Supplementary Data

Optimization of RI-MP2 auxiliary basis functions for 6-31G** and 6-311G** basis sets

for first-, second-, and third-row elements

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Table S1. Exponents of auxiliary basis functions optimized for the 6-31G** basis set[a]

type	H	He	Li	Be	B	C	N	O	F	Ne
s	13.087376	19.248269	44.408083	125.555856	143.984140	120.498651	151.440439	327.922894	573.951315	342.098276
	1.185515	3.746353	12.013820	32.426072	44.596243	45.116782	59.396988	103.186715	168.382717	110.242196
	0.368163	0.729165	3.250126	8.374361	13.812805	16.892505	23.296302	32.469517	49.399206	35.525879
			0.879264	2.162764	4.278244	6.324846	9.137125	10.217106	14.492471	11.448321
			0.237869	0.558556	1.325101	2.368132	3.583704	3.214992	4.251722	3.689256
			0.064351	0.144253	0.410424	0.886670	1.405577	1.011654	1.247347	1.188874
p	2.288385	4.523992	2.289800	4.997162	8.590813	13.216186	20.411097	24.005447	28.763485	33.148687
	1.311828	1.648567	0.708943	1.599968	2.638957	3.884909	5.431907	6.308031	7.280992	7.457743
			0.219495	0.512270	0.810644	1.141972	1.445567	1.657593	1.843060	1.677832
			0.067958	0.164016	0.249017	0.335684	0.384702	0.435574	0.466540	0.377476
d	1.875349	1.472906	0.641872	1.479514	2.746101	3.750089	4.255896	5.263808	7.084925	9.258256
			0.340209	0.508390	0.854346	1.207332	1.417789	1.743135	2.352044	2.997447
			0.180320	0.174693	0.265798	0.388698	0.472315	0.577247	0.780828	0.970451
f			0.235054	0.607087	0.911700	1.344106	1.485662	1.582739	1.686449	1.790922
g			0.299999	0.518946	0.637363	0.769479	0.979199	1.297901	1.287498	0.921868

Table S1. (continued)

type	Na	Mg	Al	Si	P	S	Cl	Ar
s	86.336180	184.332273	133.983279	222.876013	635.975307	345.597110	383.876581	397.702742
	24.398958	42.424145	28.607331	72.405071	180.513806	106.894156	118.767601	126.437368
	6.895246	9.763933	6.108071	23.522021	51.236634	33.062662	36.745516	40.196877
	1.948625	2.247173	1.304160	7.641529	14.542891	10.226374	11.368698	12.779362
	0.550689	0.517188	0.278457	2.482481	4.127822	3.163046	3.517362	4.062806
	0.155627	0.119031	0.059454	0.806476	1.171632	0.978339	1.088237	1.291644
	0.043981	0.027395	0.012694	0.261998	0.332553	0.302603	0.336690	0.410639
p	1.902174	1.822390	38.467497	45.746892	55.706954	63.546100	77.779577	10.054096
	0.762683	0.684182	9.079408	11.227286	13.878548	16.023875	19.576299	4.456528
	0.305800	0.256863	2.142995	2.755421	3.457631	4.040603	4.927148	1.975378
	0.122611	0.096435	0.505807	0.676240	0.861417	1.018884	1.240111	0.875596
	0.049161	0.036205	0.119385	0.165964	0.214609	0.256923	0.312123	0.388112
d	13.224919	6.491104	15.604294	12.961918	15.725920	17.787941	20.131474	22.797455
	3.418644	2.048807	4.762967	2.810770	3.522654	4.170908	4.909666	5.770279
	0.883720	0.646671	1.453821	0.609511	0.789085	0.977993	1.197370	1.460519
	0.228442	0.204111	0.443756	0.132171	0.176758	0.229319	0.292015	0.369673
f	2.682661	2.667018	1.867749	2.584156	3.353072	3.895639	4.997096	5.915528
	0.645994	0.237331	0.413588	0.628890	0.814023	1.017971	1.195450	1.371509
g	0.214407	0.212396	0.308735	0.532589	0.624289	0.693729	0.830367	1.588712

[a] No auxiliary basis function is contracted, i.e. contraction coefficients are 1.0.

Table S2. Exponents of auxiliary basis functions optimized for the 6-311G** basis set[a]

type	H	He	Li	Be	B	C	N	O	F	Ne
s	8.818862	16.99693	39.425059	55.535690	127.537268	170.836443	336.104794	569.712517	753.094295	388.358977
	1.986986	5.210089	8.105551	21.676359	27.013690	44.874653	64.951756	96.705444	126.498813	134.190741
	0.576353	1.597055	2.078955	8.460587	7.184714	13.663231	15.830335	21.215821	27.514137	46.367294
	0.266483	0.489547	0.660358	3.302286	2.385215	4.747730	4.841886	6.024881	7.765555	16.021418
			0.252811	1.288928	0.962511	1.834876	1.810679	2.166607	2.783462	5.535925
			0.110380	0.503087	0.446087	0.760324	0.781529	0.927309	1.190549	1.912843
			0.050561	0.196362	0.217512	0.322826	0.355601	0.423752	0.544295	0.660950
p	2.124511	3.647386	3.269739	5.767863	11.640290	18.302316	25.589469	35.115268	45.832633	60.124512
	1.021228	1.23071	1.097371	2.123635	4.155040	6.516678	9.152577	12.364373	16.018072	20.812645
			0.368294	0.781889	1.483155	2.320313	3.273600	4.353597	5.598165	7.204486
			0.123605	0.287879	0.529417	0.826165	1.170867	1.532937	1.956506	2.493898
			0.041483	0.105992	0.188977	0.294162	0.418784	0.539760	0.683780	0.863285
d	1.404201	0.325685	0.758916	0.954831	2.795844	3.666356	5.024607	6.814857	8.851759	10.818027
			0.267187	0.347948	0.734371	0.949403	1.300811	1.740326	2.282026	3.053121
			0.094067	0.126795	0.513776	0.496685	0.476812	0.644186	0.792351	0.861668
f			0.295338	0.452052	0.717054	1.116969	1.616769	2.293055	3.085941	4.039873
g			0.315668	0.502136	0.536060	0.790582	1.054812	1.246127	1.206853	0.161682

Table S2. (continued)

type	Na	Mg	Al	Si	P	S	Cl	Ar
s	246.374077	271.623196	414.931287	165.788833	162.477869	288.508216	215.291479	253.252499
	72.280470	83.934136	92.599596	62.778013	64.535636	90.942288	73.788479	86.188808
	21.205422	25.936442	24.010599	23.771679	25.633327	28.666427	25.290084	29.332428
	6.221182	8.014606	7.176302	9.001443	10.181467	9.036105	8.667862	9.982634
	1.825151	2.476589	2.433856	3.408509	4.044043	2.848321	2.970802	3.397366
	0.535457	0.765289	0.913350	1.290674	1.606280	0.897835	1.018205	1.156217
	0.157091	0.236482	0.366147	0.488730	0.638009	0.283012	0.348977	0.393493
	0.046087	0.073075	0.150199	0.185064	0.253415	0.089210	0.119608	0.133916
p	29.005563	33.304147	31.508068	36.053358	43.112850	14.864010	25.636012	53.144683
	8.944753	10.177141	10.877948	12.662363	15.615208	7.210436	11.306402	21.081781
	2.758388	3.109949	3.755538	4.447171	5.655732	3.497737	4.986529	8.362859
	0.850633	0.950344	1.296574	1.561899	2.048471	1.696730	2.199238	3.317434
	0.262319	0.290408	0.447633	0.548557	0.741944	0.823073	0.969943	1.315981
	0.080894	0.088743	0.154542	0.192660	0.268727	0.399267	0.427780	0.522032
d	11.786196	14.642323	20.112171	26.213808	35.200955	46.433857	16.564331	17.055521
	3.283910	3.739684	4.304604	4.471963	4.348965	4.752038	2.873470	5.398090
	0.914974	0.955124	1.303383	1.426371	1.087310	1.149678	1.045894	1.708501
	0.254933	0.243941	0.457953	0.640682	0.412647	0.510053	0.600519	0.540742
f	0.836538	0.241102	2.004802	2.690868	3.105546	4.099417	4.825916	5.525111
	0.165860	0.085366	0.714091	0.704784	0.911330	1.006448	1.174831	1.428824
g	0.089345	0.333097	0.360943	0.432505	0.485848	0.495784	0.059532	0.078483

[a] No auxiliary basis function is contracted, i.e. contraction coefficients are 1.0.

Table S3. RI errors (ΔE_{RI}) in mHartree for the RI-MP2/6-31G** (as Cartesian Gaussian functions) calculations of 114 small molecules

Molecule	$E_{MP2}^{(2)}$ [a]	This work[b]		SVP[c]	cc-pVDZ[d]
H_2	-0.026394	0.007	(0.007)	0.053	0.032
He_2	-0.050965	0.007	(0.007)	0.079	0.055
Li_2	-0.018524	0.012	(0.021)	0.527	0.013
Li_8	-0.137287	0.020	(0.035)	0.828	0.032
LiH	-0.020255	0.033	(0.064)	0.200	0.028
LiF	-0.192224	-0.077	(-0.068)	-0.931	-0.518
LiCl	-0.136800	-0.014	(-0.017)	-0.048	-0.082
Li_4H_4	-0.095617	0.079	(0.232)	0.314	0.100
Li_4Cl_4	-0.580848	-0.061	(-0.123)	-0.388	-0.263
$Li_4(CH_3)_4$	-0.692801	0.073	(0.145)	0.335	0.221
$LiBH_4$	-0.136451	0.035	(0.070)	0.118	0.044
Li_2O	-0.229467	-0.086	(-0.110)	-0.755	-0.189
Li_2S	-0.138231	-0.016	(-0.051)	-0.119	-0.077
Be_4	-0.187396	0.010	(0.007)	-0.357	-0.002
BeH_2	-0.048712	0.024	(0.040)	0.459	0.046
$Be(CH_3)_2$	-0.338724	0.053	(0.101)	0.518	0.166
Be_2H_4	-0.109838	0.040	(0.110)	0.692	0.082
Be_2F_4	-0.780000	-0.223	(-0.221)	-3.270	-1.526
$BeF_2(H_2O)_2$	-0.791903	-0.168	(-0.125)	-1.941	-0.812
BeS	-0.159515	-0.018	(-0.079)	-0.224	-0.138
BH_3	-0.093085	0.032	(0.065)	0.113	0.097
BF_3	-0.584883	-0.158	(-0.176)	-1.665	-1.022
B_2H_6	-0.218066	0.063	(0.116)	0.149	0.094
B_4H_4	-0.370488	0.043	(0.118)	0.083	-0.024
$B_3N_3H_6$	-0.742667	0.033	(0.218)	0.042	0.209
BH_3CO	-0.407749	-0.045	(-0.073)	-0.206	-0.083
BH_3NH_3	-0.299424	0.041	(0.103)	0.148	0.126
CH_4	-0.163160	0.034	(0.052)	0.127	0.095
C_2H_6	-0.305712	0.066	(0.113)	0.224	0.169
C_2H_4	-0.279830	0.057	(0.105)	0.173	0.120
C_2H_2	-0.262700	0.011	(-0.008)	0.003	-0.033
C_4H_4	-0.535584	0.036	(0.092)	0.082	0.049
C_6H_6	-0.794727	0.093	(0.263)	0.383	0.216
CH_3N	-0.307541	0.028	(0.050)	0.045	0.077
C_2H_3N	-0.440465	0.014	(0.030)	-0.002	0.043
CH_3OH	-0.337170	0.011	(0.047)	-0.057	0.076
CH_2O	-0.315727	-0.006	(-0.006)	-0.182	0.009

CH_2O_2	-0.509011	-0.027	(-0.033)	-0.416	-0.058
CH_3NO	-0.478506	-0.016	(-0.015)	-0.222	0.012
N_2	-0.314313	-0.030	(-0.115)	-0.186	-0.125
N_4	-0.700961	-0.105	(-0.263)	-0.555	-0.278
NH_3	-0.187702	0.014	(0.035)	0.070	0.071
H_2N_2	-0.336777	0.018	(0.028)	-0.042	0.042
H_4N_2	-0.354865	0.019	(0.057)	0.045	0.111
HCN	-0.292137	-0.013	(-0.060)	-0.101	-0.074
HNC	-0.277186	-0.017	(-0.049)	-0.147	-0.041
HNO	-0.347418	-0.004	(0.005)	-0.220	-0.013
HNO_2	-0.554175	-0.068	(-0.138)	-0.599	-0.149
HNO_3	-0.737203	-0.108	(-0.215)	-0.820	-0.221
H_2O	-0.198092	-0.021	(0.003)	-0.094	0.033
H_2O_2	-0.379757	-0.039	(0.004)	-0.285	0.013
CO	-0.285220	-0.050	(-0.107)	-0.291	-0.109
CO_2	-0.478080	-0.132	(-0.213)	-0.617	-0.234
H_2CO_3	-0.667277	-0.095	(-0.138)	-0.646	-0.140
F_2	-0.361093	-0.051	(-0.010)	-0.975	-0.552
HF	-0.184064	-0.041	(-0.016)	-0.484	-0.245
CF_4	-0.807480	-0.184	(-0.247)	-2.156	-1.323
NF_3	-0.697106	-0.131	(-0.135)	-1.683	-0.983
NH_4F	-0.377116	-0.032	(0.022)	-0.483	-0.200
OF_2	-0.548130	-0.076	(-0.038)	-1.212	-0.628
Ne_2	-0.300909	-0.065	(-0.030)	-2.444	-1.990
Na_2	-0.019140	0.011	(0.031)	1.087	0.046
NaH	-0.020331	0.163	(0.196)	0.408	0.058
NaF	-0.189834	-0.075	(-0.063)	-0.916	-0.573
NaCl	-0.134775	-0.038	(-0.031)	-0.008	-0.074
Na_3N	-0.214095	0.040	(0.089)	0.393	0.043
Na_3P	-0.160205	-0.095	(-0.207)	0.031	0.013
Na_2O	-0.246108	-0.119	(-0.178)	-0.694	-0.199
Na_2S	-0.136922	-0.095	(-0.151)	-0.044	-0.075
Mg_4	-0.133859	0.008	(0.060)	3.534	-0.064
MgH_2	-0.043995	0.074	(0.169)	0.793	0.055
MgF_2	-0.384951	-0.181	(-0.147)	-1.886	-1.104
$MgCl_2$	-0.281644	-0.050	(-0.085)	-0.232	-0.180
AlH_3	-0.071207	0.089	(0.249)	0.135	0.127
AlF_3	-0.575691	-0.178	(-0.174)	-2.256	-1.664
$AlCl_3$	-0.431705	-0.026	(-0.051)	-0.195	-0.283
AlN	-0.201558	0.003	(-0.047)	-0.103	-0.038

Al_2O_3	-0.690126	-0.171	(-0.279)	-1.468	-0.634
Al_2S_3	-0.461228	-0.037	(-0.252)	-0.201	-0.367
SiH_4	-0.108994	0.054	(0.278)	0.168	0.118
Si_2H_6	-0.201310	0.080	(0.560)	0.343	0.255
SiF_4	-0.773797	-0.241	(-0.354)	-2.938	-2.090
$SiCl_4$	-0.594487	-0.057	(-0.156)	-0.334	-0.445
SiO_2	-0.468277	-0.107	(-0.236)	-0.932	-0.387
SiS_2	-0.319897	-0.062	(-0.250)	-0.230	-0.342
P_2	-0.220022	-0.024	(-0.251)	-0.208	-0.266
PH_3	-0.124952	0.055	(0.181)	0.091	0.070
P_2H_4	-0.230868	0.086	(0.328)	0.170	0.132
CH_2PH	-0.252891	0.059	(0.140)	0.117	0.080
HCP	-0.248352	0.000	(-0.127)	-0.090	-0.104
H_3PO_4	-0.848821	-0.161	(-0.373)	-1.348	-0.492
PF_3	-0.627986	-0.181	(-0.246)	-2.248	-1.549
PF_5	-0.989144	-0.291	(-0.492)	-3.547	-2.437
S_2	-0.246390	0.025	(0.041)	-0.044	-0.105
S_5	-0.622614	0.016	(0.121)	-0.063	-0.202
H_2S	-0.135479	0.049	(0.114)	0.047	0.000
H_2S_2	-0.251760	0.055	(0.179)	0.064	-0.011
SF_2	-0.473119	-0.091	(-0.062)	-1.440	-0.972
SF_4	-0.858997	-0.226	(-0.372)	-2.945	-2.045
SF_6	-1.220390	-0.336	(-0.728)	-4.139	-2.921
CH_3SH	-0.278623	0.066	(0.159)	0.165	0.095
CH_2S	-0.260640	0.023	(0.038)	0.038	-0.021
CS_2	-0.379959	-0.091	(-0.248)	-0.260	-0.345
CHNS	-0.411008	-0.062	(-0.159)	-0.221	-0.178
H_2SO_4	-0.885760	-0.173	(-0.540)	-1.574	-0.686
Cl_2	-0.259764	0.002	(0.087)	-0.081	-0.111
HCl	-0.139386	0.012	(0.049)	-0.034	-0.065
CH_3Cl	-0.280319	0.033	(0.094)	0.083	0.035
NCl_3	-0.565691	-0.025	(0.076)	-0.265	-0.197
OCl_2	-0.448459	-0.030	(0.046)	-0.417	-0.220
CCl_4	-0.662291	-0.049	(0.046)	-0.179	-0.253
ClF	-0.309928	-0.036	(0.023)	-0.707	-0.492
ClF_3	-0.713539	-0.132	(-0.170)	-2.232	-1.533
Ar_2	-0.274741	-0.032	(0.056)	-0.307	-0.132

[a] MP2 correlation energy in Hartree. [b] ΔE_{RI} without *g*-type functions are given in parentheses. [c] Calculated in this study with SVP auxiliary basis functions[17]. [d] Calculated in this study with cc-pVDZ auxiliary basis functions[18].

Table S4. RI errors (ΔE_{RI}) in mHartree for the RI-MP2/6-311G** (as spherical Gaussian functions) calculations of 114 small molecules

Molecule	$E_{MP2}^{(2)}$ [a]	This work[b]		SVP[c]	cc-pVDZ[d]
H_2	-0.027911	0.006	(0.006)	0.023	0.070
He_2	-0.049385	0.007	(0.007)	0.064	1.210
Li_2	-0.018579	0.016	(0.019)	0.535	0.062
Li_8	-0.140213	0.039	(0.067)	0.880	0.141
LiH	-0.022708	0.024	(0.038)	0.223	0.084
LiF	-0.224864	-0.097	(-0.110)	-0.115	-0.007
LiCl	-0.145678	-0.018	(-0.052)	-0.021	-0.115
Li_4H_4	-0.107093	0.071	(0.154)	0.336	0.311
Li_4Cl_4	-0.616751	-0.041	(-0.218)	-0.329	-0.384
$Li_4(CH_3)_4$	-0.734059	0.098	(0.177)	0.171	0.286
$LiBH_4$	-0.145456	0.042	(0.068)	0.112	0.088
Li_2O	-0.244203	-0.114	(-0.158)	-0.219	-0.040
Li_2S	-0.144967	0.032	(-0.072)	-0.136	-0.093
Be_4	-0.192585	0.046	(0.066)	-0.246	0.031
BeH_2	-0.052408	0.029	(0.042)	0.413	0.052
$Be(CH_3)_2$	-0.357283	0.082	(0.140)	0.326	0.164
Be_2H_4	-0.117107	0.049	(0.096)	0.642	0.125
Be_2F_4	-0.919417	-0.429	(-0.574)	-0.529	-0.110
$BeF_2(H_2O)_2$	-0.903808	-0.253	(-0.326)	-0.119	0.004
BeS	-0.166460	0.049	(-0.002)	-0.248	-0.147
BH_3	-0.097799	0.066	(0.088)	0.104	0.101
BF_3	-0.693887	-0.255	(-0.378)	-0.176	-0.113
B_2H_6	-0.228657	0.08	(0.110)	0.130	0.126
B_4H_4	-0.383016	0.089	(0.169)	0.215	0.126
$B_3N_3H_6$	-0.781447	0.044	(0.182)	0.257	0.256
BH_3CO	-0.437500	-0.044	(-0.097)	0.042	-0.024
BH_3NH_3	-0.317410	0.066	(0.107)	0.147	0.164
CH_4	-0.170817	0.05	(0.073)	0.092	0.107
C_2H_6	-0.320303	0.07	(0.119)	0.153	0.177
C_2H_4	-0.291361	0.114	(0.172)	0.157	0.148
C_2H_2	-0.273514	0.043	(0.049)	-0.018	-0.012
C_4H_4	-0.560294	0.056	(0.106)	0.111	0.075
C_6H_6	-0.827856	0.225	(0.367)	0.320	0.288
CH_3N	-0.321713	0.035	(0.052)	0.096	0.092
C_2H_3N	-0.459628	0.035	(0.057)	0.060	0.063
CH_3OH	-0.362801	0.014	(0.029)	0.146	0.107
CH_2O	-0.338928	-0.016	(-0.024)	0.098	0.037

CH_2O_2	-0.547855	-0.052	(-0.106)	0.116	0.003
CH_3NO	-0.510726	-0.031	(-0.046)	0.116	0.060
N_2	-0.330608	-0.073	(-0.175)	-0.023	-0.129
N_4	-0.727391	-0.157	(-0.375)	-0.234	-0.294
NH_3	-0.198359	0.015	(0.021)	0.078	0.082
H_2N_2	-0.353605	-0.008	(-0.012)	0.094	0.059
H_4N_2	-0.374557	0.015	(0.038)	0.133	0.133
HCN	-0.304769	-0.04	(-0.093)	-0.020	-0.075
HNC	-0.290900	-0.014	(-0.062)	-0.019	-0.037
HNO	-0.374092	-0.035	(-0.048)	0.110	0.017
HNO_2	-0.598741	-0.113	(-0.194)	0.073	-0.048
HNO_3	-0.799819	-0.154	(-0.280)	0.083	-0.090
H_2O	-0.218889	-0.011	(0.000)	0.107	0.052
H_2O_2	-0.416699	-0.035	(-0.016)	0.183	0.070
CO	-0.308792	-0.069	(-0.149)	0.000	-0.092
CO_2	-0.518563	-0.153	(-0.263)	-0.025	-0.155
H_2CO_3	-0.728569	-0.109	(-0.216)	0.108	-0.052
F_2	-0.429055	-0.068	(-0.072)	-0.062	0.012
HF	-0.221505	-0.045	(-0.039)	-0.029	0.016
CF_4	-0.948475	-0.258	(-0.434)	-0.245	-0.135
NF_3	-0.803058	-0.177	(-0.214)	-0.087	-0.011
NH_4F	-0.425777	-0.03	(-0.013)	0.037	0.109
OF_2	-0.631243	-0.102	(-0.104)	0.018	0.025
Ne_2	-0.418165	-0.124	(-0.123)	-0.050	0.007
Na_2	-0.018636	0.061	(0.078)	1.093	0.062
NaH	-0.022642	0.098	(0.105)	0.339	0.165
NaF	-0.221429	-0.094	(-0.097)	-0.055	0.000
NaCl	-0.143405	0.023	(0.001)	0.047	-0.110
Na_3N	-0.219683	0.138	(0.182)	0.506	0.065
Na_3P	-0.162409	0.185	(0.215)	0.088	0.020
Na_2O	-0.258861	-0.159	(-0.178)	-0.062	-0.032
Na_2S	-0.142932	0.012	(-0.132)	-0.008	-0.102
Mg_4	-0.134615	0.312	(0.316)	3.469	-0.002
MgH_2	-0.048252	0.126	(0.159)	0.740	0.183
MgF_2	-0.449856	-0.219	(-0.252)	-0.202	-0.043
$MgCl_2$	-0.296587	-0.007	(-0.088)	-0.135	-0.268
AlH_3	-0.078769	0.201	(0.237)	0.189	0.301
AlF_3	-0.677767	-0.328	(-0.437)	-0.195	-0.141
$AlCl_3$	-0.456022	0.117	(0.040)	-0.103	-0.385
AlN	-0.209793	-0.002	(-0.028)	0.013	0.011

Al_2O_3	-0.740441	-0.384	(-0.568)	0.067	-0.202
Al_2S_3	-0.480109	-0.083	(-0.240)	-0.197	-0.440
SiH_4	-0.118567	0.258	(0.364)	0.210	0.287
Si_2H_6	-0.216468	0.398	(0.670)	0.398	0.512
SiF_4	-0.908865	-0.394	(-0.572)	-0.371	-0.235
$SiCl_4$	-0.626265	0.237	(0.139)	-0.209	-0.540
SiO_2	-0.504253	-0.196	(-0.323)	-0.032	-0.177
SiS_2	-0.331890	0.017	(-0.118)	-0.239	-0.387
P_2	-0.227299	0.662	(0.563)	-0.202	-0.313
PH_3	-0.135669	0.261	(0.277)	0.093	0.160
P_2H_4	-0.247305	0.548	(0.615)	0.158	0.230
CH_2PH	-0.265975	0.341	(0.379)	0.090	0.094
HCP	-0.257867	0.332	(0.287)	-0.137	-0.127
H_3PO_4	-0.924535	-0.221	(-0.440)	0.036	-0.179
PF_3	-0.729228	-0.174	(-0.267)	-0.243	-0.108
PF_5	-1.156051	-0.465	(-0.697)	-0.462	-0.261
S_2	-0.256663	0.297	(0.264)	-0.043	-0.129
S_5	-0.641772	0.428	(0.671)	-0.088	-0.290
H_2S	-0.145601	0.189	(0.190)	0.032	0.037
H_2S_2	-0.266059	0.358	(0.370)	0.038	-0.002
SF_2	-0.542491	0.054	(0.034)	-0.095	-0.015
SF_4	-0.991442	-0.214	(-0.310)	-0.303	-0.140
SF_6	-1.416670	-0.517	(-0.734)	-0.619	-0.399
CH_3SH	-0.294495	0.231	(0.275)	0.117	0.097
CH_2S	-0.272984	0.177	(0.172)	0.006	-0.051
CS_2	-0.398154	0.053	(-0.009)	-0.330	-0.423
CHNS	-0.431118	0.007	(-0.068)	-0.167	-0.209
H_2SO_4	-0.959976	-0.188	(-0.487)	-0.093	-0.337
Cl_2	-0.274506	0.273	(0.264)	-0.037	-0.153
HCl	-0.149580	0.119	(0.119)	-0.007	-0.061
CH_3Cl	-0.295502	0.141	(0.165)	0.067	-0.004
NCl_3	-0.595119	0.29	(0.286)	-0.082	-0.245
OCl_2	-0.476899	0.214	(0.210)	0.034	-0.145
CCl_4	-0.703439	0.311	(0.248)	-0.154	-0.420
ClF	-0.349348	0.098	(0.097)	-0.049	-0.054
ClF_3	-0.815678	-0.109	(-0.123)	-0.156	-0.057
Ar_2	-0.294766	0.51	(0.521)	-0.282	-0.182

[a] MP2 correlation energy in Hartree. [b] ΔE_{RI} without *g*-type functions are given in parentheses. [c] Calculated in this study with SVP auxiliary basis functions[17]. [d] Calculated in this study with cc-pVDZ auxiliary basis functions[18].