114,24.5418,13.4767,7.37556,4.25461,2.6068,1.29897,0.584075,
0.330108,0.180505,0.119148,0.0691447,0.0401233
p,Mg,433.198,123.479,41.7765,33.4832,22.9099,12.3366,8.97499,5.61338,2.42395,1.15789,0.531815,0.293408,
0.194135,0.130156,0.0845925,0.054956
d,Mg,81.7514,28.3542,19.8185,10.1999,8.2488,2.95615,1.94982,1.2873,0.58346,0.344419,0.22243,0.151929,
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0.09125,0.0548064
f,Mg,31.8104,12.8760,6.95067,4.34398,2.76214,1.25072,0.575997,0.334257,0.216355,0.12609,0.0734838
g,Mg,16.3225,8.72565,5.06665,2.5501,1.0726,0.552581,0.30805,0.146581,0.0697491
h,Mg,10.4401,2.96262,1.51258,0.45792,0.292537,0.196604
i,Mg,5.97088,2.57957,1.07457,0.769869
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cc-pwCVDZ/MP2FIT ABS in MOLPRO format

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s,Li,99.9253,30.4075,14.9763,7.58805,3.98647,2.5668,0.787336,0.345354,0.160474,0.0923455
p,Li,24.0101,6.71598,3.99706,2.33264,0.772809,0.183739,0.0783946
d,Li,3.87398,1.49284,0.575267,0.241521,0.142015
f,Li,1.61775,0.361631

s,Be,142.716,41.8746,21.4043,8.51217,4.30354,3.10685,1.0695,0.43143,0.213349,0.124175
p,Be,35.6755,9.76007,4.21747,2.64058,0.788905,0.316492,0.126019
d,Be,4.2173,2.31369,0.700086,0.353642,0.170008
f,Be,2.02219,0.452039

s,Na,294.906,159.646,55.518,35.0886,15.3653,9.68068,5.65459,1.83236,0.640241,0.329007,0.130603,0.0504624
p,Na,109.933,51.3091,18.6641,5.34079,3.13814,1.72797,0.908608,0.410309,0.102451,0.0616833
d,Na,28.5633,16.944,8.94061,4.70522,2.08557,1.08925,0.528614,0.155416
f,Na,6.12765,2.31497,1.17888,0.682956,0.27357

s,Mg,406.591,200.427,100.478,44.0693,22.107,11.9447,6.90059,2.30732,0.79142,0.442013,0.194707,0.0832303
p,Mg,127.033,59.6825,19.5551,9.00677,5.11369,3.761,1.17635,0.594066,0.210529,0.0895356
d,Mg,31.8814,22.3994,10.2021,6.43683,2.43961,1.18113,0.749498,0.259159
f,Mg,7.40658,2.891,0.928774,0.601439,0.326783
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cc-pwCVTZ/MP2FIT ABS in MOLPRO format

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s,Li,224.500,98.0209,42.7996,20.4906,9.80609,6.23005,1.97995,1.32156,0.81248,0.302821,0.132817,0.0687151
p,Li,28.4029,9.98153,5.34928,2.74212,1.4928,0.995132,0.455449,0.190615,0.0859203
d,Li,8.86060,3.90895,1.71086,0.950364,0.273703,0.148839,0.0746477
f,Li,2.64905,0.979494,0.362171,0.182526
g,Li,0.300000

s,Be,249.463,115.41,46.1748,27.4201,12.0268,8.95789,3.30036,1.74388,1.07939,0.450645,0.186293,0.102049
p,Be,33.2632,12.9585,6.65163,3.56324,2.10073,1.15263,0.550086,0.2445,0.107562
d,Be,11.6407,5.02291,2.88642,1.698,0.488912,0.265357,0.100698
f,Be,3.32571,1.67053,0.452696,0.254672
g,Be,0.500000

s,Na,486.432,262.945,149.620,59.3272,24.4106,13.8553,10.3153,3.82467,2.02943,1.21138,0.626025,0.231136,
0.099616,0.0608538
p,Na,121.060,45.9602,24.3319,11.7584,5.92673,3.16342,2.44801,1.25173,0.555056,0.323653,0.131738,0.0679466
d,Na,38.8902,23.7262,13.9795,7.20337,4.87595,2.54853,0.965966,0.423426,0.250862,0.102838
f,Na,8.74658,3.71955,2.443545,1.16754,0.529388,0.265125,0.146659
g,Na,5.48634,1.44688,0.514372

s,Mg,515.399,247.482,138.454,82.3065,47.6771,31.8882,17.9990,12.3628,4.99341,1.70781,0.790449,0.275153,
0.123443,0.0771233
p,Mg,145.327,58.6402,30.6960,16.3965,7.1768,3.49873,2.11780,1.51822,0.806848,0.326559,0.15472,0.0724774
d,Mg,61.9729,29.9212,16.2135,9.11394,5.57856,3.17149,1.48838,0.572001,0.392816,0.18472
f,Mg,11.0847,4.60912,3.30483,1.54347,0.64499,0.334225,0.174575
g,Mg,3.84017,1.76455,0.717219
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cc-pwCVQZ/MP2FIT ABS in MOLPRO format

```
s,Li,353.892,109.055,64.9667,20.8783,13.6826,6.48699,4.22075,1.9545,1.04023,0.429079,0.161718,0.0829282
p,Li,69.5061,25.7524,17.5494,7.76894,5.44422,3.65992,1.87561,0.775204,0.371484,0.163201,0.076565
d,Li,22.2298,10.4756,6.80179,4.50953,2.21726,1.0076,0.497801,0.202532,0.11806
f,Li,4.41399,2.78579,1.81962,1.03442,0.532421,0.277415,0.11709
g,Li,4.36658,0.973573,0.413563,0.203462
h,Li,0.428565

s,Be,479.978,136.646,58.3449,28.3921,15.5143,8.68918,4.21824,3.7802,1.16278,0.430644,0.18601,0.0973907
p,Be,106.326,48.6208,22.2394,13.2640,6.38157,4.19726,2.5546,1.01598,0.444495,0.201832,0.0948127
d,Be,53.8212,20.6066,8.49613,5.36850,3.04272,1.18451,0.584073,0.278041,0.162619
f,Be,12.0828,4.52273,3.40182,1.48135,0.623318,0.344031,0.140547
g,Be,6.45232,1.86007,0.53622,0.272843
h,Be,0.535704

s,Na,609.215,214.738,98.3291,48.6437,28.3770,16.3062,9.60658,2.58893,3.49236,1.31021,0.608485,0.352171,
0.185033,0.0882043,0.0506201
p,Na,200.293,67.8947,25.5016,16.2568,9.43552,6.26963,2.87851,2.29751,1.32529,0.534763,0.280666,0.139646,
0.0670942
d,Na,57.8740,29.3304,12.6688,8.491,3.54451,3.17181,1.40043,0.717681,0.407893,0.269587,0.121099
f,Na,17.0121,7.89065,4.8028,2.1908,1.51538,0.838895,0.358626,0.215661,0.117546
g,Na,11.2370,5.74341,2.31628,1.36508,0.578782,0.297583
h,Na,9.86624,5.61323,0.648943

s,Mg,703.635,265.858,74.0329,65.1123,44.3085,23.5047,11.5247,8.174275,4.82385,1.95043,0.74041,0.429062,
0.228177,0.126216,0.066462
p,Mg,223.939,72.0405,45.366,21.3035,10.9998,6.73673,2.99693,2.25791,1.14991,0.348795,0.208905,0.106035,
0.0588464
d,Mg,69.3680,35.2442,19.4010,10.9473,5.97030,3.99744,2.10185,1.00886,0.467248,0.268153,0.155964
f,Mg,21.9202,11.1046,5.8836,2.84658,2.28141,1.31819,0.439446,0.25776,0.129503
g,Mg,13.4222,7.31963,2.67583,1.46206,1.09711,0.384743
h,Mg,5.10463,2.44242,1.0598
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cc-pwCV5Z/MP2FIT ABS in MOLPRO format

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s,Li,499.975,115.553,49.8112,24.2286,14.4799,7.79537,4.74962,2.89136,1.42394,0.705917,0.380123,0.246901,
0.123532,0.0642881
p,Li,40.3767,20.0939,12.0087,6.08149,4.19963,2.34726,1.59978,1.02995,0.52019,0.223276,0.121261,0.0727775
d,Li,44.9679,24.3192,14.3724,6.96358,4.16211,2.68153,1.35163,0.771893,0.339644,0.173452,0.101078
f,Li,22.9007,10.5581,5.31933,3.22949,1.34929,0.76464,0.415519,0.25928,0.156013
g,Li,6.46499,3.53875,1.81964,0.856517,0.43491,0.196188
h,Li,2.60102,1.18528,0.598672,0.427119
i,Li,0.598672

s,Be,692.470,155.476,64.8482,33.6165,24.6783,9.86575,6.20800,5.18723,2.04825,0.941824,0.494373,0.304521,
0.168188,0.0908364
p,Be,66.2143,29.2263,19.7040,8.19087,6.13730,3.2447,2.11521,1.27464,0.594885,0.289372,0.148487,0.0785465
d,Be,55.2100,30.8319,17.3608,9.7761,6.18372,3.81802,1.73383,0.897386,0.453927,0.238389,0.136955
f,Be,30.7915,19.2209,6.44691,4.09104,1.76139,0.874992,0.497082,0.330842,0.205294
g,Be,8.01931,3.92822,2.35614,0.727039,0.51533,0.380351
h,Be,3.36781,1.50462,0.672211,0.511708
i,Be,0.672211

s,Na,955.488,400.873,166.641,74.4967,36.4625,14.9579,10.7936,5.29936,2.71610,1.93777,1.01712,0.414619,
0.224350,0.136222,0.0806265,0.0473961
p,Na,406.554,93.4239,42.8202,25.3469,13.2957,8.52195,3.87851,2.91225,2.13627,1.02399,0.437132,0.223328,
0.140095,0.0951487,0.0559091
d,Na,106.059,32.4304,14.9817,9.71975,4.81039,3.46822,1.55938,1.02764,0.540694,0.288717,0.170367,0.115665,
0.0740876
f,Na,22.9370,8.68901,5.41015,3.58510,1.87207,0.920046,0.457874,0.285729,0.176785,0.105124
g,Na,12.3596,6.52564,3.44004,2.00507,0.833273,0.446755,0.245535,0.122323
h,Na,7.54404,2.50072,1.09862,0.513689,0.260977
i,Na,9.71738,6.35811,0.682035

s,Mg,1204.16,540.416,221.088,102.127,43.1114,24.5418,13.4767,7.37556,4.25461,2.6068,1.29897,0.584075,
0.330108,0.180505,0.119148,0.0691447
p,Mg,433.198,123.479,41.7765,33.4832,22.9099,12.3366,8.97499,5.61338,2.42395,1.15789,0.531815,0.293408,
0.194135,0.130156,0.0845925
d,Mg,81.7514,28.3542,19.8185,10.1999,8.2488,2.95615,1.94982,1.2873,0.58346,0.344419,0.22243,0.151929,
0.09125
f,Mg,31.8104,12.8760,6.95067,4.34398,2.76214,1.25072,0.575997,0.334257,0.216355,0.12609
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g,Mg,16.3225,8.72565,5.06665,2.5501,1.0726,0.552581,0.30805,0.146581
h,Mg,10.4401,2.96262,1.51258,0.45792,0.292537
i,Mg,5.97088,2.57957,1.07457
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