

Supporting Information of

Pair natural orbital and canonical coupled cluster reaction enthalpies involving light to heavy alkaline and alkali – earth metals: the importance of sub- valence correlation

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Figures S1 – S6 Mentioned in the Main Text

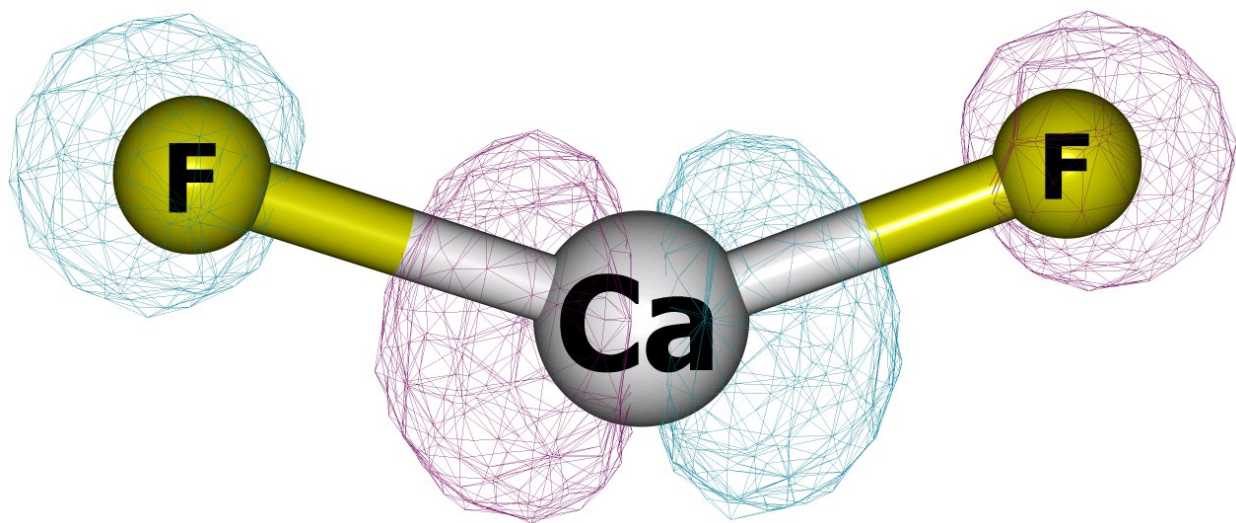


Figure S1. The MO 13 of CaF_2 complex.

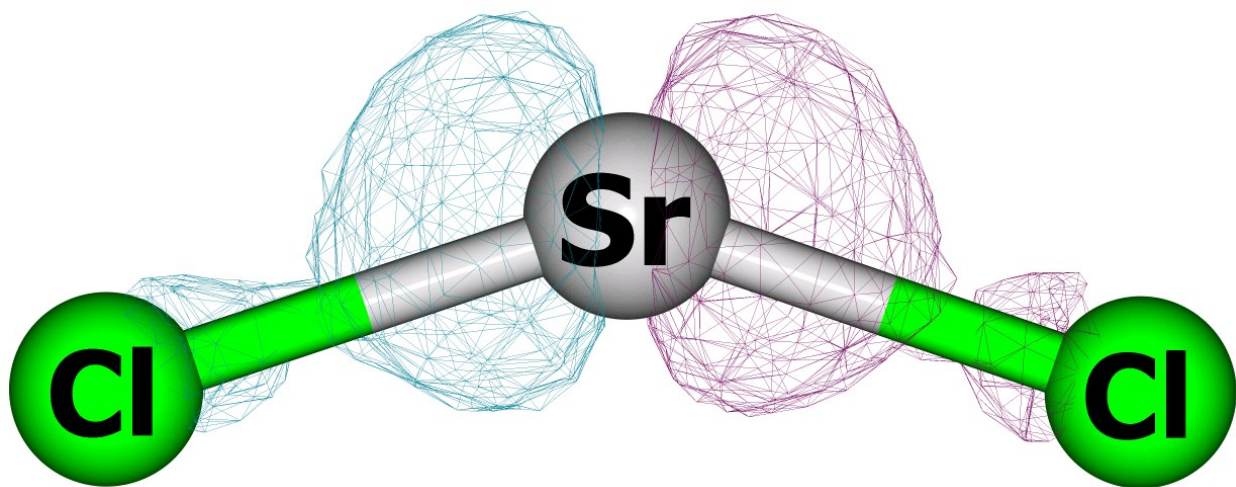


Figure S2. The MO 11 of SrCl_2 complex.

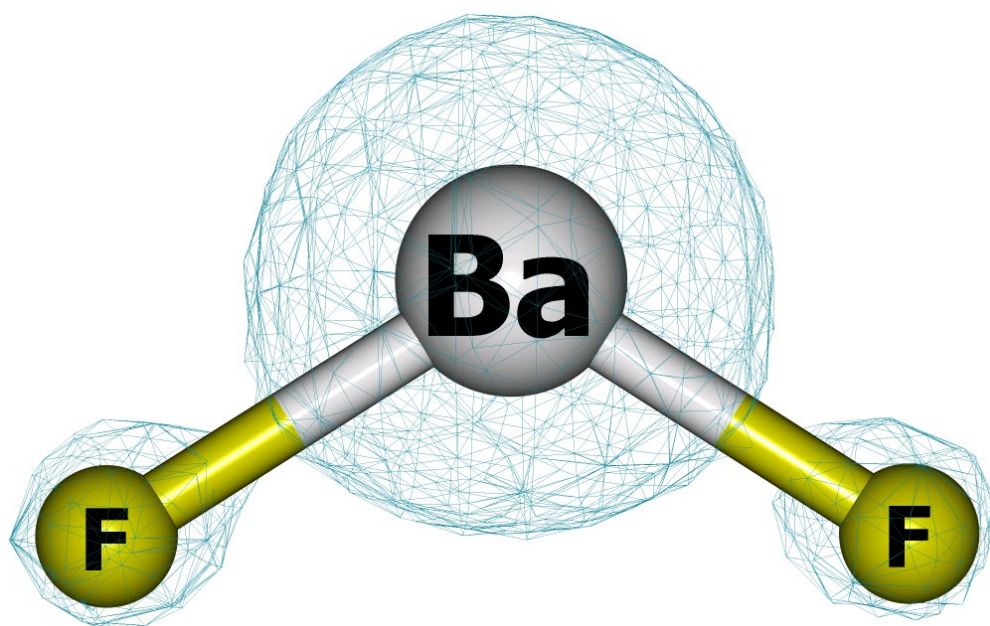


Figure S3. The MO 3 of BaF₂ complex.

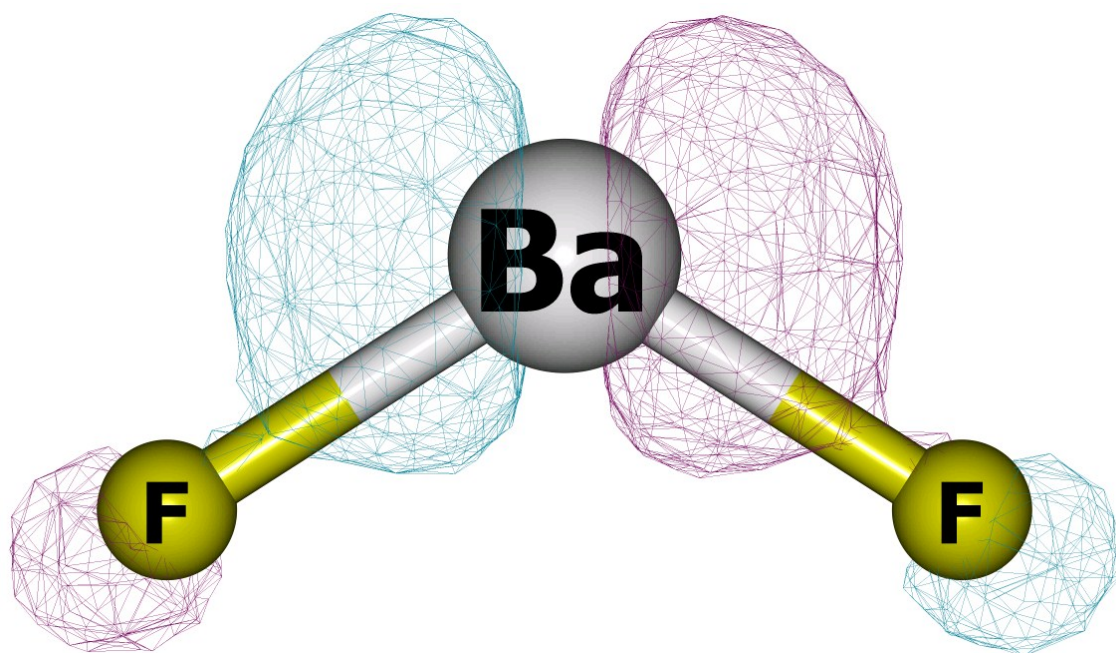


Figure S4. The MO 8 of BaF₂ complex.

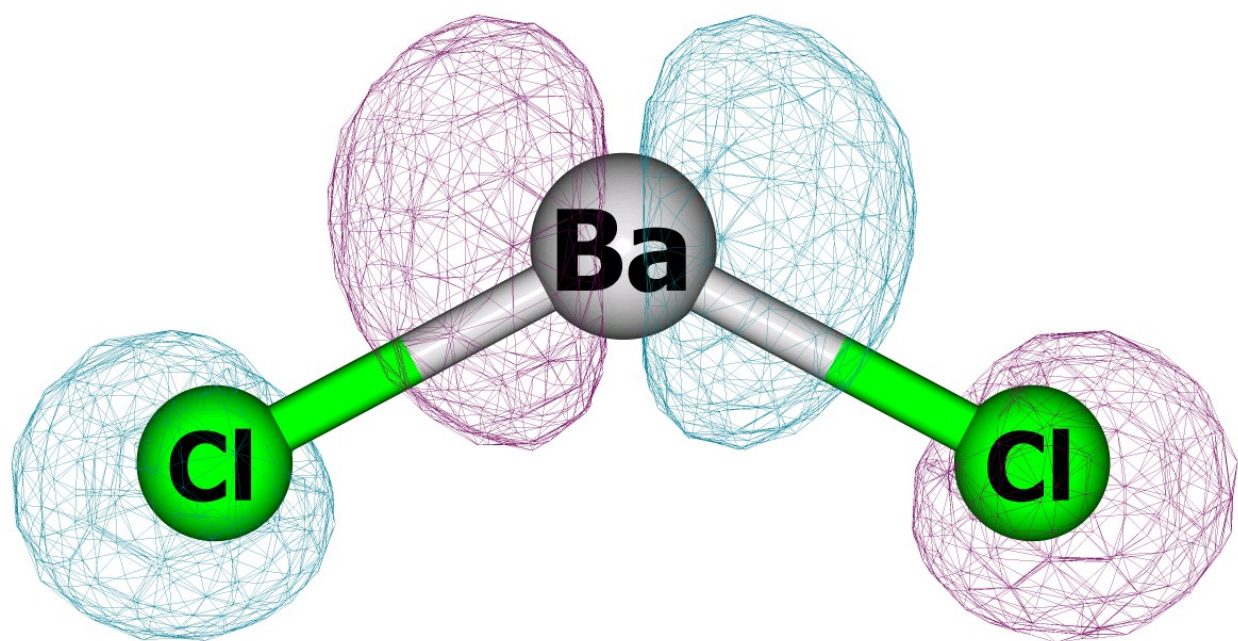


Figure S5. The MO 16 of BaCl_2 complex.

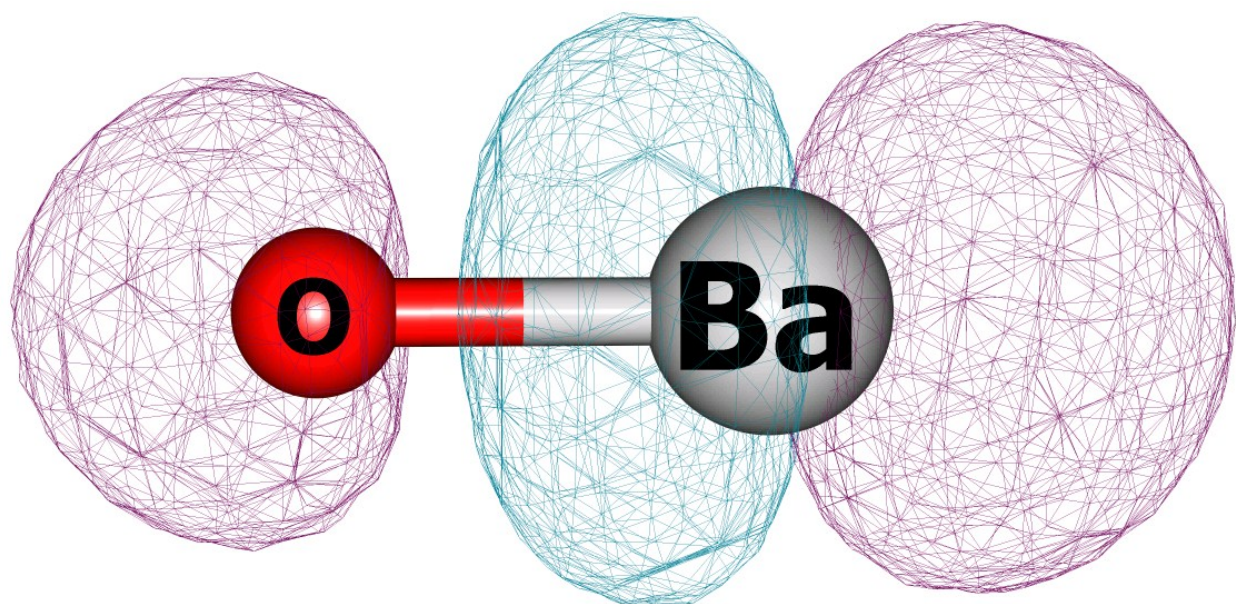


Figure S6. The MO 6 of BaO complex.

Table S1. DLPNO-CCSD(T) reaction enthalpies errors (kcal/mol) with respect to CCSD(T)

Unsigned Error (kcal/mol)							Signed Error (kcal/mol)					
	TZ(FC)	QZ(FC)	CBS(FC)	TZ(AE)	QZ(AE)	CBS(AE)	TZ(FC)	QZ(FC)	CBS(FC)	TZ(AE)	QZ(AE)	CBS(AE)
1	0.0	0.1	0.1	0.1	0.1	0.2	0.0	0.1	0.1	0.1	0.1	0.2
2	0.1	0.1	0.2	0.2	0.2	0.3	0.1	0.1	0.2	0.2	0.2	0.3
3	0.0	0.1	0.1	0.1	0.1	0.2	0.0	0.1	0.1	0.1	0.1	0.2
4	0.0	0.2	0.4	0.1	0.3	0.4	0.0	0.2	0.4	0.1	0.3	0.4
5	0.1	0.0	0.1	0.1	0.1	0.2	-0.1	0.0	0.1	-0.1	0.1	0.2
6	0.0	0.1	0.2	0.0	0.2	0.4	0.0	0.1	0.2	0.0	0.2	0.4
7	0.8	0.7	0.7	0.8	0.6	0.5	-0.8	-0.7	-0.7	-0.8	-0.6	-0.5
8	0.0	0.1	0.1	0.1	0.1	0.2	0.0	0.1	0.1	0.1	0.1	0.2
9	0.7	0.7	0.8	0.7	0.8	0.8	-0.7	-0.7	-0.8	-0.7	-0.8	-0.8
10	0.1	0.1	0.2	0.1	0.1	0.2	0.1	0.1	0.2	0.1	0.1	0.2
11	0.0	0.0	0.0	0.1	0.1	0.0	0.0	0.0	0.0	-0.1	-0.1	0.0
12	0.1	0.1	0.1	0.1	0.1	0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1
13	0.1	0.1	0.2	0.1	0.2	0.2	-0.1	-0.1	-0.2	-0.1	-0.2	-0.2
14	0.2	0.2	0.3	0.2	0.2	0.3	-0.2	-0.2	-0.3	-0.2	-0.2	-0.3
15	0.1	0.1	0.1	0.0	0.1	0.1	-0.1	-0.1	-0.1	0.0	-0.1	-0.1
16	0.1	0.0	0.0	0.0	0.0	0.0	-0.1	0.0	0.0	0.0	0.0	0.0
17	0.0	0.1	0.2	0.0	0.2	0.2	0.0	0.1	0.2	0.0	0.2	0.2
18	0.3	0.2	0.1	0.3	0.2	0.1	-0.3	-0.2	-0.1	-0.3	-0.2	-0.1
19	0.3	0.1	0.1	0.3	0.1	0.1	-0.3	-0.1	0.1	-0.3	-0.1	0.1
20	0.0	0.1	0.2	0.1	0.2	0.2	0.0	0.1	0.2	0.1	0.2	0.2
21	0.1	0.1	0.1	0.2	0.1	0.1	-0.1	-0.1	-0.1	-0.2	-0.1	-0.1
22	0.3	0.2	0.2	0.3	0.2	0.2	-0.3	-0.2	-0.2	-0.3	-0.2	-0.2
23	0.1	0.1	0.1	0.2	0.1	0.0	-0.1	-0.1	-0.1	-0.2	-0.1	0.0
24	0.0	0.1	0.1	0.1	0.3	0.4	0.0	0.1	0.1	0.1	0.3	0.4
25	0.3	0.3	0.3	0.2	0.1	0.0	-0.3	-0.3	-0.3	-0.2	-0.1	0.0
26	0.3	0.1	0.0	0.4	0.1	0.0	-0.3	-0.1	0.0	-0.4	-0.1	0.0
27	0.2	0.1	0.1	0.2	0.2	0.1	-0.2	-0.1	-0.1	-0.2	-0.2	-0.1
28	0.0	0.1	0.1	0.1	0.2	0.2	0.0	0.1	0.1	0.1	0.2	0.2
29	0.7	0.6	0.6	1.1	1.1	1.1	-0.7	-0.6	-0.6	-1.1	-1.1	-1.1
30	0.4	0.4	0.4	0.6	0.6	0.7	-0.4	-0.4	-0.4	-0.6	-0.6	-0.7
31	0.5	0.4	0.3	0.7	0.6	0.6	-0.5	-0.4	-0.3	-0.7	-0.6	-0.6

32	0.1	0.0	0.1	0.1	0.0	0.1	-0.1	0.0	0.1	-0.1	0.0	0.1
All	0.2	0.2	0.2	0.2	0.2	0.3	-0.2	-0.1	-0.1	-0.2	-0.1	0.0

Tabulated data forming the basis of Charts 1 - 12.

Table S2. Tabulated reaction enthalpies (kcal/mol) forming the basis of Chart 1.

	CBS(FC)	CBS(FC, PNO)	CBS(AE)	CBS(AE, PNO)
1	0.6	0.8	1.8	2.0
2	0.2	0.4	0.6	0.9
3	-0.6	-0.4	-0.7	-0.5
4	1.0	1.4	1.0	1.4
5	-0.1	0.0	2.0	2.3
6	0.4	0.6	1.9	2.3
7	-0.7	-1.3	0.7	0.2
8	0.5	0.6	-0.2	0.0
9	-0.6	-1.3	-1.3	-2.1

Table S3. Tabulated data (MUE/MSE in kcal/mol) forming the basis of Chart 2.

	MSE	MUE
TZ(FC)	-0.8	2.3
QZ(FC)	-0.4	1.0
CBS(FC, TZ/QZ)	0.1	0.5
TZ(FC, PNO)	-1.0	2.3
QZ(FC, PNO)	-0.4	1.0
5Z(FC, PNO)	-0.4	0.7
CBS(FC, TZ/QZ, PNO)	0.1	0.8
CBS(FC, QZ/5Z, PNO)	-0.3	0.6
TZ(AE)	-0.4	1.8
QZ(AE)	0.2	0.6
CBS(AE, TZ/QZ)	0.7	1.1
TZ(AE, PNO)	-0.5	1.6
QZ(AE, PNO)	0.1	0.6
5Z(AE, PNO)	0.2	0.7
CBS(AE, TZ/QZ, PNO)	0.7	1.3
CBS(AE, QZ/5Z, PNO)	0.2	0.9

Table S4. Tabulated reaction enthalpies (kcal/mol) forming the basis of Chart 3.

	CBS(FC)	CBS(FC, PNO)	CBS(AE)	CBS(AE, PNO)
10	1.6	1.7	0.0	0.1
11	1.2	1.2	-0.4	-0.4
12	3.9	3.8	2.2	2.1
13	-0.3	-0.5	-0.3	-0.5
14	2.3	2.1	2.3	2.0
15	2.6	2.6	2.6	2.5
16	4.1	4.1	2.6	2.6
17	3.9	4.2	2.1	2.3
18	2.4	2.3	0.1	0.0
19	5.1	5.2	3.2	3.3

Table S5. Tabulated data (MUE/MSE in kcal/mol) forming the basis of Chart 4.

	MSE	MUE
TZ(FC)	0.6	1.8
QZ(FC)	1.6	1.7
CBS(FC, TZ/QZ)	2.4	2.5
TZ(FC, PNO)	0.5	1.8
QZ(FC, PNO)	1.6	1.7
5Z(FC, PNO)	1.9	2.0
CBS(FC, TZ/QZ, PNO)	2.4	2.5
CBS(FC, QZ/5Z, PNO)	2.2	2.3
TZ(AE)	-0.1	2.3
QZ(AE)	0.7	1.2
CBS(AE, TZ/QZ)	1.3	1.5
TZ(AE, PNO)	-0.2	2.3
QZ(AE, PNO)	0.6	1.2
5Z(AE, PNO)	0.9	1.2
CBS(AE, TZ/QZ, PNO)	1.3	1.5
CBS(AE, QZ/5Z, PNO)	1.1	1.4

Table S6. Tabulated reaction enthalpies (kcal/mol) forming the basis of Chart 5.

	CBS(FC)	CBS(FC, PNO)	CBS(AE)	CBS(AE, PNO)
21	-13.6	-13.7	6.1	6.0
22	1.1	0.9	1.7	1.5
23	-2.4	-2.5	6.5	6.4
24	-3.9	-3.8	3.4	3.8
25	-4.3	-4.6	-2.4	-2.4
26	3.8	3.8	1.6	1.6

Table S7. Tabulated reaction enthalpies (kcal/mol) forming the basis of Chart 6.

	CBS(FC)	CBS(FC, PNO)	CBS(AE)	CBS(AE, PNO)
21	-16.2	-16.3	1.1	0.9
22	-1.2	-1.4	-1.9	-2.1
23	-5.5	-5.6	1.3	1.2
24	-5.5	-5.4	-0.2	0.1
25	-6.3	-6.6	-5.7	-5.8
26	1.7	1.5	-1.3	-1.4

Table S8. Tabulated data (MUE/MSE in kcal/mol) forming the basis of Chart 7.

	MSE	MUE
TZ(FC)	-9.0	9.0
QZ(FC)	-5.5	6.1
CBS(FC, TZ/QZ)	-3.2	4.9
TZ(FC, PNO)	-9.2	9.2
QZ(FC, PNO)	-5.6	6.1
5Z(FC, PNO)	-4.6	5.4
CBS(FC, TZ/QZ, PNO)	-3.3	4.9
CBS(FC, QZ/5Z, PNO)	-3.6	5.1
TZ(AE)	-6.9	6.9
QZ(AE)	-1.1	1.9
CBS(AE, TZ/QZ)	2.8	3.6
TZ(AE, PNO)	-7.0	7.0
QZ(AE, PNO)	-1.2	1.9
5Z(AE, PNO)	0.7	2.3
CBS(AE, TZ/QZ, PNO)	2.8	3.6
CBS(AE, QZ/5Z, PNO)	2.5	3.3

Table S9. Tabulated reaction enthalpies (kcal/mol) forming the basis of Chart 8.

	CBS(FC)	CBS(FC, PNO)	CBS(AE)	CBS(AE, PNO)
27	-18.6	-18.6	7.7	7.6
28	-10.2	-10.0	7.2	7.5
29	-31.0	-31.6	-0.7	-1.8
30	0.6	0.2	-2.1	-2.8
31	1.2	0.9	-3.2	-3.8
32	0.6	0.7	-1.1	-1.0

Table S10. Tabulated reaction enthalpies (kcal/mol) forming the basis of Chart 9.

	CBS(FC)	CBS(FC, PNO)	CBS(AE)	CBS(AE, PNO)
27	-20.5	-20.6	1.3	1.2
28	-12.2	-12.1	2.7	2.8
29	-31.4	-32.0	-4.8	-5.8
30	0.4	0.0	-1.9	-2.5
31	1.0	0.6	-2.7	-3.3
32	0.6	0.6	-0.8	-0.8

Table S11. Tabulated data (MUE/MSE in kcal/mol) forming the basis of Chart 10.

	MSE	MUE
TZ(FC)	-12.0	12.7
QZ(FC)	-10.4	11.0
CBS(FC, TZ/QZ)	-9.6	10.3
TZ(FC, PNO)	-12.3	12.7
QZ(FC, PNO)	-10.6	11.0
5Z(FC, PNO)	-10.1	10.6
CBS(FC, TZ/QZ, PNO)	-9.7	10.3
CBS(FC, QZ/5Z, PNO)	-9.8	10.4
TZ(AE)	-4.8	4.8
QZ(AE)	-1.0	2.3
CBS(AE, TZ/QZ)	1.3	3.7
TZ(AE, PNO)	-5.2	5.2
QZ(AE, PNO)	-1.4	2.7
5Z(AE, PNO)	0.0	3.2
CBS(AE, TZ/QZ, PNO)	1.0	4.1
CBS(AE, QZ/5Z, PNO)	1.3	3.7

Table S12. Tabulated data (MUE/MSE in kcal/mol) forming the basis of Chart 11.

	MSE	MUE
TZ(FC)	-4.0	5.3
QZ(FC)	-2.5	4.1
CBS(FC, TZ/QZ)	-1.5	3.9
TZ(FC, PNO)	-4.1	5.3
QZ(FC, PNO)	-2.6	4.1
5Z(FC, PNO)	-2.2	3.9
CBS(FC, TZ/QZ, PNO)	-1.6	3.9
CBS(FC, QZ/5Z, PNO)	-1.9	3.9
TZ(AE)	-2.3	3.5
QZ(AE)	-0.1	1.4
CBS(AE, TZ/QZ)	1.4	2.2
TZ(AE, PNO)	-2.3	3.5
QZ(AE, PNO)	-0.1	1.4
5Z(AE, PNO)	0.5	1.7
CBS(AE, TZ/QZ, PNO)	1.4	2.2
CBS(AE, QZ/5Z, PNO)	1.2	2.1

Table S13. Tabulated data (MUE/MSE in kcal/mol) forming the basis of Chart 12.

	MSE	MUE
TZ(FC)	-0.2	0.2
QZ(FC)	-0.1	0.2
CBS(FC, TZ/QZ)	-0.1	0.2
TZ(AE)	-0.2	0.2
QZ(AE)	-0.1	0.2
CBS(AE, TZ/QZ)	0.0	0.3

Table S14. Tabulated CCSD(T)/cc-pwCVnZ(-PP) reaction enthalpies in kcal/mol.

	CCSDT/TZ(FC)	CCSDT/QZ(FC)	CCSDT/CBS(FC)	CCSDT/TZ(AE)	CCSDT/QZ(AE)	CCSDT/CBS(AE)	EXPT
1	-175.2	-178.7	-180.7	-176.1	-179.7	-181.8	-180.0
2	-100.7	-101.6	-102.4	-100.9	-102.0	-102.9	-102.3
3	-84.0	-84.8	-85.5	-83.9	-84.7	-85.4	-86.1
4	-63.4	-63.8	-64.2	-63.5	-63.8	-64.2	-63.2
5	-263.9	-266.2	-267.7	-265.5	-268.1	-269.8	-267.8
6	-162.6	-163.4	-164.2	-163.9	-164.8	-165.7	-163.8
7	12.1	12.5	12.5	11.0	11.3	11.1	11.8
8	101.3	102.7	103.5	101.6	103.3	104.2	104.0
9	276.0	278.7	280.2	276.6	279.4	280.9	279.6
10	-16.4	-17.5	-18.0	-15.4	-16.1	-16.4	-16.5
11	-21.1	-22.2	-22.8	-20.1	-20.9	-21.2	-21.5
12	-23.6	-24.6	-25.2	-22.8	-23.3	-23.6	-21.3
13	-4.7	-4.7	-4.7	-4.8	-4.7	-4.7	-5.1
14	-7.2	-7.1	-7.2	-7.4	-7.2	-7.1	-4.9
15	-2.5	-2.4	-2.5	-2.6	-2.5	-2.4	0.2
16	-205.4	-210.6	-213.5	-203.8	-209.0	-212.0	-209.4
17	-129.7	-132.1	-133.9	-128.3	-130.4	-132.1	-130.0
18	-114.2	-116.2	-117.9	-112.5	-114.2	-115.6	-115.5
19	-92.1	-93.6	-94.9	-91.0	-92.1	-93.0	-89.8
20	75.7	78.5	79.5	75.5	78.6	79.9	79.4
21	-209.1	-213.8	-216.4	-222.9	-231.1	-236.1	-230.0
22	-139.0	-141.9	-144.2	-136.4	-141.2	-144.8	-143.1
23	-212.2	-217.8	-220.9	-216.2	-224.6	-229.8	-223.3
24	-145.6	-148.0	-149.6	-148.2	-153.3	-156.9	-153.5
25	-135.6	-138.1	-140.1	-134.3	-138.7	-142.0	-144.4
26	-117.9	-120.6	-122.8	-114.0	-117.7	-120.5	-118.9
27	-209.8	-214.7	-216.7	-225.6	-236.5	-242.9	-235.2
28	-145.8	-149.3	-151.4	-157.3	-164.2	-168.7	-161.5
29	17.3	15.5	15.1	-4.3	-11.1	-15.2	-15.9
30	8.8	8.8	8.6	10.5	11.1	11.3	9.2
31	24.3	24.4	24.2	27.0	28.0	28.6	25.4
32	15.5	15.6	15.6	16.4	16.9	17.3	16.2

Table S15. Tabulated DLPNO-CCSD(T)/cc-pwCVnZ(-PP) reaction enthalpies in kcal/mol.

	DLPNO/ TZ(FC)	DLPNO/ QZ(FC)	DLPNO/ 5Z(FC)	DLPNO/CBS (TZ/QZ,FC)	DLPNO/CBS (QZ/5Z,FC)	DLPNO/ TZ(AE)	DLPNO/ QZ(AE)	DLPNO/ 5Z(AE)	DLPNO/CBS (TZ/QZ,AE)	DLPNO/CBS (QZ/5Z,AE)	EXPT
1	-175.3	-178.8	-179.7	-180.8	-180.4	-176.1	-179.8	-180.8	-182.0	-181.5	-180.0
2	-100.7	-101.8	-101.8	-102.6	-101.8	-101.1	-102.2	-102.3	-103.1	-102.4	-102.3
3	-84.0	-84.9	-84.9	-85.7	-85.0	-84.0	-84.8	-84.9	-85.6	-84.9	-86.1
4	-63.5	-64.0	-63.7	-64.6	-63.4	-63.6	-64.1	-63.7	-64.6	-63.4	-63.2
5	-263.8	-266.2	-266.9	-267.8	-267.6	-265.5	-268.2	-268.9	-270.1	-269.6	-267.8
6	-162.6	-163.5	-163.7	-164.4	-163.9	-163.9	-165.1	-165.2	-166.1	-165.5	-163.8
7	12.9	13.2	13.2	13.1	13.1	11.8	11.9	11.9	11.6	11.8	11.8
8	101.3	102.7	103.2	103.4	103.6	101.6	103.1	103.7	104.0	104.2	104.0
9	276.7	279.4	280.1	280.9	280.7	277.3	280.1	280.9	281.7	281.5	279.6
10	-16.5	-17.6	-18.0	-18.2	-18.3	-15.4	-16.2	-16.5	-16.6	-16.6	-16.5
11	-21.1	-22.2	-22.6	-22.7	-22.9	-20.1	-20.8	-21.1	-21.1	-21.2	-21.5
12	-23.5	-24.5	-25.0	-25.1	-25.4	-22.7	-23.2	-23.5	-23.5	-23.7	-21.3
13	-4.6	-4.6	-4.6	-4.5	-4.6	-4.6	-4.6	-4.6	-4.5	-4.6	-5.1
14	-7.0	-6.9	-7.0	-6.9	-7.1	-7.2	-7.0	-7.0	-6.8	-7.1	-4.9
15	-2.4	-2.4	-2.4	-2.4	-2.5	-2.6	-2.4	-2.5	-2.3	-2.5	0.2
16	-205.3	-210.5	-211.7	-213.5	-212.9	-203.7	-209.0	-210.3	-212.0	-211.7	-209.4
17	-129.7	-132.2	-132.6	-134.2	-133.2	-128.3	-130.6	-131.0	-132.3	-131.6	-130.0
18	-113.9	-116.0	-116.6	-117.8	-117.2	-112.3	-114.0	-114.5	-115.5	-115.1	-115.5
19	-91.8	-93.5	-93.8	-95.1	-94.2	-90.7	-92.0	-92.2	-93.1	-92.6	-89.8
20	75.7	78.4	79.1	79.3	79.7	75.4	78.4	79.3	79.7	80.1	79.4
21	-209.0	-213.7	-214.9	-216.3	-216.0	-222.8	-230.9	-233.2	-236.0	-235.4	-230.0
22	-138.7	-141.7	-142.8	-144.0	-144.0	-136.2	-141.0	-142.4	-144.6	-143.8	-143.1
23	-212.1	-217.7	-219.1	-220.8	-220.4	-216.0	-224.5	-227.2	-229.7	-229.8	-223.3
24	-145.6	-148.1	-148.6	-149.7	-149.2	-148.3	-153.6	-155.1	-157.3	-156.7	-153.5
25	-135.3	-137.8	-138.7	-139.8	-139.6	-134.1	-138.6	-140.2	-142.0	-141.9	-144.4
26	-117.6	-120.5	-121.4	-122.7	-122.4	-113.6	-117.5	-119.0	-120.5	-120.6	-118.9
27	-209.7	-214.6	-215.7	-216.6	-216.4	-225.4	-236.4	-239.9	-242.8	-243.2	-235.2
28	-145.8	-149.4	-150.1	-151.5	-150.8	-157.4	-164.3	-166.4	-169.0	-168.5	-161.5
29	18.0	16.1	15.4	15.7	15.2	-3.2	-10.1	-13.1	-14.1	-15.9	-15.9
30	9.2	9.2	9.0	9.1	8.8	11.1	11.7	11.6	12.0	11.5	9.2
31	24.8	24.8	24.6	24.5	24.4	27.7	28.7	28.8	29.2	28.9	25.4
32	15.6	15.6	15.6	15.4	15.6	16.6	17.0	17.2	17.2	17.4	16.2

AutoAux basis sets generated for cc-pwCV5Z(-PP) basis sets.

Auxiliary basis set for element : H
NewAuxGTO H

```
S 1
 1 303.1407225144 1.0000000000
S 1
 1 168.4115125080 1.0000000000
S 1
 1 93.5619513933 1.0000000000
S 1
 1 51.9788618852 1.0000000000
S 1
 1 28.8771454918 1.0000000000
S 1
 1 16.0428586065 1.0000000000
S 1
 1 8.9126992259 1.0000000000
S 1
 1 4.9514995699 1.0000000000
S 1
 1 2.7508330944 1.0000000000
S 1
 1 1.5282406080 1.0000000000
S 1
 1 0.8490225600 1.0000000000
S 1
 1 0.4716792000 1.0000000000
S 1
 1 0.2620440000 1.0000000000
S 1
 1 0.1455800000 1.0000000000
P 1
 1 10.2012800000 1.0000000000
P 1
 1 5.1006400000 1.0000000000
P 1
 1 2.5503200000 1.0000000000
P 1
 1 1.2751600000 1.0000000000
P 1
 1 0.6375800000 1.0000000000
P 1
 1 0.3187900000 1.0000000000
D 1
 1 11.5253952000 1.0000000000
D 1
 1 5.2388160000 1.0000000000
```

```
D 1
 1 2.3812800000 1.0000000000
D 1
 1 1.0824000000 1.0000000000
D 1
 1 0.4920000000 1.0000000000
F 1
 1 7.8688720000 1.0000000000
F 1
 1 3.5767600000 1.0000000000
F 1
 1 1.6258000000 1.0000000000
F 1
 1 0.7390000000 1.0000000000
G 1
 1 10.4989280000 1.0000000000
G 1
 1 4.7722400000 1.0000000000
G 1
 1 2.1692000000 1.0000000000
G 1
 1 0.9860000000 1.0000000000
H 1
 1 7.2367200000 1.0000000000
H 1
 1 3.1464000000 1.0000000000
H 1
 1 1.3680000000 1.0000000000
end;
```

Auxiliary basis set for element : Ca
NewAuxGTO Ca

```
S 1
 1 4663.3048079577 1.0000000000
S 1
 1 2590.7248933098 1.0000000000
S 1
 1 1439.2916073943 1.0000000000
S 1
 1 799.6064485524 1.0000000000
S 1
 1 444.2258047513 1.0000000000
S 1
 1 246.7921137507 1.0000000000
S 1
 1 137.1067298615 1.0000000000
S 1
 1 76.1704054786 1.0000000000
S 1
 1 42.3168919326 1.0000000000
S 1
 1 23.5093844070 1.0000000000
S 1
```

1	13.0607691150	1.0000000000
S 1		
1	7.2559828417	1.0000000000
S 1		
1	4.0311015787	1.0000000000
S 1		
1	2.2395008771	1.0000000000
S 1		
1	1.2441671539	1.0000000000
S 1		
1	0.6912039744	1.0000000000
S 1		
1	0.3840022080	1.0000000000
S 1		
1	0.2133345600	1.0000000000
S 1		
1	0.1185192000	1.0000000000
S 1		
1	0.0658440000	1.0000000000
S 1		
1	0.0365800000	1.0000000000
P 1		
1	868.0254803722	1.0000000000
P 1		
1	482.2363779846	1.0000000000
P 1		
1	267.9090988803	1.0000000000
P 1		
1	148.8383882668	1.0000000000
P 1		
1	82.6879934816	1.0000000000
P 1		
1	45.9377741564	1.0000000000
P 1		
1	25.5209856425	1.0000000000
P 1		
1	14.1783253569	1.0000000000
P 1		
1	7.8768474205	1.0000000000
P 1		
1	4.3760263447	1.0000000000
P 1		
1	2.4311257471	1.0000000000
P 1		
1	1.3506254150	1.0000000000
P 1		
1	0.7503474528	1.0000000000
P 1		
1	0.4168596960	1.0000000000
P 1		
1	0.2315887200	1.0000000000
P 1		
1	0.1286604000	1.0000000000

P 1		
1	0.0714780000	1.0000000000
P 1		
1	0.0397100000	1.0000000000
D 1		
1	520.2469512178	1.0000000000
D 1		
1	289.0260840099	1.0000000000
D 1		
1	160.5700466722	1.0000000000
D 1		
1	89.2055814845	1.0000000000
D 1		
1	49.5586563803	1.0000000000
D 1		
1	27.5325868779	1.0000000000
D 1		
1	15.2958815989	1.0000000000
D 1		
1	8.4977119994	1.0000000000
D 1		
1	4.7209511108	1.0000000000
D 1		
1	2.6227506171	1.0000000000
D 1		
1	1.4570836762	1.0000000000
D 1		
1	0.8094909312	1.0000000000
D 1		
1	0.4497171840	1.0000000000
D 1		
1	0.2498428800	1.0000000000
D 1		
1	0.1388016000	1.0000000000
D 1		
1	0.0771120000	1.0000000000
D 1		
1	0.0428400000	1.0000000000
F 1		
1	132.1621758101	1.0000000000
F 1		
1	60.0737162773	1.0000000000
F 1		
1	27.3062346715	1.0000000000
F 1		
1	12.4119248507	1.0000000000
F 1		
1	5.6417840230	1.0000000000
F 1		
1	2.5644472832	1.0000000000
F 1		
1	1.1656578560	1.0000000000
F 1		

1	0.5298444800	1.0000000000
F 1		
1	0.2408384000	1.0000000000
F 1		
1	0.1094720000	1.0000000000
F 1		
1	0.0497600000	1.0000000000
G 1		
1	150.5416423818	1.0000000000
G 1		
1	68.4280192645	1.0000000000
G 1		
1	31.1036451202	1.0000000000
G 1		
1	14.1380205092	1.0000000000
G 1		
1	6.4263729587	1.0000000000
G 1		
1	2.9210786176	1.0000000000
G 1		
1	1.3277630080	1.0000000000
G 1		
1	0.6035286400	1.0000000000
G 1		
1	0.2743312000	1.0000000000
G 1		
1	0.1246960000	1.0000000000
G 1		
1	0.0566800000	1.0000000000
H 1		
1	205.9437953117	1.0000000000
H 1		
1	89.5407805703	1.0000000000
H 1		
1	38.9307741610	1.0000000000
H 1		
1	16.9264235483	1.0000000000
H 1		
1	7.3593145862	1.0000000000
H 1		
1	3.1997019940	1.0000000000
H 1		
1	1.3911747800	1.0000000000
H 1		
1	0.6048586000	1.0000000000
H 1		
1	0.2629820000	1.0000000000
H 1		
1	0.1143400000	1.0000000000
I 1		
1	31.4782200000	1.0000000000
I 1		
1	10.4927400000	1.0000000000

I 1		
1	3.4975800000	1.0000000000
I 1		
1	1.1658600000	1.0000000000
I 1		
1	0.3886200000	1.0000000000
I 1		
1	0.1295400000	1.0000000000
J 1		
1	15.1632000000	1.0000000000
J 1		
1	5.0544000000	1.0000000000
J 1		
1	1.6848000000	1.0000000000
J 1		
1	0.5616000000	1.0000000000
J 1		
1	0.1872000000	1.0000000000
end;		
# Auxiliary basis set for element : Br		
NewAuxGTO Br		
S 1		
1	1547.1882019830	1.0000000000
S 1		
1	859.5490011017	1.0000000000
S 1		
1	477.5272228343	1.0000000000
S 1		
1	265.2929015746	1.0000000000
S 1		
1	147.3849453192	1.0000000000
S 1		
1	81.8805251773	1.0000000000
S 1		
1	45.4891806541	1.0000000000
S 1		
1	25.2717670300	1.0000000000
S 1		
1	14.0398705722	1.0000000000
S 1		
1	7.7999280957	1.0000000000
S 1		
1	4.3332933865	1.0000000000
S 1		
1	2.4073852147	1.0000000000
S 1		
1	1.3374362304	1.0000000000
S 1		
1	0.7430201280	1.0000000000
S 1		
1	0.4127889600	1.0000000000
S 1		

1	0.2293272000	1.0000000000
S 1		
1	0.1274040000	1.0000000000
P 1		
1	859.5490011017	1.0000000000
P 1		
1	477.5272228343	1.0000000000
P 1		
1	265.2929015746	1.0000000000
P 1		
1	147.3849453192	1.0000000000
P 1		
1	81.8805251773	1.0000000000
P 1		
1	45.4891806541	1.0000000000
P 1		
1	25.2717670300	1.0000000000
P 1		
1	14.0398705722	1.0000000000
P 1		
1	7.7999280957	1.0000000000
P 1		
1	4.3332933865	1.0000000000
P 1		
1	2.4073852147	1.0000000000
P 1		
1	1.3374362304	1.0000000000
P 1		
1	0.7430201280	1.0000000000
P 1		
1	0.4127889600	1.0000000000
P 1		
1	0.2293272000	1.0000000000
P 1		
1	0.1274040000	1.0000000000
D 1		
1	477.5272228343	1.0000000000
D 1		
1	265.2929015746	1.0000000000
D 1		
1	147.3849453192	1.0000000000
D 1		
1	81.8805251773	1.0000000000
D 1		
1	45.4891806541	1.0000000000
D 1		
1	25.2717670300	1.0000000000
D 1		
1	14.0398705722	1.0000000000
D 1		
1	7.7999280957	1.0000000000
D 1		
1	4.3332933865	1.0000000000

D 1		
1	2.4073852147	1.0000000000
D 1		
1	1.3374362304	1.0000000000
D 1		
1	0.7430201280	1.0000000000
D 1		
1	0.4127889600	1.0000000000
D 1		
1	0.2293272000	1.0000000000
D 1		
1	0.1274040000	1.0000000000
F 1		
1	238.5409445128	1.0000000000
F 1		
1	132.5227469516	1.0000000000
F 1		
1	73.6237483064	1.0000000000
F 1		
1	40.9020823925	1.0000000000
F 1		
1	22.7233791069	1.0000000000
F 1		
1	12.6240995038	1.0000000000
F 1		
1	7.0133886132	1.0000000000
F 1		
1	3.8963270074	1.0000000000
F 1		
1	2.1646261152	1.0000000000
F 1		
1	1.2025700640	1.0000000000
F 1		
1	0.6680944800	1.0000000000
F 1		
1	0.3711636000	1.0000000000
F 1		
1	0.2062020000	1.0000000000
G 1		
1	329.6969437065	1.0000000000
G 1		
1	183.1649687258	1.0000000000
G 1		
1	101.7583159588	1.0000000000
G 1		
1	56.5323977549	1.0000000000
G 1		
1	31.4068876416	1.0000000000
G 1		
1	17.4482709120	1.0000000000
G 1		
1	9.6934838400	1.0000000000
G 1		

1	5.3852688000	1.0000000000
G 1		
1	2.9918160000	1.0000000000
G 1		
1	1.6621200000	1.0000000000
G 1		
1	0.9234000000	1.0000000000
G 1		
1	0.5130000000	1.0000000000
G 1		
1	0.2850000000	1.0000000000
H 1		
1	59.3179807223	1.0000000000
H 1		
1	25.7904264010	1.0000000000
H 1		
1	11.2132288700	1.0000000000
H 1		
1	4.8753169000	1.0000000000
H 1		
1	2.1197030000	1.0000000000
H 1		
1	0.9216100000	1.0000000000
H 1		
1	0.4007000000	1.0000000000
I 1		
1	125.4852000000	1.0000000000
I 1		
1	41.8284000000	1.0000000000
I 1		
1	13.9428000000	1.0000000000
I 1		
1	4.6476000000	1.0000000000
I 1		
1	1.5492000000	1.0000000000
I 1		
1	0.5164000000	1.0000000000
J 1		
1	56.4732000000	1.0000000000
J 1		
1	18.8244000000	1.0000000000
J 1		
1	6.2748000000	1.0000000000
J 1		
1	2.0916000000	1.0000000000
J 1		
1	0.6972000000	1.0000000000
end;		
# Auxiliary basis set for element : Ba		
NewAuxGTO Ba		
S 1		
1	156.1037705841	1.0000000000

S 1		
1	86.7243169911	1.0000000000
S 1		
1	48.1801761062	1.0000000000
S 1		
1	26.7667645034	1.0000000000
S 1		
1	14.8704247241	1.0000000000
S 1		
1	8.2613470690	1.0000000000
S 1		
1	4.5896372605	1.0000000000
S 1		
1	2.5497984781	1.0000000000
S 1		
1	1.4165547100	1.0000000000
S 1		
1	0.7869748389	1.0000000000
S 1		
1	0.4372082438	1.0000000000
S 1		
1	0.2428934688	1.0000000000
S 1		
1	0.1349408160	1.0000000000
S 1		
1	0.0749671200	1.0000000000
S 1		
1	0.0416484000	1.0000000000
S 1		
1	0.0231380000	1.0000000000
P 1		
1	156.1037705841	1.0000000000
P 1		
1	86.7243169911	1.0000000000
P 1		
1	48.1801761062	1.0000000000
P 1		
1	26.7667645034	1.0000000000
P 1		
1	14.8704247241	1.0000000000
P 1		
1	8.2613470690	1.0000000000
P 1		
1	4.5896372605	1.0000000000
P 1		
1	2.5497984781	1.0000000000
P 1		
1	1.4165547100	1.0000000000
P 1		
1	0.7869748389	1.0000000000
P 1		
1	0.4372082438	1.0000000000
P 1		

1	0.2428934688	1.0000000000
P 1		
1	0.1349408160	1.0000000000
P 1		
1	0.0749671200	1.0000000000
P 1		
1	0.0416484000	1.0000000000
P 1		
1	0.0231380000	1.0000000000
D 1		
1	86.7243169911	1.0000000000
D 1		
1	48.1801761062	1.0000000000
D 1		
1	26.7667645034	1.0000000000
D 1		
1	14.8704247241	1.0000000000
D 1		
1	8.2613470690	1.0000000000
D 1		
1	4.5896372605	1.0000000000
D 1		
1	2.5497984781	1.0000000000
D 1		
1	1.4165547100	1.0000000000
D 1		
1	0.7869748389	1.0000000000
D 1		
1	0.4372082438	1.0000000000
D 1		
1	0.2428934688	1.0000000000
D 1		
1	0.1349408160	1.0000000000
D 1		
1	0.0749671200	1.0000000000
D 1		
1	0.0416484000	1.0000000000
D 1		
1	0.0231380000	1.0000000000
F 1		
1	17.7452112253	1.0000000000
F 1		
1	8.0660051024	1.0000000000
F 1		
1	3.6663659556	1.0000000000
F 1		
1	1.6665299798	1.0000000000
F 1		
1	0.7575136272	1.0000000000
F 1		
1	0.3443243760	1.0000000000
F 1		
1	0.1565110800	1.0000000000

F 1		
1	0.0711414000	1.0000000000
F 1		
1	0.0323370000	1.0000000000
G 1		
1	22.7932428319	1.0000000000
G 1		
1	10.3605649236	1.0000000000
G 1		
1	4.7093476925	1.0000000000
G 1		
1	2.1406125875	1.0000000000
G 1		
1	0.9730057216	1.0000000000
G 1		
1	0.4422753280	1.0000000000
G 1		
1	0.2010342400	1.0000000000
G 1		
1	0.0913792000	1.0000000000
G 1		
1	0.0415360000	1.0000000000
H 1		
1	34.7898254524	1.0000000000
H 1		
1	15.1260110662	1.0000000000
H 1		
1	6.5765265505	1.0000000000
H 1		
1	2.8593593698	1.0000000000
H 1		
1	1.2431997260	1.0000000000
H 1		
1	0.5405216200	1.0000000000
H 1		
1	0.2350094000	1.0000000000
H 1		
1	0.1021780000	1.0000000000
I 1		
1	28.9092240000	1.0000000000
I 1		
1	9.6364080000	1.0000000000
I 1		
1	3.2121360000	1.0000000000
I 1		
1	1.0707120000	1.0000000000
I 1		
1	0.3569040000	1.0000000000
I 1		
1	0.1189680000	1.0000000000
J 1		
1	12.1069080000	1.0000000000
J 1		

```

1 4.0356360000 1.0000000000
J 1
1 1.3452120000 1.0000000000
J 1
1 0.4484040000 1.0000000000
J 1
1 0.1494680000 1.0000000000
end;

# Auxiliary basis set for element : Cl
NewAuxGTO Cl
S 1
1 4071.0416888573 1.0000000000
S 1
1 2261.6898271430 1.0000000000
S 1
1 1256.4943484128 1.0000000000
S 1
1 698.0524157849 1.0000000000
S 1
1 387.8068976583 1.0000000000
S 1
1 215.4482764768 1.0000000000
S 1
1 119.6934869316 1.0000000000
S 1
1 66.4963816286 1.0000000000
S 1
1 36.9424342381 1.0000000000
S 1
1 20.5235745767 1.0000000000
S 1
1 11.4019858760 1.0000000000
S 1
1 6.3344365978 1.0000000000
S 1
1 3.5191314432 1.0000000000
S 1
1 1.9550730240 1.0000000000
S 1
1 1.0861516800 1.0000000000
S 1
1 0.6034176000 1.0000000000
S 1
1 0.3352320000 1.0000000000
S 1
1 0.1862400000 1.0000000000
P 1
1 1256.4943484128 1.0000000000
P 1
1 698.0524157849 1.0000000000
P 1
1 387.8068976583 1.0000000000

```

```

P 1
1 215.4482764768 1.0000000000
P 1
1 119.6934869316 1.0000000000
P 1
1 66.4963816286 1.0000000000
P 1
1 36.9424342381 1.0000000000
P 1
1 20.5235745767 1.0000000000
P 1
1 11.4019858760 1.0000000000
P 1
1 6.3344365978 1.0000000000
P 1
1 3.5191314432 1.0000000000
P 1
1 1.9550730240 1.0000000000
P 1
1 1.0861516800 1.0000000000
P 1
1 0.6034176000 1.0000000000
P 1
1 0.3352320000 1.0000000000
P 1
1 0.1862400000 1.0000000000
D 1
1 698.0524157849 1.0000000000
D 1
1 387.8068976583 1.0000000000
D 1
1 215.4482764768 1.0000000000
D 1
1 119.6934869316 1.0000000000
D 1
1 66.4963816286 1.0000000000
D 1
1 36.9424342381 1.0000000000
D 1
1 20.5235745767 1.0000000000
D 1
1 11.4019858760 1.0000000000
D 1
1 6.3344365978 1.0000000000
D 1
1 3.5191314432 1.0000000000
D 1
1 1.9550730240 1.0000000000
D 1
1 1.0861516800 1.0000000000
D 1
1 0.6034176000 1.0000000000
D 1
1 0.3352320000 1.0000000000
D 1
1 0.1862400000 1.0000000000

```

1	0.3352320000	1.0000000000
D 1		
1	0.1862400000	1.0000000000
F 1		
1	188.2900972767	1.0000000000
F 1		
1	85.5864078531	1.0000000000
F 1		
1	38.9029126605	1.0000000000
F 1		
1	17.6831421184	1.0000000000
F 1		
1	8.0377918720	1.0000000000
F 1		
1	3.6535417600	1.0000000000
F 1		
1	1.6607008000	1.0000000000
F 1		
1	0.7548640000	1.0000000000
F 1		
1	0.3431200000	1.0000000000
G 1		
1	226.7032087519	1.0000000000
G 1		
1	103.0469130691	1.0000000000
G 1		
1	46.8395059405	1.0000000000
G 1		
1	21.2906845184	1.0000000000
G 1		
1	9.6775838720	1.0000000000
G 1		
1	4.3989017600	1.0000000000
G 1		
1	1.9995008000	1.0000000000
G 1		
1	0.9088640000	1.0000000000
G 1		
1	0.4131200000	1.0000000000
H 1		
1	194.0750504790	1.0000000000
H 1		
1	84.3804567300	1.0000000000
H 1		
1	36.6871551000	1.0000000000
H 1		
1	15.9509370000	1.0000000000
H 1		
1	6.9351900000	1.0000000000
H 1		
1	3.0153000000	1.0000000000
H 1		
1	1.3110000000	1.0000000000

H 1		
1	0.5700000000	1.0000000000
I 1		
1	155.5200000000	1.0000000000
I 1		
1	51.8400000000	1.0000000000
I 1		
1	17.2800000000	1.0000000000
I 1		
1	5.7600000000	1.0000000000
I 1		
1	1.9200000000	1.0000000000
I 1		
1	0.6400000000	1.0000000000
end;		

Auxiliary basis set for element : Pb
NewAuxGTO Pb

S 1		
1	773.4483735542	1.0000000000
S 1		
1	429.6935408634	1.0000000000
S 1		
1	238.7186338130	1.0000000000
S 1		
1	132.6214632295	1.0000000000
S 1		
1	73.6785906830	1.0000000000
S 1		
1	40.9325503795	1.0000000000
S 1		
1	22.7403057664	1.0000000000
S 1		
1	12.6335032035	1.0000000000
S 1		
1	7.0186128909	1.0000000000
S 1		
1	3.8992293838	1.0000000000
S 1		
1	2.1662385466	1.0000000000
S 1		
1	1.2034658592	1.0000000000
S 1		
1	0.6685921440	1.0000000000
S 1		
1	0.3714400800	1.0000000000
S 1		
1	0.2063556000	1.0000000000
S 1		
1	0.1146420000	1.0000000000
S 1		
1	0.0636900000	1.0000000000
P 1		

1	238.7186338130	1.0000000000
P 1		
1	132.6214632295	1.0000000000
P 1		
1	73.6785906830	1.0000000000
P 1		
1	40.9325503795	1.0000000000
P 1		
1	22.7403057664	1.0000000000
P 1		
1	12.6335032035	1.0000000000
P 1		
1	7.0186128909	1.0000000000
P 1		
1	3.8992293838	1.0000000000
P 1		
1	2.1662385466	1.0000000000
P 1		
1	1.2034658592	1.0000000000
P 1		
1	0.6685921440	1.0000000000
P 1		
1	0.3714400800	1.0000000000
P 1		
1	0.2063556000	1.0000000000
P 1		
1	0.1146420000	1.0000000000
P 1		
1	0.0636900000	1.0000000000
D 1		
1	132.6214632295	1.0000000000
D 1		
1	73.6785906830	1.0000000000
D 1		
1	40.9325503795	1.0000000000
D 1		
1	22.7403057664	1.0000000000
D 1		
1	12.6335032035	1.0000000000
D 1		
1	7.0186128909	1.0000000000
D 1		
1	3.8992293838	1.0000000000
D 1		
1	2.1662385466	1.0000000000
D 1		
1	1.2034658592	1.0000000000
D 1		
1	0.6685921440	1.0000000000
D 1		
1	0.3714400800	1.0000000000
D 1		
1	0.2063556000	1.0000000000

D 1		
1	0.1146420000	1.0000000000
D 1		
1	0.0636900000	1.0000000000
F 1		
1	120.8252536331	1.0000000000
F 1		
1	67.1251409073	1.0000000000
F 1		
1	37.2917449485	1.0000000000
F 1		
1	20.7176360825	1.0000000000
F 1		
1	11.5097978236	1.0000000000
F 1		
1	6.3943321242	1.0000000000
F 1		
1	3.5524067357	1.0000000000
F 1		
1	1.9735592976	1.0000000000
F 1		
1	1.0964218320	1.0000000000
F 1		
1	0.6091232400	1.0000000000
F 1		
1	0.3384018000	1.0000000000
F 1		
1	0.1880010000	1.0000000000
F 1		
1	0.1044450000	1.0000000000
G 1		
1	93.3177314350	1.0000000000
G 1		
1	51.8431841306	1.0000000000
G 1		
1	28.8017689614	1.0000000000
G 1		
1	16.0009827564	1.0000000000
G 1		
1	8.8894348646	1.0000000000
G 1		
1	4.9385749248	1.0000000000
G 1		
1	2.7436527360	1.0000000000
G 1		
1	1.5242515200	1.0000000000
G 1		
1	0.8468064000	1.0000000000
G 1		
1	0.4704480000	1.0000000000
G 1		
1	0.2613600000	1.0000000000
G 1		

1	0.1452000000	1.0000000000
H 1		
1	30.6582326119	1.0000000000
H 1		
1	13.3296663530	1.0000000000
H 1		
1	5.7955071100	1.0000000000
H 1		
1	2.5197857000	1.0000000000
H 1		
1	1.0955590000	1.0000000000
H 1		
1	0.4763300000	1.0000000000
H 1		
1	0.2071000000	1.0000000000
I 1		
1	21.7890000000	1.0000000000
I 1		
1	7.2630000000	1.0000000000
I 1		
1	2.4210000000	1.0000000000
I 1		
1	0.8070000000	1.0000000000
I 1		
1	0.2690000000	1.0000000000
J 1		
1	31.5495000000	1.0000000000
J 1		
1	10.5165000000	1.0000000000
J 1		
1	3.5055000000	1.0000000000
J 1		
1	1.1685000000	1.0000000000
J 1		
1	0.3895000000	1.0000000000
end;		
# Auxiliary basis set for element : Li		
NewAuxGTO Li		
S 1		
1	1145.4526318880	1.0000000000
S 1		
1	636.3625732711	1.0000000000
S 1		
1	353.5347629284	1.0000000000
S 1		
1	196.4082016269	1.0000000000
S 1		
1	109.1156675705	1.0000000000
S 1		
1	60.6198153169	1.0000000000
S 1		
1	33.6776751761	1.0000000000

S 1		
1	18.7098195423	1.0000000000
S 1		
1	10.3943441901	1.0000000000
S 1		
1	5.7746356612	1.0000000000
S 1		
1	3.2081309229	1.0000000000
S 1		
1	1.7822949572	1.0000000000
S 1		
1	0.9901638651	1.0000000000
S 1		
1	0.5500910362	1.0000000000
S 1		
1	0.3056061312	1.0000000000
S 1		
1	0.1697811840	1.0000000000
S 1		
1	0.0943228800	1.0000000000
S 1		
1	0.0524016000	1.0000000000
S 1		
1	0.0291120000	1.0000000000
P 1		
1	353.5347629284	1.0000000000
P 1		
1	196.4082016269	1.0000000000
P 1		
1	109.1156675705	1.0000000000
P 1		
1	60.6198153169	1.0000000000
P 1		
1	33.6776751761	1.0000000000
P 1		
1	18.7098195423	1.0000000000
P 1		
1	10.3943441901	1.0000000000
P 1		
1	5.7746356612	1.0000000000
P 1		
1	3.2081309229	1.0000000000
P 1		
1	1.7822949572	1.0000000000
P 1		
1	0.9901638651	1.0000000000
P 1		
1	0.5500910362	1.0000000000
P 1		
1	0.3056061312	1.0000000000
P 1		
1	0.1697811840	1.0000000000
P 1		

1	0.0943228800	1.0000000000
P 1		
1	0.0524016000	1.0000000000
P 1		
1	0.0291120000	1.0000000000
D 1		
1	196.4082016269	1.0000000000
D 1		
1	109.1156675705	1.0000000000
D 1		
1	60.6198153169	1.0000000000
D 1		
1	33.6776751761	1.0000000000
D 1		
1	18.7098195423	1.0000000000
D 1		
1	10.3943441901	1.0000000000
D 1		
1	5.7746356612	1.0000000000
D 1		
1	3.2081309229	1.0000000000
D 1		
1	1.7822949572	1.0000000000
D 1		
1	0.9901638651	1.0000000000
D 1		
1	0.5500910362	1.0000000000
D 1		
1	0.3056061312	1.0000000000
D 1		
1	0.1697811840	1.0000000000
D 1		
1	0.0943228800	1.0000000000
D 1		
1	0.0524016000	1.0000000000
D 1		
1	0.0291120000	1.0000000000
F 1		
1	37.7304556084	1.0000000000
F 1		
1	17.1502070947	1.0000000000
F 1		
1	7.7955486794	1.0000000000
F 1		
1	3.5434312179	1.0000000000
F 1		
1	1.6106505536	1.0000000000
F 1		
1	0.7321138880	1.0000000000
F 1		
1	0.3327790400	1.0000000000
F 1		
1	0.1512632000	1.0000000000

F 1		
1	0.0687560000	1.0000000000
G 1		
1	58.5832875521	1.0000000000
G 1		
1	26.6287670691	1.0000000000
G 1		
1	12.1039850314	1.0000000000
G 1		
1	5.5018113779	1.0000000000
G 1		
1	2.5008233536	1.0000000000
G 1		
1	1.1367378880	1.0000000000
G 1		
1	0.5166990400	1.0000000000
G 1		
1	0.2348632000	1.0000000000
G 1		
1	0.1067560000	1.0000000000
H 1		
1	49.8466445441	1.0000000000
H 1		
1	21.6724541496	1.0000000000
H 1		
1	9.4228061520	1.0000000000
H 1		
1	4.0968722400	1.0000000000
H 1		
1	1.7812488000	1.0000000000
H 1		
1	0.7744560000	1.0000000000
H 1		
1	0.3367200000	1.0000000000
H 1		
1	0.1464000000	1.0000000000
I 1		
1	44.8092000000	1.0000000000
I 1		
1	14.9364000000	1.0000000000
I 1		
1	4.9788000000	1.0000000000
I 1		
1	1.6596000000	1.0000000000
I 1		
1	0.5532000000	1.0000000000
I 1		
1	0.1844000000	1.0000000000
end;		
# Auxiliary basis set for element : F		
NewAuxGTO F		
S 1		

1	12386.2492621034	1.0000000000
S 1		
1	6881.2495900574	1.0000000000
S 1		
1	3822.9164389208	1.0000000000
S 1		
1	2123.8424660671	1.0000000000
S 1		
1	1179.9124811484	1.0000000000
S 1		
1	655.5069339713	1.0000000000
S 1		
1	364.1705188730	1.0000000000
S 1		
1	202.3169549294	1.0000000000
S 1		
1	112.3983082941	1.0000000000
S 1		
1	62.4435046078	1.0000000000
S 1		
1	34.6908358932	1.0000000000
S 1		
1	19.2726866074	1.0000000000
S 1		
1	10.7070481152	1.0000000000
S 1		
1	5.9483600640	1.0000000000
S 1		
1	3.3046444800	1.0000000000
S 1		
1	1.8359136000	1.0000000000
S 1		
1	1.0199520000	1.0000000000
S 1		
1	0.5666400000	1.0000000000
S 1		
1	0.3148000000	1.0000000000
P 1		
1	3822.9164389208	1.0000000000
P 1		
1	2123.8424660671	1.0000000000
P 1		
1	1179.9124811484	1.0000000000
P 1		
1	655.5069339713	1.0000000000
P 1		
1	364.1705188730	1.0000000000
P 1		
1	202.3169549294	1.0000000000
P 1		
1	112.3983082941	1.0000000000
P 1		
1	62.4435046078	1.0000000000
P 1		
1	34.6908358932	1.0000000000
P 1		
1	19.2726866074	1.0000000000
P 1		
1	10.7070481152	1.0000000000
P 1		
1	5.9483600640	1.0000000000
P 1		
1	3.3046444800	1.0000000000
P 1		
1	1.8359136000	1.0000000000
P 1		
1	1.0199520000	1.0000000000
P 1		
1	0.5666400000	1.0000000000
P 1		
1	0.3148000000	1.0000000000
F 1		
1	340.4499194173	1.0000000000
F 1		

P 1		
1	34.6908358932	1.0000000000
P 1		
1	19.2726866074	1.0000000000
P 1		
1	10.7070481152	1.0000000000
P 1		
1	5.9483600640	1.0000000000
P 1		
1	3.3046444800	1.0000000000
P 1		
1	1.8359136000	1.0000000000
P 1		
1	1.0199520000	1.0000000000
P 1		
1	0.5666400000	1.0000000000
P 1		
1	0.3148000000	1.0000000000
D 1		
1	2123.8424660671	1.0000000000
D 1		
1	1179.9124811484	1.0000000000
D 1		
1	655.5069339713	1.0000000000
D 1		
1	364.1705188730	1.0000000000
D 1		
1	202.3169549294	1.0000000000
D 1		
1	112.3983082941	1.0000000000
D 1		
1	62.4435046078	1.0000000000
D 1		
1	34.6908358932	1.0000000000
D 1		
1	19.2726866074	1.0000000000
D 1		
1	10.7070481152	1.0000000000
D 1		
1	5.9483600640	1.0000000000
D 1		
1	3.3046444800	1.0000000000
D 1		
1	1.8359136000	1.0000000000
D 1		
1	1.0199520000	1.0000000000
D 1		
1	0.5666400000	1.0000000000
D 1		
1	0.3148000000	1.0000000000
F 1		
1	340.4499194173	1.0000000000
F 1		

1	154.7499633715	1.0000000000
F 1		
1	70.3408924416	1.0000000000
F 1		
1	31.9731329280	1.0000000000
F 1		
1	14.5332422400	1.0000000000
F 1		
1	6.6060192000	1.0000000000
F 1		
1	3.0027360000	1.0000000000
F 1		
1	1.3648800000	1.0000000000
F 1		
1	0.6204000000	1.0000000000
G 1		
1	508.1505889434	1.0000000000
G 1		
1	230.9775404288	1.0000000000
G 1		
1	104.9897911040	1.0000000000
G 1		
1	47.7226323200	1.0000000000
G 1		
1	21.6921056000	1.0000000000
G 1		
1	9.8600480000	1.0000000000
G 1		
1	4.4818400000	1.0000000000
G 1		
1	2.0372000000	1.0000000000
G 1		
1	0.9260000000	1.0000000000
H 1		
1	430.0294539561	1.0000000000
H 1		
1	186.9693278070	1.0000000000
H 1		
1	81.2910120900	1.0000000000
H 1		
1	35.3439183000	1.0000000000
H 1		
1	15.3669210000	1.0000000000
H 1		
1	6.6812700000	1.0000000000
H 1		
1	2.9049000000	1.0000000000
H 1		
1	1.2630000000	1.0000000000
I 1		
1	388.8000000000	1.0000000000
I 1		
1	129.6000000000	1.0000000000

I 1		
1	43.2000000000	1.0000000000
I 1		
1	14.4000000000	1.0000000000
I 1		
1	4.8000000000	1.0000000000
I 1		
1	1.6000000000	1.0000000000
end;		

Auxiliary basis set for element : Sr
NewAuxGTO Sr

S 1		
1	353.7533540844	1.0000000000
S 1		
1	196.5296411580	1.0000000000
S 1		
1	109.1831339767	1.0000000000
S 1		
1	60.6572966537	1.0000000000
S 1		
1	33.6984981409	1.0000000000
S 1		
1	18.7213878561	1.0000000000
S 1		
1	10.4007710312	1.0000000000
S 1		
1	5.7782061284	1.0000000000
S 1		
1	3.2101145158	1.0000000000
S 1		
1	1.7833969532	1.0000000000
S 1		
1	0.9907760851	1.0000000000
S 1		
1	0.5504311584	1.0000000000
S 1		
1	0.3057950880	1.0000000000
S 1		
1	0.1698861600	1.0000000000
S 1		
1	0.0943812000	1.0000000000
S 1		
1	0.0524340000	1.0000000000
S 1		
1	0.0291300000	1.0000000000
P 1		
1	109.1831339767	1.0000000000
P 1		
1	60.6572966537	1.0000000000
P 1		
1	33.6984981409	1.0000000000
P 1		

1	18.7213878561	1.0000000000
P 1		
1	10.4007710312	1.0000000000
P 1		
1	5.7782061284	1.0000000000
P 1		
1	3.2101145158	1.0000000000
P 1		
1	1.7833969532	1.0000000000
P 1		
1	0.9907760851	1.0000000000
P 1		
1	0.5504311584	1.0000000000
P 1		
1	0.3057950880	1.0000000000
P 1		
1	0.1698861600	1.0000000000
P 1		
1	0.0943812000	1.0000000000
P 1		
1	0.0524340000	1.0000000000
P 1		
1	0.0291300000	1.0000000000
D 1		
1	60.6572966537	1.0000000000
D 1		
1	33.6984981409	1.0000000000
D 1		
1	18.7213878561	1.0000000000
D 1		
1	10.4007710312	1.0000000000
D 1		
1	5.7782061284	1.0000000000
D 1		
1	3.2101145158	1.0000000000
D 1		
1	1.7833969532	1.0000000000
D 1		
1	0.9907760851	1.0000000000
D 1		
1	0.5504311584	1.0000000000
D 1		
1	0.3057950880	1.0000000000
D 1		
1	0.1698861600	1.0000000000
D 1		
1	0.0943812000	1.0000000000
D 1		
1	0.0524340000	1.0000000000
D 1		
1	0.0291300000	1.0000000000
D 1		
F 1		
1	15.9853419610	1.0000000000

F 1		
1	7.2660645277	1.0000000000
F 1		
1	3.3027566035	1.0000000000
F 1		
1	1.5012530016	1.0000000000
F 1		
1	0.6823877280	1.0000000000
F 1		
1	0.3101762400	1.0000000000
F 1		
1	0.1409892000	1.0000000000
F 1		
1	0.0640860000	1.0000000000
F 1		
1	0.0291300000	1.0000000000
G 1		
1	15.9853419610	1.0000000000
G 1		
1	7.2660645277	1.0000000000
G 1		
1	3.3027566035	1.0000000000
G 1		
1	1.5012530016	1.0000000000
G 1		
1	0.6823877280	1.0000000000
G 1		
1	0.3101762400	1.0000000000
G 1		
1	0.1409892000	1.0000000000
G 1		
1	0.0640860000	1.0000000000
G 1		
1	0.0291300000	1.0000000000
H 1		
1	12.9775662092	1.0000000000
H 1		
1	5.6424200909	1.0000000000
H 1		
1	2.4532261265	1.0000000000
H 1		
1	1.0666200550	1.0000000000
H 1		
1	0.4637478500	1.0000000000
H 1		
1	0.2016295000	1.0000000000
H 1		
1	0.0876650000	1.0000000000
I 1		
1	7.9270650000	1.0000000000
I 1		
1	2.6423550000	1.0000000000
I 1		

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1 0.8807850000 1.0000000000
I 1
1 0.2935950000 1.0000000000
I 1
1 0.0978650000 1.0000000000
J 1
1 4.2228000000 1.0000000000
J 1
1 1.4076000000 1.0000000000
J 1
1 0.4692000000 1.0000000000
J 1
1 0.1564000000 1.0000000000
end;

```

```

# Auxiliary basis set for element : I
NewAuxGTO I

```

```

S 1
1 1316.3802291809 1.0000000000
S 1
1 731.3223495449 1.0000000000
S 1
1 406.2901941916 1.0000000000
S 1
1 225.7167745509 1.0000000000
S 1
1 125.3982080838 1.0000000000
S 1
1 69.6656711577 1.0000000000
S 1
1 38.7031506432 1.0000000000
S 1
1 21.5017503573 1.0000000000
S 1
1 11.9454168652 1.0000000000
S 1
1 6.6363427029 1.0000000000
S 1
1 3.6868570572 1.0000000000
S 1
1 2.0482539206 1.0000000000
S 1
1 1.1379188448 1.0000000000
S 1
1 0.6321771360 1.0000000000
S 1
1 0.3512095200 1.0000000000
S 1
1 0.1951164000 1.0000000000
S 1
1 0.1083980000 1.0000000000
P 1
1 406.2901941916 1.0000000000

```

```

P 1
1 225.7167745509 1.0000000000
P 1
1 125.3982080838 1.0000000000
P 1
1 69.6656711577 1.0000000000
P 1
1 38.7031506432 1.0000000000
P 1
1 21.5017503573 1.0000000000
P 1
1 11.9454168652 1.0000000000
P 1
1 6.6363427029 1.0000000000
P 1
1 3.6868570572 1.0000000000
P 1
1 2.0482539206 1.0000000000
P 1
1 1.1379188448 1.0000000000
P 1
1 0.6321771360 1.0000000000
P 1
1 0.3512095200 1.0000000000
P 1
1 0.1951164000 1.0000000000
P 1
1 0.1083980000 1.0000000000
D 1
1 225.7167745509 1.0000000000
D 1
1 125.3982080838 1.0000000000
D 1
1 69.6656711577 1.0000000000
D 1
1 38.7031506432 1.0000000000
D 1
1 21.5017503573 1.0000000000
D 1
1 11.9454168652 1.0000000000
D 1
1 6.6363427029 1.0000000000
D 1
1 3.6868570572 1.0000000000
D 1
1 2.0482539206 1.0000000000
D 1
1 1.1379188448 1.0000000000
D 1
1 0.6321771360 1.0000000000
D 1
1 0.3512095200 1.0000000000
D 1

```

1	0.1951164000	1.0000000000
D 1		
1	0.1083980000	1.0000000000
F 1		
1	223.7300323364	1.0000000000
F 1		
1	124.2944624091	1.0000000000
F 1		
1	69.0524791162	1.0000000000
F 1		
1	38.3624883979	1.0000000000
F 1		
1	21.3124935544	1.0000000000
F 1		
1	11.8402741969	1.0000000000
F 1		
1	6.5779301094	1.0000000000
F 1		
1	3.6544056163	1.0000000000
F 1		
1	2.0302253424	1.0000000000
F 1		
1	1.1279029680	1.0000000000
F 1		
1	0.6266127600	1.0000000000
F 1		
1	0.3481182000	1.0000000000
F 1		
1	0.1933990000	1.0000000000
G 1		
1	160.5418456938	1.0000000000
G 1		
1	89.1899142743	1.0000000000
G 1		
1	49.5499523746	1.0000000000
G 1		
1	27.5277513192	1.0000000000
G 1		
1	15.2931951774	1.0000000000
G 1		
1	8.4962195430	1.0000000000
G 1		
1	4.7201219683	1.0000000000
G 1		
1	2.6222899824	1.0000000000
G 1		
1	1.4568277680	1.0000000000
G 1		
1	0.8093487600	1.0000000000
G 1		
1	0.4496382000	1.0000000000
G 1		
1	0.2497990000	1.0000000000

H 1		
1	49.5624156372	1.0000000000
H 1		
1	21.5488763640	1.0000000000
H 1		
1	9.3690766800	1.0000000000
H 1		
1	4.0735116000	1.0000000000
H 1		
1	1.7710920000	1.0000000000
H 1		
1	0.7700400000	1.0000000000
H 1		
1	0.3348000000	1.0000000000
I 1		
1	95.0616000000	1.0000000000
I 1		
1	31.6872000000	1.0000000000
I 1		
1	10.5624000000	1.0000000000
I 1		
1	3.5208000000	1.0000000000
I 1		
1	1.1736000000	1.0000000000
I 1		
1	0.3912000000	1.0000000000
J 1		
1	41.9742000000	1.0000000000
J 1		
1	13.9914000000	1.0000000000
J 1		
1	4.6638000000	1.0000000000
J 1		
1	1.5546000000	1.0000000000
J 1		
1	0.5182000000	1.0000000000
end;		
# Auxiliary basis set for element : Be		
NewAuxGTO Be		
S 1		
1	2653.5217605980	1.0000000000
S 1		
1	1474.1787558878	1.0000000000
S 1		
1	818.9881977154	1.0000000000
S 1		
1	454.9934431752	1.0000000000
S 1		
1	252.7741350974	1.0000000000
S 1		
1	140.4300750541	1.0000000000
S 1		

1	78.0167083634	1.0000000000
S 1		
1	43.3426157574	1.0000000000
S 1		
1	24.0792309764	1.0000000000
S 1		
1	13.3773505424	1.0000000000
S 1		
1	7.4318614125	1.0000000000
S 1		
1	4.1288118958	1.0000000000
S 1		
1	2.2937843866	1.0000000000
S 1		
1	1.2743246592	1.0000000000
S 1		
1	0.7079581440	1.0000000000
S 1		
1	0.3933100800	1.0000000000
S 1		
1	0.2185056000	1.0000000000
S 1		
1	0.1213920000	1.0000000000
S 1		
1	0.0674400000	1.0000000000
P 1		
1	818.9881977154	1.0000000000
P 1		
1	454.9934431752	1.0000000000
P 1		
1	252.7741350974	1.0000000000
P 1		
1	140.4300750541	1.0000000000
P 1		
1	78.0167083634	1.0000000000
P 1		
1	43.3426157574	1.0000000000
P 1		
1	24.0792309764	1.0000000000
P 1		
1	13.3773505424	1.0000000000
P 1		
1	7.4318614125	1.0000000000
P 1		
1	4.1288118958	1.0000000000
P 1		
1	2.2937843866	1.0000000000
P 1		
1	1.2743246592	1.0000000000
P 1		
1	0.7079581440	1.0000000000
P 1		
1	0.3933100800	1.0000000000
P 1		

P 1		
1	0.2185056000	1.0000000000
P 1		
1	0.1213920000	1.0000000000
P 1		
1	0.0674400000	1.0000000000
D 1		
1	454.9934431752	1.0000000000
D 1		
1	252.7741350974	1.0000000000
D 1		
1	140.4300750541	1.0000000000
D 1		
1	78.0167083634	1.0000000000
D 1		
1	43.3426157574	1.0000000000
D 1		
1	24.0792309764	1.0000000000
D 1		
1	13.3773505424	1.0000000000
D 1		
1	7.4318614125	1.0000000000
D 1		
1	4.1288118958	1.0000000000
D 1		
1	2.2937843866	1.0000000000
D 1		
1	1.2743246592	1.0000000000
D 1		
1	0.7079581440	1.0000000000
D 1		
1	0.3933100800	1.0000000000
D 1		
1	0.2185056000	1.0000000000
D 1		
1	0.1213920000	1.0000000000
D 1		
1	0.0674400000	1.0000000000
F 1		
1	101.6410929634	1.0000000000
F 1		
1	46.2004968015	1.0000000000
F 1		
1	21.0002258189	1.0000000000
F 1		
1	9.5455571904	1.0000000000
F 1		
1	4.3388896320	1.0000000000
F 1		
1	1.9722225600	1.0000000000
F 1		
1	0.8964648000	1.0000000000
F 1		

```

1 0.4074840000 1.0000000000
F 1
1 0.1852200000 1.0000000000
G 1
1 132.5362097641 1.0000000000
G 1
1 60.2437317110 1.0000000000
G 1
1 27.3835144141 1.0000000000
G 1
1 12.4470520064 1.0000000000
G 1
1 5.6577509120 1.0000000000
G 1
1 2.5717049600 1.0000000000
G 1
1 1.1689568000 1.0000000000
G 1
1 0.5313440000 1.0000000000
G 1
1 0.2415200000 1.0000000000
H 1
1 52.1115936458 1.0000000000
H 1
1 22.6572146286 1.0000000000
H 1
1 9.8509628820 1.0000000000
H 1
1 4.2830273400 1.0000000000
H 1
1 1.8621858000 1.0000000000
H 1
1 0.8096460000 1.0000000000
H 1
1 0.3520200000 1.0000000000
I 1
1 100.9908000000 1.0000000000
I 1
1 33.6636000000 1.0000000000
I 1
1 11.2212000000 1.0000000000
I 1
1 3.7404000000 1.0000000000
I 1
1 1.2468000000 1.0000000000
I 1
1 0.4156000000 1.0000000000
end;

# Auxiliary basis set for element : O
NewAuxGTO O
S 1
1 10112.0268753512 1.0000000000

```

```

S 1
1 5617.7927085285 1.0000000000
S 1
1 3120.9959491825 1.0000000000
S 1
1 1733.8866384347 1.0000000000
S 1
1 963.2703546859 1.0000000000
S 1
1 535.1501970477 1.0000000000
S 1
1 297.3056650265 1.0000000000
S 1
1 165.1698139036 1.0000000000
S 1
1 91.7610077242 1.0000000000
S 1
1 50.9783376246 1.0000000000
S 1
1 28.3212986803 1.0000000000
S 1
1 15.7340548224 1.0000000000
S 1
1 8.7411415680 1.0000000000
S 1
1 4.8561897600 1.0000000000
S 1
1 2.6978832000 1.0000000000
S 1
1 1.4988240000 1.0000000000
S 1
1 0.8326800000 1.0000000000
S 1
1 0.4626000000 1.0000000000
S 1
1 0.2570000000 1.0000000000
P 1
1 3120.9959491825 1.0000000000
P 1
1 1733.8866384347 1.0000000000
P 1
1 963.2703546859 1.0000000000
P 1
1 535.1501970477 1.0000000000
P 1
1 297.3056650265 1.0000000000
P 1
1 165.1698139036 1.0000000000
P 1
1 91.7610077242 1.0000000000
P 1
1 50.9783376246 1.0000000000
P 1

```

1	28.3212986803	1.0000000000
P 1		
1	15.7340548224	1.0000000000
P 1		
1	8.7411415680	1.0000000000
P 1		
1	4.8561897600	1.0000000000
P 1		
1	2.6978832000	1.0000000000
P 1		
1	1.4988240000	1.0000000000
P 1		
1	0.8326800000	1.0000000000
P 1		
1	0.4626000000	1.0000000000
P 1		
1	0.2570000000	1.0000000000
D 1		
1	1733.8866384347	1.0000000000
D 1		
1	963.2703546859	1.0000000000
D 1		
1	535.1501970477	1.0000000000
D 1		
1	297.3056650265	1.0000000000
D 1		
1	165.1698139036	1.0000000000
D 1		
1	91.7610077242	1.0000000000
D 1		
1	50.9783376246	1.0000000000
D 1		
1	28.3212986803	1.0000000000
D 1		
1	15.7340548224	1.0000000000
D 1		
1	8.7411415680	1.0000000000
D 1		
1	4.8561897600	1.0000000000
D 1		
1	2.6978832000	1.0000000000
D 1		
1	1.4988240000	1.0000000000
D 1		
1	0.8326800000	1.0000000000
D 1		
1	0.4626000000	1.0000000000
D 1		
1	0.2570000000	1.0000000000
F 1		
1	583.714668024	1.0000000000
F 1		
1	265.3248485466	1.0000000000

F 1		
1	120.6022038848	1.0000000000
F 1		
1	54.8191835840	1.0000000000
F 1		
1	24.9178107200	1.0000000000
F 1		
1	11.3262776000	1.0000000000
F 1		
1	5.1483080000	1.0000000000
F 1		
1	2.3401400000	1.0000000000
F 1		
1	1.0637000000	1.0000000000
F 1		
1	0.4835000000	1.0000000000
G 1		
1	389.6187021056	1.0000000000
G 1		
1	177.0994100480	1.0000000000
G 1		
1	80.4997318400	1.0000000000
G 1		
1	36.5907872000	1.0000000000
G 1		
1	16.6321760000	1.0000000000
G 1		
1	7.5600800000	1.0000000000
G 1		
1	3.4364000000	1.0000000000
G 1		
1	1.5620000000	1.0000000000
G 1		
1	0.7100000000	1.0000000000
H 1		
1	325.5013127332	1.0000000000
H 1		
1	141.5223098840	1.0000000000
H 1		
1	61.5314390800	1.0000000000
H 1		
1	26.7527996000	1.0000000000
H 1		
1	11.6316520000	1.0000000000
H 1		
1	5.0572400000	1.0000000000
H 1		
1	2.1988000000	1.0000000000
H 1		
1	0.9560000000	1.0000000000
I 1		
1	292.0860000000	1.0000000000
I 1		

```

1  97.3620000000  1.0000000000
l 1
1  32.4540000000  1.0000000000
l 1
1  10.8180000000  1.0000000000
l 1
1  3.6060000000  1.0000000000
l 1
1  1.2020000000  1.0000000000
end;

```

Auxiliary basis set for element : Na
NewAuxGTO Na

```

S 1
1  1685.7417690148  1.0000000000
S 1
1  936.5232050082  1.0000000000
S 1
1  520.2906694490  1.0000000000
S 1
1  289.0503719161  1.0000000000
S 1
1  160.5835399534  1.0000000000
S 1
1  89.2130777519  1.0000000000
S 1
1  49.5628209733  1.0000000000
S 1
1  27.5349005407  1.0000000000
S 1
1  15.2971669671  1.0000000000
S 1
1  8.4984260928  1.0000000000
S 1
1  4.7213478293  1.0000000000
S 1
1  2.6229710163  1.0000000000
S 1
1  1.4572061202  1.0000000000
S 1
1  0.8095589556  1.0000000000
S 1
1  0.4497549754  1.0000000000
S 1
1  0.2498638752  1.0000000000
S 1
1  0.1388132640  1.0000000000
S 1
1  0.0771184800  1.0000000000
S 1
1  0.0428436000  1.0000000000
S 1
1  0.0238020000  1.0000000000

```

```

P 1
1  289.0503719161  1.0000000000
P 1
1  160.5835399534  1.0000000000
P 1
1  89.2130777519  1.0000000000
P 1
1  49.5628209733  1.0000000000
P 1
1  27.5349005407  1.0000000000
P 1
1  15.2971669671  1.0000000000
P 1
1  8.4984260928  1.0000000000
P 1
1  4.7213478293  1.0000000000
P 1
1  2.6229710163  1.0000000000
P 1
1  1.4572061202  1.0000000000
P 1
1  0.8095589556  1.0000000000
P 1
1  0.4497549754  1.0000000000
P 1
1  0.2498638752  1.0000000000
P 1
1  0.1388132640  1.0000000000
P 1
1  0.0771184800  1.0000000000
P 1
1  0.0428436000  1.0000000000
P 1
1  0.0238020000  1.0000000000
D 1
1  289.0503719161  1.0000000000
D 1
1  160.5835399534  1.0000000000
D 1
1  89.2130777519  1.0000000000
D 1
1  49.5628209733  1.0000000000
D 1
1  27.5349005407  1.0000000000
D 1
1  15.2971669671  1.0000000000
D 1
1  8.4984260928  1.0000000000
D 1
1  4.7213478293  1.0000000000
D 1
1  2.6229710163  1.0000000000
D 1

```

1	1.4572061202	1.0000000000
D 1		
1	0.8095589556	1.0000000000
D 1		
1	0.4497549754	1.0000000000
D 1		
1	0.2498638752	1.0000000000
D 1		
1	0.1388132640	1.0000000000
D 1		
1	0.0771184800	1.0000000000
D 1		
1	0.0428436000	1.0000000000
D 1		
1	0.0238020000	1.0000000000
F 1		
1	74.2482641634	1.0000000000
F 1		
1	33.7492109834	1.0000000000
F 1		
1	15.3405504470	1.0000000000
F 1		
1	6.9729774759	1.0000000000
F 1		
1	3.1695352163	1.0000000000
F 1		
1	1.4406978256	1.0000000000
F 1		
1	0.6548626480	1.0000000000
F 1		
1	0.2976648400	1.0000000000
F 1		
1	0.1353022000	1.0000000000
F 1		
1	0.0615010000	1.0000000000
G 1		
1	47.0840482526	1.0000000000
G 1		
1	21.4018401148	1.0000000000
G 1		
1	9.7281091431	1.0000000000
G 1		
1	4.4218677923	1.0000000000
G 1		
1	2.0099399056	1.0000000000
G 1		
1	0.9136090480	1.0000000000
G 1		
1	0.4152768400	1.0000000000
G 1		
1	0.1887622000	1.0000000000
G 1		
1	0.0858010000	1.0000000000

H 1		
1	42.0495942704	1.0000000000
H 1		
1	18.2824322915	1.0000000000
H 1		
1	7.9488836050	1.0000000000
H 1		
1	3.4560363500	1.0000000000
H 1		
1	1.5026245000	1.0000000000
H 1		
1	0.6533150000	1.0000000000
H 1		
1	0.2840500000	1.0000000000
H 1		
1	0.1235000000	1.0000000000
I 1		
1	35.9154000000	1.0000000000
I 1		
1	11.9718000000	1.0000000000
I 1		
1	3.9906000000	1.0000000000
I 1		
1	1.3302000000	1.0000000000
I 1		
1	0.4434000000	1.0000000000
I 1		
1	0.1478000000	1.0000000000
end;		
# Auxiliary basis set for element : Mg		
NewAuxGTO Mg		
S 1		
1	2815.9437331328	1.0000000000
S 1		
1	1564.4131850738	1.0000000000
S 1		
1	869.1184361521	1.0000000000
S 1		
1	482.8435756401	1.0000000000
S 1		
1	268.2464309111	1.0000000000
S 1		
1	149.0257949506	1.0000000000
S 1		
1	82.7921083059	1.0000000000
S 1		
1	45.9956157255	1.0000000000
S 1		
1	25.5531198475	1.0000000000
S 1		
1	14.1961776931	1.0000000000
S 1		

1	7.8867653850	1.0000000000
S 1		
1	4.3815363250	1.0000000000
S 1		
1	2.4341868472	1.0000000000
S 1		
1	1.3523260262	1.0000000000
S 1		
1	0.7512922368	1.0000000000
S 1		
1	0.4173845760	1.0000000000
S 1		
1	0.2318803200	1.0000000000
S 1		
1	0.1288224000	1.0000000000
S 1		
1	0.0715680000	1.0000000000
S 1		
1	0.0397600000	1.0000000000
P 1		
1	1564.4131850738	1.0000000000
P 1		
1	869.1184361521	1.0000000000
P 1		
1	482.8435756401	1.0000000000
P 1		
1	268.2464309111	1.0000000000
P 1		
1	149.0257949506	1.0000000000
P 1		
1	82.7921083059	1.0000000000
P 1		
1	45.9956157255	1.0000000000
P 1		
1	25.5531198475	1.0000000000
P 1		
1	14.1961776931	1.0000000000
P 1		
1	7.8867653850	1.0000000000
P 1		
1	4.3815363250	1.0000000000
P 1		
1	2.4341868472	1.0000000000
P 1		
1	1.3523260262	1.0000000000
P 1		
1	0.7512922368	1.0000000000
P 1		
1	0.4173845760	1.0000000000
P 1		
1	0.2318803200	1.0000000000
P 1		
1	0.1288224000	1.0000000000

P 1		
1	0.0715680000	1.0000000000
P 1		
1	0.0397600000	1.0000000000
D 1		
1	869.1184361521	1.0000000000
D 1		
1	482.8435756401	1.0000000000
D 1		
1	268.2464309111	1.0000000000
D 1		
1	149.0257949506	1.0000000000
D 1		
1	82.7921083059	1.0000000000
D 1		
1	45.9956157255	1.0000000000
D 1		
1	25.5531198475	1.0000000000
D 1		
1	14.1961776931	1.0000000000
D 1		
1	7.8867653850	1.0000000000
D 1		
1	4.3815363250	1.0000000000
D 1		
1	2.4341868472	1.0000000000
D 1		
1	1.3523260262	1.0000000000
D 1		
1	0.7512922368	1.0000000000
D 1		
1	0.4173845760	1.0000000000
D 1		
1	0.2318803200	1.0000000000
D 1		
1	0.1288224000	1.0000000000
D 1		
1	0.0715680000	1.0000000000
D 1		
1	0.0397600000	1.0000000000
F 1		
1	150.0394183872	1.0000000000
F 1		
1	68.1997356305	1.0000000000
F 1		
1	30.9998798321	1.0000000000
F 1		
1	14.0908544691	1.0000000000
F 1		
1	6.4049338496	1.0000000000
F 1		
1	2.9113335680	1.0000000000
F 1		

1	1.3233334400	1.0000000000	end;
F 1			
1	0.6015152000	1.0000000000	
F 1			
1	0.2734160000	1.0000000000	
F 1			
1	0.1242800000	1.0000000000	
G 1			
1	96.1864311339	1.0000000000	
G 1			
1	43.7211050609	1.0000000000	
G 1			
1	19.8732295731	1.0000000000	
G 1			
1	9.0332861696	1.0000000000	
G 1			
1	4.1060391680	1.0000000000	
G 1			
1	1.8663814400	1.0000000000	
G 1			
1	0.8483552000	1.0000000000	
G 1			
1	0.3856160000	1.0000000000	
G 1			
1	0.1752800000	1.0000000000	
H 1			
1	85.4543090688	1.0000000000	
H 1			
1	37.1540474212	1.0000000000	
H 1			
1	16.1539336614	1.0000000000	
H 1			
1	7.0234494180	1.0000000000	
H 1			
1	3.0536736600	1.0000000000	
H 1			
1	1.3276842000	1.0000000000	
H 1			
1	0.5772540000	1.0000000000	
H 1			
1	0.2509800000	1.0000000000	
I 1			
1	75.5244000000	1.0000000000	
I 1			
1	25.1748000000	1.0000000000	
I 1			
1	8.3916000000	1.0000000000	
I 1			
1	2.7972000000	1.0000000000	
I 1			
1	0.9324000000	1.0000000000	
I 1			
1	0.3108000000	1.0000000000	

Energies and Cartesian coordinates (Å) of the individual compounds.

BaCl₂

Enthalpy correction = 0.00686862570117
E(PBE/L3) = -9060.28564548
E(HF/cc-pwCVTZ(-PP)) = -944.35384957
T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.006421815
T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.017743
E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -945.651363103694
T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.006077971
T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.018212
E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -944.789541787486
T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.006053216
T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.030231
E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -945.650955876881
T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.005893206
T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.025453
E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -944.788812456975
E(HF/cc-pwCVQZ(-PP)) = -944.36273612
T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.006275928
T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.015516
E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -945.879654465133
T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.005397317
T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.011749
E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -944.839498529085
T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.005916390
T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.026956
E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -945.888960215188
T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.005226331
T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.020449
E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -944.839506830110
E(HF/cc-pwCV5Z(-PP)) = -944.36403569
T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.006068831
T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.029291
E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -945.979591755921
T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.005087603
T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.025420
E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -944.852648322512
E(HF/Sapporo-QZ(AUG, decont)) = -9050.86515571
T1 (Sapporo-QZ(AUG, decont)/AE) = 0.003718247
T2 (Sapporo-QZ(AUG, decont)/AE) = 0.025380
E(CCSD(T)/Sapporo-QZ(AUG, decont)/AE) = -9053.334330370064

Ba	-0.53889336	-0.12381664	0.64737421
Cl	1.64285979	1.45429654	1.08589018

C1 -1.10396644 -1.33047990 -1.73326439

BaF2

Enthalpy correction = 0.00729681922489
E(PBE/L3) = -8337.03153435
E(HF/cc-pwCVTZ(-PP)) = -224.21478865
T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.013409547
T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.024104
E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -225.135292370232
T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.015119770
T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.021208
E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -224.762337135923
T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.013002984
T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.023100
E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -225.133679857490
T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.014910788
T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.019846
E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -224.761421887558
E(HF/cc-pwCVQZ(-PP)) = -224.23583732
T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.013059236
T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.021591
E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -225.239696792982
T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.014317467
T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.018454
E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -224.824915433629
T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.012640972
T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.026973
E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -225.237040176613
T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.014041440
T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.018454
E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -224.824416709693
E(HF/cc-pwCV5Z(-PP)) = -224.24113766
T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.012656604
T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.026550
E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -225.282634170578
T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.013783542
T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.023330
E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -224.844559056834
E(HF/Sapporo-QZ(AUG, decont)) = -8328.11481605
T1 (Sapporo-QZ(AUG, decont)/AE) = 0.007572422
T2 (Sapporo-QZ(AUG, decont)/AE) = 0.023909
E(CCSD(T)/Sapporo-QZ(AUG, decont)/AE) = -8330.058386733745

Ba -0.58164910 0.54075051 0.03256986
F 1.35674749 0.81027451 1.07770574
F -0.77509840 -1.35102502 -1.11027559

Ba

Enthalpy correction = 0.00330459586945

E(PBE/L3) = -8137.05139123
 E(HF/cc-pwCVTZ(-PP)) = -25.09500665
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.025569720
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.071925
 E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -25.356881103362
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.017419768
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.099178
 E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -25.119113755545
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.025596848
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.066894
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -25.356283477046
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.017409933
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.099907
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -25.119138844639
 E(HF/cc-pwCVQZ(-PP)) = -25.09501581
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.026553687
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.067045
 E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -25.375829868764
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.018172903
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.076942
 E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -25.119178563414
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.025718779
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.074875
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -25.375531625847
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.018073628
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.122227
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -25.119187384992
 E(HF/cc-pwCV5Z(-PP)) = -25.09501407
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.025436092
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.074491
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -25.391448801636
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.018070424
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.120648
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -25.119172803388
 E(HF/Sapporo-QZ(AUG, decont)) = -8128.80301162
 T1 (Sapporo-QZ(AUG, decont)/AE) = 0.009656941
 T2 (Sapporo-QZ(AUG, decont)/AE) = 0.078239
 E(CCSD(T)/Sapporo-QZ(AUG, decont)/AE) = -8130.007149912769

Ba 1.05330017 0.00000000 -0.79661357

BaO

Enthalpy correction = 0.00494310938297
 E(PBE/L3) = -8212.34250984
 E(HF/cc-pwCVTZ(-PP)) = -99.97655755
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.023155697
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.042534
 E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -100.571416357958
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.026673051
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.035054
 E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -100.246312546065
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.022430561

T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.030011
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -100.568909719005
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.026408498
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.026046
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -100.244947857197
 E(HF/cc-pwCVQZ(-PP)) = -99.98678166
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.021640043
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.032385
 E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -100.630784663794
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.024512751
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.022150
 E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -100.272495295561
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.020833134
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.030615
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -100.627779768455
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.024183334
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.020266
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -100.271403765170
 E(HF/cc-pwCV5Z(-PP)) = -99.98978478
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.020399964
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.025298
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -100.658999330313
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.023267092
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.021882
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -100.280127999442

Ba 0.56466743 0.57246890 0.57953605
 O -0.56466743 -0.57246890 -0.57953605

BeCl2

Enthalpy correction = 0.00917930902601
 E(PBE/L3) = -937.87865351
 E(HF/cc-pwCVTZ(-PP)) = -933.84190044
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.005880257
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.020975
 E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -934.967023183169
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.008339073
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.021239
 E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -934.318229307237
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.005709921
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.025020
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -934.967339757963
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.008206327
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.025474
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -934.317416123498
 E(HF/cc-pwCVQZ(-PP)) = -933.84889226
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.005555175
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.018142
 E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -935.172179341322
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.007505131
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.018940
 E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -934.364200137753

T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.005381674
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.028003
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -935.179966662632
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.007279319
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.028552
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -934.364218747485
 E(HF/cc-pwCV5Z(-PP)) = -933.84998100
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.005311414
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.025743
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -935.254690842955
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.007069957
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.026293
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -934.376520100618

Be	-0.000000006	0.000000006	-0.000000000
C1	1.08387149	1.20343096	-0.78717083
C1	-1.08387143	-1.20343102	0.78717083

BeF2

Enthalpy correction = 0.0108866649669
 E(PBE/L3) = -214.67083209
 E(HF/cc-pwCVTZ(-PP)) = -213.76898547
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.011041108
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.021715
 E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -214.505359838295
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.012871066
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.021396
 E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -214.351719870650
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.010802509
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.019152
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -214.504772411705
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.012632377
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.019226
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -214.350925884707
 E(HF/cc-pwCVQZ(-PP)) = -213.78537689
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.010303981
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.021756
 E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -214.582780881809
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.012014182
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.021623
 E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -214.410357206068
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.009935478
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.022247
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -214.578931293597
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.011602485
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.022349
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -214.410056295971
 E(HF/cc-pwCV5Z(-PP)) = -213.78992888
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.009820843
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.027317
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -214.607138711591
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.011507259

T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.027466
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -214.429636093656

Be	0.00000000	-0.00000001	-0.00000001
F	0.83381914	0.92579594	-0.60556821
F	-0.83381914	-0.92579593	0.60556822

Be

Enthalpy correction = 0.00330459586945
 E(PBE/L3) = -14.63267345
 E(HF/cc-pwCVTZ(-PP)) = -14.57287348
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.016412418
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.125457
 E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -14.659693443988
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.021385471
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.128273
 E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -14.618764395683
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.016398596
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.125262
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -14.659938744426
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.021407792
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.128168
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -14.618797378546
 E(HF/cc-pwCVQZ(-PP)) = -14.57296813
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.016838447
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.112175
 E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -14.664966577170
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.021673001
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.114881
 E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -14.619008063765
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.016804681
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.113593
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -14.663063377247
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.021673952
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.116329
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -14.619004483937
 E(HF/cc-pwCV5Z(-PP)) = -14.57301210
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.016796567
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.115020
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -14.666102419871
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.021597912
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.117926
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -14.619029401597

Be	1.05330017	0.00000000	-0.79661357
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BeO

Enthalpy correction = 0.0067043281489
 E(PBE/L3) = -89.89447775
 E(HF/cc-pwCVTZ(-PP)) = -89.44434580

T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.034594865
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.095232
 E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -89.851650025304
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.042882767
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.097770
 E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -89.755952406833
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.032825800
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.078273
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -89.850393434153
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.040991920
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.081244
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -89.754449464186
 E(HF/cc-pwCVQZ(-PP)) = -89.45040837
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.031949218
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.087326
 E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -89.886037762292
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.039713406
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.090234
 E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -89.778781528630
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.029372521
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.069156
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -89.882071597766
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.036739154
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.072265
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -89.777557090787
 E(HF/cc-pwCV5Z(-PP)) = -89.45230876
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.028118046
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.065829
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -89.895514347022
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.035098155
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.068658
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -89.785281985677

Be -0.40277823 -0.44720784 0.29252111
 O 0.40277823 0.44720784 -0.29252111

Br2

Enthalpy correction = 0.00442185109638
 E(PBE/L3) = -5213.04000549
 E(HF/cc-pwCVTZ(-PP)) = -831.00661808
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.006351618
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.107341
 E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -832.876803790475
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.007497980
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.109690
 E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -832.294201485963
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.006200590
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.083390
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -832.876249691687
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.007312958
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.085079
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -832.293790920636

E(HF/cc-pwCVQZ(-PP)) = -831.01037244
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.006488968
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.096480
 E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -833.233218622936
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.007745023
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.098704
 E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -832.456731072126
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.006252942
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.083310
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -833.239434393328
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.007460298
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.085073
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -832.462467942093
 E(HF/cc-pwCV5Z(-PP)) = -831.01082673
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.006224416
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.081738
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -833.382623174434
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.007456994
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.083495
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -832.518270909432

Br 0.70775097 0.27864113 0.86954506
 Br -0.70775097 -0.27864113 -0.86954506

CaBr2

Enthalpy correction = 0.00734558261091
 E(PBE/L3) = -5893.57509643
 E(HF/cc-pwCVTZ(-PP)) = -1507.99182877
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.005977706
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.024933
 E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -1510.245370294772
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.006354108
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.017757
 E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -1509.302042378389
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.005510957
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.026568
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -1510.243939389272
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.006127100
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.019253
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -1509.301236872239
 E(HF/cc-pwCVQZ(-PP)) = -1507.99537414
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.006004325
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.016529
 E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -1510.765388933262
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.006441621
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.013002
 E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -1509.469562124763
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.005501542
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.034257
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -1510.771661116937
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.006235415
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.024021

E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -1509.475055987423
 E(HF/cc-pwCV5Z(-PP)) = -1507.99587414
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.005526425
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.037169
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -1511.024991325237
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.006281556
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.023712
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -1509.532629006999

Ca	-0.04349751	0.04415242	-0.00179693
Br	1.65957685	1.67549549	-1.14491675
Br	-1.74657362	-1.58719233	1.14132407

CaF2

Enthalpy correction = 0.00761824324324
 E(PBE/L3) = -880.29061576
 E(HF/cc-pwCVTZ(-PP)) = -875.87468671
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.010991825
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.023292
 E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -876.926021991627
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.013995281
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.018796
 E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -876.429171231011
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.010540641
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.029745
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -876.924600476221
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.013670041
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.029388
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -876.428260969703
 E(HF/cc-pwCVQZ(-PP)) = -875.89350117
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.010736032
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.025615
 E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -877.163028841679
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.013187457
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.019118
 E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -876.491756020268
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.010316169
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.033072
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -877.161133704239
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.012900338
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.020269
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -876.491308920498
 E(HF/cc-pwCV5Z(-PP)) = -875.89832440
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.010311001
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.032752
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -877.296684097381
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.012707899
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.021910
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -876.511654074573

Ca	-0.20269513	0.33180764	0.22817431
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F	1.23121169	1.08859326	-0.93466054
F	-1.02851656	-1.42040091	0.70648622

Ca

Enthalpy correction = 0.00330459586945
 E(PBE/L3) = -680.32210120
 E(HF/cc-pwCVTZ(-PP)) = -676.75793693
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.014095687
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.094402
 E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -677.151517727370
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.017994308
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.118773
 E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -676.786729798031
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.012524757
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.083312
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -677.151103299511
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.018026001
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.118690
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -676.786757889565
 E(HF/cc-pwCVQZ(-PP)) = -676.75814267
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.014852495
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.086663
 E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -677.307536199344
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.018763187
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.110501
 E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -676.787050585494
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.013394651
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.079708
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -677.307954670526
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.018882922
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.110773
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -676.787150511358
 E(HF/cc-pwCV5Z(-PP)) = -676.75817447
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.014344712
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.072858
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -677.415863396174
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.018789884
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.105598
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -676.787128295099

Ca	1.05330017	0.00000000	-0.79661357
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C12

Enthalpy correction = 0.00472160249873
 E(PBE/L3) = -922.98054340
 E(HF/cc-pwCVTZ(-PP)) = -919.00101810
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.006056563
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.094580
 E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -920.044982146836

T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.008569066
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.097318
 E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -919.439189546315
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.005991123
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.076408
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -920.045023217083
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.008500481
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.078489
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -919.438422951171
 E(HF/cc-pwCVQZ(-PP)) = -919.00848577
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.006319673
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.087433
 E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -920.243381550143
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.008782568
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.090104
 E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -919.483605381390
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.006232533
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.076505
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -920.252700079201
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.008669285
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.078693
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -919.483467480678
 E(HF/cc-pwCV5Z(-PP)) = -919.00969136
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.006261234
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.076666
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -920.324141417294
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.008644490
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.078853
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -919.495492644338
 E(HF/Sapporo-QZ(AUG, decont)) = -921.80425901
 T1 (Sapporo-QZ(AUG, decont)/AE) = 0.006159586
 T2 (Sapporo-QZ(AUG, decont)/AE) = 0.076441
 E(CCSD(T)/Sapporo-QZ(AUG, decont)/AE) = -923.063112319635

C1 0.61786206 0.24325192 0.75910727
 C1 -0.61786206 -0.24325192 -0.75910727

F2

Enthalpy correction = 0.00558101733809
 E(PBE/L3) = -199.61290022
 E(HF/cc-pwCVTZ(-PP)) = -198.75131293
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.009407924
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.170320
 E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -199.420508332188
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.010700506
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.171335
 E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -199.310421340326
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.009358336
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.146904
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -199.419774196047
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.010643406

T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.147731
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -199.309722442655
 E(HF/cc-pwCVQZ(-PP)) = -198.76717404
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.010003279
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.161517
 E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -199.488568324465
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.011418776
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.162555
 E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -199.365199776852
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.009879529
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.144538
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -199.486457383550
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.011286570
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.145376
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -199.364858634841
 E(HF/cc-pwCV5Z(-PP)) = -198.77154719
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.010330694
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.144249
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -199.510472002928
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.011839041
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.145109
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -199.383282359323
 E(HF/Sapporo-QZ(AUG, decont)) = -198.93941465
 T1 (Sapporo-QZ(AUG, decont)/AE) = 0.010513616
 T2 (Sapporo-QZ(AUG, decont)/AE) = 0.145263
 E(CCSD(T)/Sapporo-QZ(AUG, decont)/AE) = -199.664532740717

F	0.43512335	0.17130781	0.53459392
F	-0.43512335	-0.17130781	-0.53459392

H2

Enthalpy correction = 0.0131372705252
 E(PBE/L3) = -1.16635211
 E(HF/cc-pwCVTZ(-PP)) = -1.13278713
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.005793266
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.056909
 E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -1.172285066355
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.005793266
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.056909
 E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -1.172285066355
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.005789191
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.056913
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -1.172283428658
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.005789191
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.056913
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -1.172283428658
 E(HF/cc-pwCVQZ(-PP)) = -1.13327638
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.005899992
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.055658
 E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -1.173735901994
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.005899992

T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.055658
 E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -1.173735901994
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.005911576
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.055647
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -1.173775742926
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.005911576
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.055647
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -1.173775742926
 E(HF/cc-pwCV5Z(-PP)) = -1.13342305
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.005939060
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.059885
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -1.174162953613
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.005940422
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.059881
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -1.174165085319

H	0.26835626	-0.22594463	-0.13467326
H	-0.26835626	0.22594463	0.13467326

H2O

Enthalpy correction = 0.0246226415094
 E(PBE/L3) = -76.43706376
 E(HF/cc-pwCVTZ(-PP)) = -76.05607196
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.006050920
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.046928
 E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -76.389882357589
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.006766084
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.047062
 E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -76.336826949598
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.006031179
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.032880
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -76.389667699738
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.006748469
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.032976
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -76.336585669191
 E(HF/cc-pwCVQZ(-PP)) = -76.06364279
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.006733823
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.041706
 E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -76.420832373165
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.007526949
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.041892
 E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -76.361537362966
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.006699817
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.039725
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -76.419840046550
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.007493280
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.039913
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -76.361495070004
 E(HF/cc-pwCV5Z(-PP)) = -76.06582876
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.007446631
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.040122
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -76.430646366023

T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.008380456
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.040286
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -76.369557993881

O	-0.22372605	-0.20723197	-0.26073737
H	-0.49921059	0.50805428	0.33325693
H	0.72293664	-0.30082231	-0.07251956

HBr

Enthalpy correction = 0.00913229857216
 E(PBE/L3) = -2607.12167432
 E(HF/cc-pwCVTZ(-PP)) = -416.09346061
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.005882321
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.053177
 E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -417.045902229691
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.006917065
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.053655
 E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -416.754687861754
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.005827039
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.046747
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -417.045790887179
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.006857274
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.047129
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -416.754614426772
 E(HF/cc-pwCVQZ(-PP)) = -416.09530375
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.006220465
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.041875
 E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -417.224269284096
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.007440293
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.042274
 E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -416.836124136531
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.006101153
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.049504
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -417.227612938536
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.007304210
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.049945
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -416.839188819861
 E(HF/cc-pwCV5Z(-PP)) = -416.09558812
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.006168745
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.062058
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -417.299018424448
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.007404004
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.062589
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -416.866910296179

Br	0.51115758	-0.43037308	-0.25652191
H	-0.51115758	0.43037308	0.25652191

HCl

Enthalpy correction = 0.00989227434982

E(PBE/L3) = -462.10770134
 E(HF/cc-pwCVTZ(-PP)) = -460.10777792
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.004862566
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.043338
 E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -460.646225269966
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.006165343
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.043929
 E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -460.343194876264
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.004841139
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.038355
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -460.646416578420
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.006153219
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.038707
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -460.342921129191
 E(HF/cc-pwCVQZ(-PP)) = -460.11160257
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.005303102
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.035762
 E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -460.745880669318
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.006489208
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.036499
 E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -460.365804329676
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.005299622
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.038011
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -460.750734590226
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.006457526
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.038407
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -460.365867578111
 E(HF/cc-pwCV5Z(-PP)) = -460.11225960
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.005427027
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.053906
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -460.786325901727
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.006555755
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.054687
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -460.371727222710

 C1 0.46070703 -0.38789586 -0.23120356
 H -0.46070703 0.38789586 0.23120356

HF

Enthalpy correction = 0.0124612761346
 E(PBE/L3) = -100.48893857
 E(HF/cc-pwCVTZ(-PP)) = -100.05739811
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.005894351
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.040706
 E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -100.400408283552
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.006738609
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.040851
 E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -100.345050878656
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.005892664
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.038422
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -100.400197345423
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.006744115

T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.038533
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -100.344845305912
 E(HF/cc-pwCVQZ(-PP)) = -100.06699482
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.006576385
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.036877
 E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -100.438059668078
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.007547217
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.037029
 E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -100.376036431357
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.006542903
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.047878
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -100.437189823838
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.007519575
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.048085
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -100.376039488866
 E(HF/cc-pwCV5Z(-PP)) = -100.06970575
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.007265434
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.042567
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -100.450259523878
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.008370044
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.042753
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -100.386306917057

 F 0.33169902 -0.27927657 -0.16646151
 H -0.33169902 0.27927657 0.16646151

HI

Enthalpy correction = 0.00842507011729
 E(PBE/L3) = -7118.07053376
 E(HF/cc-pwCVTZ(-PP)) = -295.24523125
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.007515512
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.071692
 E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -296.173734906562
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.008651910
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.072401
 E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -295.918935591766
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.007439115
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.060111
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -296.173055636815
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.008574597
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.060623
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -295.918292887339
 E(HF/cc-pwCVQZ(-PP)) = -295.24626271
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.008369949
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.062091
 E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -296.355238335844
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.009658553
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.062767
 E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -296.005423153693
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.008234757
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.061330
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -296.357487404516

T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.009509684
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.061919
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -296.007563459963
 E(HF/cc-pwCV5Z(-PP)) = -295.24640508
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.008456715
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.056552
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -296.434731097818
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.009741219
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.057104
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -296.037913339004

I	0.58136955	-0.48948861	-0.29175745
H	-0.58136955	0.48948861	0.29175745

I2

Enthalpy correction = 0.00433022055074
 E(PBE/L3) = -14234.97060895
 E(HF/cc-pwCVTZ(-PP)) = -589.34665100
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.007453071
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.103548
 E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -591.166741164155
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.008612443
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.105838
 E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -590.657225397038
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.007273056
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.078372
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -591.164912390202
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.008400985
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.079970
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -590.655498108049
 E(HF/cc-pwCVQZ(-PP)) = -589.34864753
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.007967816
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.094652
 E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -591.530077564176
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.009217399
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.096906
 E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -590.830570166914
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.007653968
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.077085
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -591.533715637394
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.008840575
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.078769
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -590.834034171993
 E(HF/cc-pwCV5Z(-PP)) = -589.34884859
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.007808039
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.076521
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -591.689225678015
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.009003896
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.078229
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -590.895703351225

I	0.82485733	0.32474584	1.01342230
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I -0.82485733 -0.32474584 -1.01342230

LiBr

Enthalpy correction = 0.00475283656298
E(PBE/L3) = -2614.09533453
E(HF/cc-pwCVTZ(-PP)) = -423.04401335
T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.005333223
T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.027632
E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -424.029701266958
T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.006130806
T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.027855
E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -423.699239802903
T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.005211545
T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.020882
E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -424.029565657855
T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.006022798
T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.021045
E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -423.698924071843
E(HF/cc-pwCVQZ(-PP)) = -423.04569551
T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.005208592
T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.020829
E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -424.214704722018
T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.006229111
T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.020937
E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -423.782814903519
T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.005090964
T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.025733
E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -424.216647046056
T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.006131616
T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.025950
E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -423.785653744728
E(HF/cc-pwCV5Z(-PP)) = -423.04592885
T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.005090889
T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.022231
E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -424.291147342855
T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.006198351
T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.022437
E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -423.814111845030

Li 0.40318385 -0.79813176 0.62209893
Br -0.40318385 0.79813176 -0.62209893

LiCl

Enthalpy correction = 0.00489354920959
E(PBE/L3) = -469.07777359
E(HF/cc-pwCVTZ(-PP)) = -467.05179230
T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.004499763
T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.029482
E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -467.625263947382
T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.006093728

T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.030284
 E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -467.282817327117
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.004369041
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.030550
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -467.625581982247
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.005910764
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.031287
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -467.282467947972
 E(HF/cc-pwCVQZ(-PP)) = -467.05542139
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.004172249
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.029432
 E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -467.731422818200
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.004989554
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.030105
 E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -467.307425386836
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.004089514
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.030663
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -467.735098555225
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.004795678
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.031480
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -467.307483124133
 E(HF/cc-pwCV5Z(-PP)) = -467.05601204
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.004060587
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.029249
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -467.773719192404
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.004544294
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.030084
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -467.314007385235

 Li 0.37533895 -0.74301076 0.57913521
 Cl -0.37533895 0.74301076 -0.57913521

LiF

Enthalpy correction = 0.00540142146864
 E(PBE/L3) = -107.44970330
 E(HF/cc-pwCVTZ(-PP)) = -106.98259016
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.012600802
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.028143
 E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -107.368596890673
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.015339143
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.028192
 E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -107.273280864998
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.012271624
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.020494
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -107.368386780557
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.014956044
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.020577
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -107.272872569752
 E(HF/cc-pwCVQZ(-PP)) = -106.99089864
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.011659683
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.015253
 E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -107.410498531447

T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.014233992
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.015340
 E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -107.303821281256
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.011310955
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.019269
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -107.408298929453
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.013817430
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.019332
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -107.303650919431
 E(HF/cc-pwCV5Z(-PP)) = -106.99303100
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.010840540
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.019990
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -107.423405972744
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.013255903
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.020082
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -107.313537908478

Li	0.29125280	-0.57655610	0.44939314
F	-0.29125280	0.57655610	-0.44939314

LiH

Enthalpy correction = 0.00642624936257
 E(PBE/L3) = -8.04774428
 E(HF/cc-pwCVTZ(-PP)) = -7.98694842
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.007954757
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.043831
 E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -8.062056431048
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.010456275
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.043996
 E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -8.022797882494
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.007786058
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.046949
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -8.062275853877
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.010213022
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.047310
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -8.022798422922
 E(HF/cc-pwCVQZ(-PP)) = -7.98725234
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.007596054
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.032630
 E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -8.067751873100
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.009708223
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.032627
 E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -8.024042868784
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.007348178
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.039410
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -8.066613414253
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.009392554
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.039675
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -8.024071774167
 E(HF/cc-pwCV5Z(-PP)) = -7.98734936
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.007235035
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.045741

E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -8.069295374488
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.009151750
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.045835
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -8.024399348099

Li	0.29731811	-0.58856283	0.45875171
H	-0.29731811	0.58856283	-0.45875171

MgBr2

Enthalpy correction = 0.00761664966854
 E(PBE/L3) = -5413.48703653
 E(HF/cc-pwCVTZ(-PP)) = -1030.80720997
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.005961151
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.018246
 E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -1032.970564477191
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.006641469
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.016987
 E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -1032.123195029810
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.005628506
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.028963
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -1032.969684112441
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.006343480
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.028957
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -1032.122353791010
 E(HF/cc-pwCVQZ(-PP)) = -1030.81123293
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.005685780
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.020461
 E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -1033.404047638745
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.006558260
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.020711
 E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -1032.289972882197
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.005354858
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.027664
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -1033.410407219298
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.006289222
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.027659
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -1032.295485022967
 E(HF/cc-pwCV5Z(-PP)) = -1030.81198085
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.005308543
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.027247
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -1033.588582621755
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.006326902
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.027260
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -1032.352533542257

Mg	-0.00001708	0.00001676	-0.00000050
Br	1.48504139	1.48188605	-1.01822369
Br	-1.48502432	-1.48190281	1.01822419

MgCl2

Enthalpy correction = 0.00788962901581
 E(PBE/L3) = -1123.45303304
 E(HF/cc-pwCVTZ(-PP)) = -1118.82703683
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.005292720
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.018356
 E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -1120.163774721552
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.006962531
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.018749
 E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -1119.292908489564
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.005079563
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.026325
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -1120.163984084818
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.006719925
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.026679
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -1119.292156487194
 E(HF/cc-pwCVQZ(-PP)) = -1118.83499723
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.004888802
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.018116
 E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -1120.440034157539
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.005913510
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.018482
 E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -1119.342129353862
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.004690401
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.027563
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -1120.450019785239
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.005658748
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.027984
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -1119.342228675370
 E(HF/cc-pwCV5Z(-PP)) = -1118.83642150
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.004593735
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.024372
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -1120.556363811063
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.005377874
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.024755
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -1119.355337116226

Mg	0.00000050	0.00000082	0.00000022
Cl	1.31537205	1.46046778	-0.95530040
Cl	-1.31537255	-1.46046860	0.95530018

MgF2

Enthalpy correction = 0.00874203212647
 E(PBE/L3) = -400.20486448
 E(HF/cc-pwCVTZ(-PP)) = -398.70478616
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.010866986
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.022359
 E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -399.659600052215
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.014038379
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.020366
 E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -399.284788747045
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.010576901
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.023549

E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -399.658925141617
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.013700134
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.023611
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -399.284041449656
 E(HF/cc-pwCVQZ(-PP)) = -398.72433764
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.010291960
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.020039
 E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -399.810480336427
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.013280559
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.018834
 E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -399.348790214835
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.009935498
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.021669
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -399.808764033296
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.012860466
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.021801
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -399.348461955684
 E(HF/cc-pwCV5Z(-PP)) = -398.72914695
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.009663324
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.021227
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -399.869061538830
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.012523472
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.021364
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -399.369105483000

Mg	0.00000001	-0.00000000	0.00000002
F	1.06026827	1.17722419	-0.77002883
F	-1.06026829	-1.17722418	0.77002881

Mg

Enthalpy correction = 0.00330459586945
 E(PBE/L3) = -200.27843625
 E(HF/cc-pwCVTZ(-PP)) = -199.61334754
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.010788008
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.085149
 E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -199.914534371417
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.016607225
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.093552
 E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -199.647177527805
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.010773368
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.085022
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -199.914663493435
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.016704633
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.093476
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -199.647247719769
 E(HF/cc-pwCVQZ(-PP)) = -199.61423295
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.011477601
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.062797
 E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -199.988966815895
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.017195232
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.069635
 E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -199.648192750819

T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.011479947
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.064242
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -199.989396371651
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.017233608
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.071264
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -199.648252007668
 E(HF/cc-pwCV5Z(-PP)) = -199.61460519
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.011639230
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.096272
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -200.023536339807
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.017266808
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.106649
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -199.648632946495

Mg 1.05330017 0.00000000 -0.79661357

MgI2

Enthalpy correction = 0.00699818332483
 E(PBE/L3) = -14435.38500360
 E(HF/cc-pwCVTZ(-PP)) = -789.10986073
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.006739066
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.020781
 E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -791.225647446880
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.007638797
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.021107
 E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -790.450514822507
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.006448960
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.031574
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -791.223475192824
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.007350988
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.031715
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -790.448346371453
 E(HF/cc-pwCVQZ(-PP)) = -789.11203306
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.006950182
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.019247
 E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -791.665098499987
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.008106866
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.019561
 E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -790.627299579104
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.006653163
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.027664
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -791.669030511650
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.007843668
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.027808
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -790.630714071664
 E(HF/cc-pwCV5Z(-PP)) = -789.11250355
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.006783419
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.029721
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -791.859117799273
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.008064693
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.029889
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -790.693223540923

Mg	-0.00036560	0.00039644	-0.00002425
I	1.71898296	1.51713793	-1.10704919
I	-1.71861736	-1.51753437	1.10707345

NaBr

Enthalpy correction = 0.00439715068842
 E(PBE/L3) = -2769.00363644
 E(HF/cc-pwCVTZ(-PP)) = -577.45084161
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.005609455
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.024360
 E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -578.668371294201
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.006135011
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.024583
 E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -578.104914699299
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.005313587
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.019761
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -578.667878346289
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.006033344
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.020017
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -578.104625623317
 E(HF/cc-pwCVQZ(-PP)) = -577.45331216
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.005213642
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.019683
 E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -578.911971264265
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.006179120
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.019828
 E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -578.189443284484
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.004973740
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.027410
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -578.915885025658
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.006104303
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.027531
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -578.192280126337
 E(HF/cc-pwCV5Z(-PP)) = -577.45374001
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.004893958
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.024882
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -579.018567242891
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.006163949
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.019720
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -578.221081366009

Na	0.46648564	-0.92344227	0.71977145
Br	-0.46648564	0.92344227	-0.71977145

NaCl

Enthalpy correction = 0.00446758669046
 E(PBE/L3) = -623.98259637
 E(HF/cc-pwCVTZ(-PP)) = -621.45514820
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.005181560

T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.031155
 E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -622.260418839759
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.006273434
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.031708
 E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -621.685203875010
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.004984481
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.027002
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -622.260424646601
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.006070310
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.027436
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -621.684870845057
 E(HF/cc-pwCVQZ(-PP)) = -621.45965948
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.004560526
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.027997
 E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -622.425357165086
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.004953329
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.028536
 E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -621.710936556840
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.004424254
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.035098
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -622.431056070505
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.004832517
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.036100
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -621.711004560228
 E(HF/cc-pwCV5Z(-PP)) = -621.46043939
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.004287215
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.033052
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -622.497874254163
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.004510624
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.034017
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -621.717872983294

Na	0.43989470	-0.87080356	0.67874253
Cl	-0.43989470	0.87080356	-0.67874253

NaF

Enthalpy correction = 0.00470024859765
 E(PBE/L3) = -262.33887042
 E(HF/cc-pwCVTZ(-PP)) = -261.36991629
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.011657781
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.024429
 E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -261.987752807255
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.016847548
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.024473
 E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -261.658561379676
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.011254856
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.025482
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -261.987261582082
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.016371857
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.025530
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -261.658158674000
 E(HF/cc-pwCVQZ(-PP)) = -261.37946955

T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.010743421
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.015781
 E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -262.089510013124
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.015598178
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.016839
 E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -261.690971306112
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.010331221
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.018901
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -262.089292908337
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.015099246
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.018643
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -261.690763716939
 E(HF/cc-pwCV5Z(-PP)) = -261.38208936
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.010013142
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.022874
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -262.133229111082
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.014698564
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.022985
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -261.701463428155

Na	0.35987497	-0.71239869	0.55527481
F	-0.35987497	0.71239869	-0.55527481

NaI

Enthalpy correction = 0.00436225140235
 E(PBE/L3) = -7279.95709428
 E(HF/cc-pwCVTZ(-PP)) = -456.60835008
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.006188225
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.023666
 E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -457.801033101869
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.007066566
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.023921
 E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -457.273740650428
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.006029234
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.023642
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -457.799937654661
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.006985026
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.024077
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -457.272775530914
 E(HF/cc-pwCVQZ(-PP)) = -456.60979975
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.006405316
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.019182
 E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -458.047512625772
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.007931718
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.019641
 E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -457.363262524020
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.006288184
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.018905
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -458.050257884154
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.007880399
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.019302
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -457.365068099607

E(HF/cc-pwCV5Z(-PP)) = -456.61008020
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.006402674
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.017413
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -458.158851397768
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.008173853
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.017837
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -457.396590132415

Na	0.50497678	-0.99963828	0.77916196
I	-0.50497678	0.99963828	-0.77916196

PbBr2

Enthalpy correction = 0.00676615884753
 E(PBE/L3) = -26109.81493105
 E(HF/cc-pwCVTZ(-PP)) = -1022.98322092
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.010209769
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.043377
 E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -1025.565126408197
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.009764677
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.042659
 E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -1024.342352680088
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.009136269
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.050486
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -1025.562912381182
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.008586492
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.075743
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -1024.340893274039
 E(HF/cc-pwCVQZ(-PP)) = -1022.98737729
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.009970992
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.038270
 E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -1026.067879530491
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.009294358
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.039894
 E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -1024.510721219151
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.008880887
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.050486
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -1026.074863567214
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.008182208
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.076556
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -1024.515485477247
 E(HF/cc-pwCV5Z(-PP)) = -1022.98790879
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.008728812
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.050744
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -1026.280327443131
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.008022098
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.076523
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -1024.573136651964

Pb	0.02450399	0.07408920	1.10839889
Br	1.97682931	-0.47808197	-0.56868923
Br	-2.00133329	0.40399277	-0.53970966

PbCl2

Enthalpy correction = 0.00695196965834
E(PBE/L3) = -21819.77301567
E(HF/cc-pwCVTZ(-PP)) = -1110.99574581
T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.010712727
T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.040208
E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -1112.749967038278
T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.012617338
T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.039342
E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -1111.501217513709
T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.010277759
T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.050981
E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -1112.749256260386
T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.012251297
T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.076802
E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -1111.500072130981
E(HF/cc-pwCVQZ(-PP)) = -1111.00421909
T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.010471766
T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.035377
E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -1113.095594367169
T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.011604096
T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.036604
E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -1111.551504709832
T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.009872194
T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.051178
E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -1113.106664017625
T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.010988646
T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.077635
E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -1111.551075420710
E(HF/cc-pwCV5Z(-PP)) = -1111.00542850
T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.009760961
T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.051411
E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -1113.240178103736
T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.010725391
T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.077583
E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -1111.564596437172

Pb	0.02341406	0.07079845	1.05916320
Cl	1.85592510	-0.44950781	-0.54318726
Cl	-1.87933916	0.37870936	-0.51597594

PbI2

Enthalpy correction = 0.00670321264661
E(PBE/L3) = -35131.72058050
E(HF/cc-pwCVTZ(-PP)) = -781.29308147
T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.010820468
T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.047526
E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -783.828917946675
T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.010853455
T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.044072

E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -782.680653685821
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.009755507
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.049337
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -783.825218420692
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.009703491
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.074078
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -782.677763262770
 E(HF/cc-pwCVQZ(-PP)) = -781.29525592
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.010739720
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.041283
 E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -784.337771389929
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.010660703
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.041724
 E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -782.859740246024
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.009632703
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.049406
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -784.342138133918
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.009574950
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.074607
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -782.862303969102
 E(HF/cc-pwCV5Z(-PP)) = -781.29550254
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.009546948
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.049639
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -784.559594259918
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.009532123
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.074540
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -782.925784444543

Pb	0.02614168	0.07904598	1.18254873
I	2.14654258	-0.51837236	-0.60700710
I	-2.17268426	0.43932638	-0.57554163

SrBr2

Enthalpy correction = 0.00676552141764
 E(PBE/L3) = -8392.85015812
 E(HF/cc-pwCVTZ(-PP)) = -861.57290551
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.006271539
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.014700
 E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -863.680542969696
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.006365019
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.014849
 E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -862.876610196466
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.005765376
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.023688
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -863.679297598206
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.006119443
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.020772
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -862.875737216275
 E(HF/cc-pwCVQZ(-PP)) = -861.57639268
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.006179825
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.013304
 E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -864.087893915909

T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.006476726
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.013474
 E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -863.043245723861
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.005682844
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.029712
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -864.094652546916
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.006259654
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.018538
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -863.048619095176
 E(HF/cc-pwCV5Z(-PP)) = -861.57683437
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.005685524
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.027769
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -864.256707656069
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.006306028
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.020483
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -863.105689236952

Sr	0.25492944	0.32450223	-0.26690999
Br	-0.73160407	1.75268768	1.88458553
Br	0.47667463	-2.07718990	-1.61767555

SrCl2

Enthalpy correction = 0.00691292707802
 E(PBE/L3) = -4102.81528855
 E(HF/cc-pwCVTZ(-PP)) = -949.58787359
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.005831979
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.017596
 E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -950.870615157017
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.006773005
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.017956
 E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -950.037348128000
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.005462126
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.030812
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -950.870498604814
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.006613361
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.024246
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -950.036697211464
 E(HF/cc-pwCVQZ(-PP)) = -949.59569988
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.005679220
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.012544
 E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -951.121131333499
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.006042574
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.012734
 E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -950.085636261475
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.005345436
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.029567
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -951.131589118424
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.005833814
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.019423
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -950.085772368833
 E(HF/cc-pwCV5Z(-PP)) = -949.59678497
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.005393877

T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.027203
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -951.221739922505
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.005646329
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.021652
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -950.098517679377

Sr	0.07045708	0.38657936	-0.39843405
Cl	-0.59415250	1.57833084	1.81928866
Cl	0.52369542	-1.96491020	-1.42085461

SrF2

Enthalpy correction = 0.007394027282
 E(PBE/L3) = -3379.56064842
 E(HF/cc-pwCVTZ(-PP)) = -229.44856998
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.012690229
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.026914
 E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -230.354152814114
 T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.014314964
 T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.023289
 E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -230.014390684932
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.012211005
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.027518
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -230.352848569489
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.014055618
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.019327
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -230.013509186173
 E(HF/cc-pwCVQZ(-PP)) = -229.46773148
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.012298239
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.023373
 E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -230.479579395213
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.013517697
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.020271
 E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -230.078167830381
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.011840606
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.026985
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -230.478059207912
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.013229878
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.019629
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -230.077750333362
 E(HF/cc-pwCV5Z(-PP)) = -229.47253831
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.011729814
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.028321
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -230.522633769602
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.012961276
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.020489
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -230.098341027074

Sr	-0.56940361	-0.29094532	0.12171762
F	-0.14011107	1.49200146	1.17048451
F	0.70951469	-1.20105614	-1.29220213

Sr

Enthalpy correction = 0.00330459586945
E(PBE/L3) = -3179.60079874
E(HF/cc-pwCVTZ(-PP)) = -30.34122374
T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.022008213
T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.069376
E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -30.590628521064
T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.017371432
T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.091945
E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -30.367265942293
T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.022207090
T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.058692
E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -30.590296159092
T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.017441385
T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.099180
E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -30.367296727443
E(HF/cc-pwCVQZ(-PP)) = -30.34125454
T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.023282194
T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.063609
E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -30.634569328938
T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.017642531
T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.085485
E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -30.367366789616
T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.021110947
T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = 0.057508
E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -30.635279965602
T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.017766165
T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = 0.103843
E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -30.367477393326
E(HF/cc-pwCV5Z(-PP)) = -30.34121577
T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.022489430
T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = 0.083491
E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -30.651556473808
T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.017596051
T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = 0.081354
E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -30.367333289217

Sr 1.05330017 0.00000000 -0.79661357

SrI2

Enthalpy correction = 0.00671054309026
E(PBE/L3) = -17414.74852054
E(HF/cc-pwCVTZ(-PP)) = -619.88010558
T1 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.006938558
T2 (CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.026888
E(CCSD(T)/cc-pwCVTZ(-PP)/AE) = -621.938052617009
T1 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.007232494
T2 (CCSD(T)/cc-pwCVTZ(-PP)/FC) = 0.027294
E(CCSD(T)/cc-pwCVTZ(-PP)/FC) = -621.211380752239
T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.006423253
T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = 0.021084

E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/AE) = -621.935320728672
 T1 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC)= 0.007007355
 T2 (DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC)= 0.019932
 E(DLPNO-CCSD(T)/cc-pwCVTZ(-PP)/FC) = -621.209196469647
 E(HF/cc-pwCVQZ(-PP)) = -619.88159354
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/AE)= 0.007320923
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/AE)= 0.018877
 E(CCSD(T)/cc-pwCVQZ(-PP)/AE) = -622.351230551768
 T1 (CCSD(T)/cc-pwCVQZ(-PP)/FC)= 0.007997710
 T2 (CCSD(T)/cc-pwCVQZ(-PP)/FC)= 0.019202
 E(CCSD(T)/cc-pwCVQZ(-PP)/FC) = -621.389205714431
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE)= 0.006784857
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE)= 0.030476
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/AE) = -622.355344533074
 T1 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC)= 0.007799301
 T2 (DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC)= 0.023714
 E(DLPNO-CCSD(T)/cc-pwCVQZ(-PP)/FC) = -621.392526663513
 E(HF/cc-pwCV5Z(-PP)) = -619.88174972
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE)= 0.007017486
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE)= 0.029418
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/AE) = -622.529499726770
 T1 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC)= 0.008072962
 T2 (DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC)= 0.024007
 E(DLPNO-CCSD(T)/cc-pwCV5Z(-PP)/FC) = -621.455597440133

Sr	-0.03950195	0.00347844	-0.01743200
I	-0.66015073	2.15334434	1.97944825
I	0.69965268	-2.15682277	-1.96201625