

Electronic Supplementary Information

Improving the Theoretical Description of Ln(III)/An(III) Separation with Phosphinic Acid Ligands: A Benchmarking Study of Structure and Selectivity

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A. Comparison of MP2 f-in-valence (SC ECP) Reaction Energies

Table S1: MP2 SC ECP Energies of $\text{Am}(\text{H}_2\text{PO}_2)_3 + \text{Eu}(\text{H}_2\text{PX}_2)_3 \rightarrow \text{Am}(\text{H}_2\text{PX}_2)_3 + \text{Eu}(\text{H}_2\text{PO}_2)_3$ reactions, kcal/mol. 74 electrons were correlated for all species (see main body of text). MP2 calculations without RI approximation (columns 1 and 2) were calculated using MOLPRO software,^{1,2} and RI-MP2 calculations (column 3) were calculated using ORCA.³⁻⁵

	ROHF MP2 SC ECP	UHF MP2 SC ECP	UHF RI-MP2 SC ECP
X=S			
aug-cc-pVDZ	-3.96	-3.94	-4.24
aug-cc-pVTZ	-4.03	-4.00	-4.30
X=Se			
aug-cc-pVDZ	-4.62	-4.65	-5.07
aug-cc-pVTZ	-4.32	-4.35	-4.74
X=Te			
aug-cc-pVDZ	-6.02	-6.05	-6.09
aug-cc-pVTZ	-4.60	-4.59	-4.77

B. DFT Second-Order Stabilization Energies ($E^{(2)}$)

Table S2: DFT Second-Order Stabilization Energies for Forward and Back Donation.

Forward donation, kcal/mol (L→M)

	Eu(H₂PO₂)₃	Eu(H₂PS₂)₃	Eu(H₂PSe₂)₃	Eu(H₂PTe₂)₃
B3LYP	176.94	664.04	704.6	699.02
B5050LYP	294.28	970.65	1140.98	1263.42
	Am(H₂PO₂)₃	Am(H₂PS₂)₃	Am(H₂PSe₂)₃	Am(H₂PTe₂)₃
B3LYP	175.97	645.3	757.29	1007.01
B5050LYP	258.52	916.77	1056.65	1243.56

Back donation, kcal/mol (M→L)

	Eu(H₂PO₂)₃	Eu(H₂PS₂)₃	Eu(H₂PSe₂)₃	Eu(H₂PTe₂)₃
B3LYP	55.25	19.43	13.89	9.28
B5050LYP	25.36	5.5	3.24	0.83
	Am(H₂PO₂)₃	Am(H₂PS₂)₃	Am(H₂PSe₂)₃	Am(H₂PTe₂)₃
B3LYP	128.27	65.67	46.97	29.64
B5050LYP	86.67	43.54	27.55	14.2

C. Additional Basis Functions for Am(III) and Eu(III) in aug-cc-pwCVTZ Calculations

The following basis functions were added to the Dolg ECP28MWB_ANO basis set^{6,7} for Eu(III) in aug-cc-pwCVnZ calculations presented in Table 3 of the main body of text:

s,Eu,1.0527690E+01,6.6356370E+00
p,Eu,9.0665380E+00,6.0491120E+00
d,Eu,1.4506110E+01,7.6754510E+00
f,Eu,7.3173440E+00,3.0372840E+00
g,Eu,9.2594070E+00

The following basis functions were added to the Dolg ECP60MWB_ANO basis set^{8,9} for Am(III) in aug-cc-pwCVnZ calculations presented in Table 3 of the main body of text:

s,Am,8.7069655E+00,5.3198651E+00
p,Am,6.8589925E+00,3.7470795E+00
d,Am,7.3983569E+00,4.2739044E+00
f,Am,9.6480742E+00,4.6241999E+00
g,Am,4.7742905E+00

D. Recontracted cc-pVTZ-PP Basis Sets for Am(III) and Eu(III)

The following basis set for Eu(III) was constructed by re-contracting the cc-pVTZ-DK3 set in the presence of the ECP28MWB ECP using the procedure outlined in Ref. ¹⁰.

S	30	
1	6.9855600E+07	1.38885E-08
2	1.8422660E+07	3.57883E-08
3	6.1949800E+06	1.80190E-07
4	2.2928270E+06	3.84669E-07
5	9.1381600E+05	1.76236E-06
6	3.8128830E+05	3.07212E-06
7	1.6555900E+05	1.40276E-05
8	7.4280470E+04	2.06713E-05
9	3.4342950E+04	9.51601E-05
10	1.6316470E+04	1.17809E-04
11	7.9497860E+03	5.58477E-04
12	3.9636570E+03	5.45111E-04
13	2.0184970E+03	2.76572E-03
14	1.0481120E+03	1.58540E-03
15	5.5373610E+02	1.03513E-02
16	2.9670960E+02	-2.02035E-03
17	1.5886880E+02	2.75114E-02
18	8.7062830E+01	-3.49489E-02
19	4.7924070E+01	9.26072E-03
20	2.5489300E+01	4.41874E-01
21	1.4533130E+01	-1.06482E+00
22	8.0949100E+00	1.36174E-02
23	4.2748700E+00	7.38190E-01
24	2.2631260E+00	5.65356E-01
25	1.0266980E+00	5.12784E-02

26	5.3394470E-01	7.33721E-02
27	2.5806550E-01	2.00561E-02
28	6.5975540E-02	8.14713E-03
29	3.3914920E-02	3.66000E-03
30	1.6765960E-02	2.30871E-03
S	30	
1	6.9855600E+07	-1.62121E-08
2	1.8422660E+07	-4.58252E-08
3	6.1949800E+06	-2.01225E-07
4	2.2928270E+06	-5.15859E-07
5	9.1381600E+05	-1.91904E-06
6	3.8128830E+05	-4.26583E-06
7	1.6555900E+05	-1.50458E-05
8	7.4280470E+04	-2.96009E-05
9	3.4342950E+04	-1.00678E-04
10	1.6316470E+04	-1.75427E-04
11	7.9497860E+03	-5.81002E-04
12	3.9636570E+03	-8.67839E-04
13	2.0184970E+03	-2.80125E-03
14	1.0481120E+03	-3.09088E-03
15	5.5373610E+02	-9.81180E-03
16	2.9670960E+02	-3.24439E-03
17	1.5886880E+02	-2.13555E-02
18	8.7062830E+01	2.14798E-02
19	4.7924070E+01	-2.15588E-02
20	2.5489300E+01	-2.07020E-01
21	1.4533130E+01	5.78025E-01
22	8.0949100E+00	-1.83288E-02
23	4.2748700E+00	-5.28647E-01
24	2.2631260E+00	-6.37713E-01
25	1.0266980E+00	2.53244E-01
26	5.3394470E-01	6.47471E-01
27	2.5806550E-01	2.39602E-01
28	6.5975540E-02	1.57366E-01
29	3.3914920E-02	1.48055E-01
30	1.6765960E-02	4.89031E-02
S	30	
1	6.9855600E+07	1.07459E-08
2	1.8422660E+07	3.07188E-08
3	6.1949800E+06	1.32602E-07
4	2.2928270E+06	3.47612E-07
5	9.1381600E+05	1.26024E-06
6	3.8128830E+05	2.88535E-06
7	1.6555900E+05	9.85976E-06
8	7.4280470E+04	2.00858E-05
9	3.4342950E+04	6.58467E-05
10	1.6316470E+04	1.19504E-04
11	7.9497860E+03	3.79069E-04
12	3.9636570E+03	5.94960E-04
13	2.0184970E+03	1.82032E-03
14	1.0481120E+03	2.15494E-03

15	5.5373610E+02	6.30822E-03
16	2.9670960E+02	2.63851E-03
17	1.5886880E+02	1.31960E-02
18	8.7062830E+01	-1.24198E-02
19	4.7924070E+01	1.48520E-02
20	2.5489300E+01	1.09164E-01
21	1.4533130E+01	-3.17197E-01
22	8.0949100E+00	5.96779E-03
23	4.2748700E+00	3.19196E-01
24	2.2631260E+00	3.92614E-01
25	1.0266980E+00	-1.71389E-01
26	5.3394470E-01	-5.78091E-01
27	2.5806550E-01	-3.54665E-01
28	6.5975540E-02	5.00209E-01
29	3.3914920E-02	4.95438E-01
30	1.6765960E-02	1.62714E-01
S	30	
1	6.9855600E+07	3.03656E-08
2	1.8422660E+07	8.75859E-08
3	6.1949800E+06	3.72949E-07
4	2.2928270E+06	9.95171E-07
5	9.1381600E+05	3.53452E-06
6	3.8128830E+05	8.28450E-06
7	1.6555900E+05	2.76054E-05
8	7.4280470E+04	5.78139E-05
9	3.4342950E+04	1.84066E-04
10	1.6316470E+04	3.45017E-04
11	7.9497860E+03	1.05755E-03
12	3.9636570E+03	1.72622E-03
13	2.0184970E+03	5.06184E-03
14	1.0481120E+03	6.33650E-03
15	5.5373610E+02	1.73790E-02
16	2.9670960E+02	8.64577E-03
17	1.5886880E+02	3.49297E-02
18	8.7062830E+01	-3.08817E-02
19	4.7924070E+01	5.25364E-02
20	2.5489300E+01	1.60051E-01
21	1.4533130E+01	-5.63842E-01
22	8.0949100E+00	-2.92780E-02
23	4.2748700E+00	9.36827E-01
24	2.2631260E+00	5.60139E-01
25	1.0266980E+00	-1.49601E+00
26	5.3394470E-01	-8.64676E-01
27	2.5806550E-01	1.54104E+00
28	6.5975540E-02	9.77856E-01
29	3.3914920E-02	-1.12837E+00
30	1.6765960E-02	-1.80940E-01
S	30	
1	6.9855600E+07	-5.47770E-08
2	1.8422660E+07	-1.60018E-07
3	6.1949800E+06	-6.68222E-07

4	2.2928270E+06	-1.82855E-06
5	9.1381600E+05	-6.30704E-06
6	3.8128830E+05	-1.52837E-05
7	1.6555900E+05	-4.91350E-05
8	7.4280470E+04	-1.07021E-04
9	3.4342950E+04	-3.26849E-04
10	1.6316470E+04	-6.41273E-04
11	7.9497860E+03	-1.87237E-03
12	3.9636570E+03	-3.22913E-03
13	2.0184970E+03	-8.91750E-03
14	1.0481120E+03	-1.20459E-02
15	5.5373610E+02	-3.02089E-02
16	2.9670960E+02	-1.83745E-02
17	1.5886880E+02	-5.75511E-02
18	8.7062830E+01	4.50856E-02
19	4.7924070E+01	-8.81008E-02
20	2.5489300E+01	-2.20849E-01
21	1.4533130E+01	8.87523E-01
22	8.0949100E+00	-8.90782E-02
23	4.2748700E+00	-1.76129E+00
24	2.2631260E+00	-9.32897E-02
25	1.0266980E+00	4.10348E+00
26	5.3394470E-01	-3.53813E+00
27	2.5806550E-01	-1.62827E-01
28	6.5975540E-02	2.55950E+00
29	3.3914920E-02	-1.70694E+00
30	1.6765960E-02	-2.25223E-01
S	30	
1	6.9855600E+07	-1.09333E-07
2	1.8422660E+07	-3.07540E-07
3	6.1949800E+06	-1.36042E-06
4	2.2928270E+06	-3.45412E-06
5	9.1381600E+05	-1.29931E-05
6	3.8128830E+05	-2.85165E-05
7	1.6555900E+05	-1.01962E-04
8	7.4280470E+04	-1.97605E-04
9	3.4342950E+04	-6.82853E-04
10	1.6316470E+04	-1.16926E-03
11	7.9497860E+03	-3.94519E-03
12	3.9636570E+03	-5.77327E-03
13	2.0184970E+03	-1.90570E-02
14	1.0481120E+03	-2.04986E-02
15	5.5373610E+02	-6.69915E-02
16	2.9670960E+02	-2.10247E-02
17	1.5886880E+02	-1.46109E-01
18	8.7062830E+01	1.56948E-01
19	4.7924070E+01	-3.36276E-01
20	2.5489300E+01	1.11115E-01
21	1.4533130E+01	6.83475E-01
22	8.0949100E+00	6.39465E-01
23	4.2748700E+00	-5.41518E+00

24	2.2631260E+00	6.33243E+00
25	1.0266980E+00	-1.07294E+00
26	5.3394470E-01	-4.33676E+00
27	2.5806550E-01	4.57985E+00
28	6.5975540E-02	-2.89401E+00
29	3.3914920E-02	1.24107E+00
30	1.6765960E-02	3.54559E-01
P	24	
1	1.4590550E+07	-3.25601E-10
2	2.4896360E+06	4.85118E-09
3	5.5880580E+05	-2.48765E-08
4	1.4833850E+05	2.59818E-07
5	4.4801660E+04	-4.89034E-07
6	1.5127620E+04	7.40871E-06
7	5.6543160E+03	-3.14915E-06
8	2.3098440E+03	1.29836E-04
9	1.0153770E+03	7.45006E-06
10	4.7331040E+02	1.41004E-03
11	2.3064360E+02	-1.32461E-04
12	1.1634230E+02	9.38624E-03
13	6.0094260E+01	-1.20715E-02
14	3.1423980E+01	8.32368E-02
15	1.6915250E+01	-2.32935E-01
16	9.0665380E+00	9.69098E-03
17	4.7398210E+00	5.98084E-01
18	2.4537310E+00	4.11708E-01
19	1.1847470E+00	1.07231E-01
20	5.8203120E-01	2.57456E-02
21	2.7857010E-01	2.78586E-02
22	1.1871710E-01	1.35598E-03
23	4.9701490E-02	9.72008E-04
24	2.0385000E-02	-2.36148E-04
P	24	
1	1.4590550E+07	1.11996E-10
2	2.4896360E+06	-1.90875E-09
3	5.5880580E+05	7.56620E-09
4	1.4833850E+05	-1.09462E-07
5	4.4801660E+04	7.49015E-08
6	1.5127620E+04	-3.34637E-06
7	5.6543160E+03	-2.00092E-06
8	2.3098440E+03	-6.10615E-05
9	1.0153770E+03	-5.16678E-05
10	4.7331040E+02	-6.72652E-04
11	2.3064360E+02	-3.43887E-04
12	1.1634230E+02	-4.32644E-03
13	6.0094260E+01	3.79204E-03
14	3.1423980E+01	-3.94480E-02
15	1.6915250E+01	1.27422E-01
16	9.0665380E+00	-4.02599E-02
17	4.7398210E+00	-3.62657E-01
18	2.4537310E+00	-2.77355E-01

19	1.1847470E+00	2.07750E-01
20	5.8203120E-01	5.62839E-01
21	2.7857010E-01	3.71999E-01
22	1.1871710E-01	6.35342E-02
23	4.9701490E-02	-8.65124E-04
24	2.0385000E-02	1.23224E-03
P	24	
1	1.4590550E+07	-2.30589E-11
2	2.4896360E+06	4.12954E-10
3	5.5880580E+05	-1.47548E-09
4	1.4833850E+05	2.42075E-08
5	4.4801660E+04	-7.66526E-09
6	1.5127620E+04	7.55323E-07
7	5.6543160E+03	6.68369E-07
8	2.3098440E+03	1.39351E-05
9	1.0153770E+03	1.47233E-05
10	4.7331040E+02	1.54070E-04
11	2.3064360E+02	1.03342E-04
12	1.1634230E+02	9.81220E-04
13	6.0094260E+01	-7.45765E-04
14	3.1423980E+01	9.00545E-03
15	1.6915250E+01	-3.02190E-02
16	9.0665380E+00	1.15844E-02
17	4.7398210E+00	8.88424E-02
18	2.4537310E+00	6.81455E-02
19	1.1847470E+00	-7.48708E-02
20	5.8203120E-01	-1.85273E-01
21	2.7857010E-01	-1.71119E-01
22	1.1871710E-01	1.59105E-01
23	4.9701490E-02	6.30813E-01
24	2.0385000E-02	3.63283E-01
P	24	
1	1.4590550E+07	-9.11003E-11
2	2.4896360E+06	1.54705E-09
3	5.5880580E+05	-6.17742E-09
4	1.4833850E+05	8.85721E-08
5	4.4801660E+04	-6.30722E-08
6	1.5127620E+04	2.70343E-06
7	5.6543160E+03	1.55924E-06
8	2.3098440E+03	4.92929E-05
9	1.0153770E+03	4.10761E-05
10	4.7331040E+02	5.42938E-04
11	2.3064360E+02	2.78196E-04
12	1.1634230E+02	3.47367E-03
13	6.0094260E+01	-2.90306E-03
14	3.1423980E+01	3.13198E-02
15	1.6915250E+01	-1.07095E-01
16	9.0665380E+00	5.76097E-02
17	4.7398210E+00	2.93423E-01
18	2.4537310E+00	2.43185E-01
19	1.1847470E+00	-5.45609E-01

20	5.8203120E-01	-4.58379E-01
21	2.7857010E-01	2.28829E-01
22	1.1871710E-01	5.92841E-01
23	4.9701490E-02	3.48067E-01
24	2.0385000E-02	5.73974E-03
P	24	
1	1.4590550E+07	-6.70494E-11
2	2.4896360E+06	1.63103E-09
3	5.5880580E+05	-2.51505E-09
4	1.4833850E+05	1.06390E-07
5	4.4801660E+04	1.45024E-07
6	1.5127620E+04	3.62518E-06
7	5.6543160E+03	7.48156E-06
8	2.3098440E+03	6.98908E-05
9	1.0153770E+03	1.30912E-04
10	4.7331040E+02	7.85195E-04
11	2.3064360E+02	9.93597E-04
12	1.1634230E+02	4.85781E-03
13	6.0094260E+01	-1.83266E-03
14	3.1423980E+01	4.76841E-02
15	1.6915250E+01	-1.82542E-01
16	9.0665380E+00	1.21308E-01
17	4.7398210E+00	5.78220E-01
18	2.4537310E+00	2.08623E-01
19	1.1847470E+00	-1.36379E+00
20	5.8203120E-01	1.52837E-02
21	2.7857010E-01	1.37585E+00
22	1.1871710E-01	-3.67860E-01
23	4.9701490E-02	-6.51834E-01
24	2.0385000E-02	-1.49142E-03
P	24	
1	1.4590550E+07	5.97444E-10
2	2.4896360E+06	-5.45694E-09
3	5.5880580E+05	5.98553E-08
4	1.4833850E+05	-1.88525E-07
5	4.4801660E+04	2.23620E-06
6	1.5127620E+04	-2.15203E-06
7	5.6543160E+03	5.00333E-05
8	2.3098440E+03	-3.07052E-06
9	1.0153770E+03	6.87715E-04
10	4.7331040E+02	1.10775E-04
11	2.3064360E+02	5.64967E-03
12	1.1634230E+02	-8.15106E-04
13	6.0094260E+01	2.13461E-02
14	3.1423980E+01	2.88007E-02
15	1.6915250E+01	-2.44623E-01
16	9.0665380E+00	1.99503E-01
17	4.7398210E+00	1.48810E+00
18	2.4537310E+00	-1.47721E+00
19	1.1847470E+00	-1.32149E+00
20	5.8203120E-01	3.00029E+00

21	2.7857010E-01	-1.60738E+00
22	1.1871710E-01	-5.09849E-01
23	4.9701490E-02	8.16563E-01
24	2.0385000E-02	-1.64995E-03
D	16	
1	1.1053090E+04	6.09662E-07
2	2.8711810E+03	3.35409E-06
3	1.0273200E+03	5.42909E-05
4	4.3276070E+02	1.95161E-04
5	2.0103890E+02	1.25049E-03
6	9.9473570E+01	3.18063E-03
7	5.1298640E+01	1.21360E-02
8	2.7084780E+01	1.60849E-02
9	1.4506110E+01	3.10871E-03
10	7.6754510E+00	2.87396E-01
11	3.9561870E+00	4.56815E-01
12	1.9833970E+00	3.01106E-01
13	9.2695730E-01	7.27458E-02
14	3.9170760E-01	2.90384E-03
15	1.5410150E-01	6.63832E-04
16	5.6087510E-02	-8.26803E-05
D	16	
1	1.1053090E+04	-2.24541E-07
2	2.8711810E+03	-6.92986E-07
3	1.0273200E+03	-1.84368E-05
4	4.3276070E+02	-5.20722E-05
5	2.0103890E+02	-4.11228E-04
6	9.9473570E+01	-8.92770E-04
7	5.1298640E+01	-4.02184E-03
8	2.7084780E+01	-3.92256E-03
9	1.4506110E+01	-5.03029E-03
10	7.6754510E+00	-9.22699E-02
11	3.9561870E+00	-1.36077E-01
12	1.9833970E+00	-4.65038E-02
13	9.2695730E-01	2.08748E-01
14	3.9170760E-01	4.46696E-01
15	1.5410150E-01	4.27911E-01
16	5.6087510E-02	1.55001E-01
D	16	
1	1.1053090E+04	-5.11310E-07
2	2.8711810E+03	6.70390E-08
3	1.0273200E+03	-3.74069E-05
4	4.3276070E+02	-5.85262E-05
5	2.0103890E+02	-7.83102E-04
6	9.9473570E+01	-1.18622E-03
7	5.1298640E+01	-7.49016E-03
8	2.7084780E+01	-4.57922E-03
9	1.4506110E+01	-1.11603E-02
10	7.6754510E+00	-1.50112E-01
11	3.9561870E+00	-2.55726E-01
12	1.9833970E+00	-1.00551E-01

13	9.2695730E-01	8.65086E-01
14	3.9170760E-01	1.54824E-01
15	1.5410150E-01	-6.36332E-01
16	5.6087510E-02	-2.51554E-01
D	16	
1	1.1053090E+04	3.75990E-06
2	2.8711810E+03	-2.60132E-05
3	1.0273200E+03	1.99660E-04
4	4.3276070E+02	-5.03343E-04
5	2.0103890E+02	3.27977E-03
6	9.9473570E+01	-4.36765E-03
7	5.1298640E+01	2.80424E-02
8	2.7084780E+01	-3.33955E-02
9	1.4506110E+01	1.01803E-01
10	7.6754510E+00	1.30314E-01
11	3.9561870E+00	6.39525E-01
12	1.9833970E+00	-8.09463E-01
13	9.2695730E-01	-6.61025E-01
14	3.9170760E-01	1.34163E+00
15	1.5410150E-01	-4.18415E-01
16	5.6087510E-02	-4.25157E-01
D	16	
1	1.1053090E+04	4.25916E-06
2	2.8711810E+03	-2.70117E-05
3	1.0273200E+03	2.32205E-04
4	4.3276070E+02	-4.82979E-04
5	2.0103890E+02	3.94806E-03
6	9.9473570E+01	-3.90237E-03
7	5.1298640E+01	3.50552E-02
8	2.7084780E+01	-3.89729E-02
9	1.4506110E+01	1.30504E-01
10	7.6754510E+00	3.74714E-01
11	3.9561870E+00	5.80465E-01
12	1.9833970E+00	-2.12453E+00
13	9.2695730E-01	1.90093E+00
14	3.9170760E-01	-5.52590E-01
15	1.5410150E-01	-5.91624E-01
16	5.6087510E-02	7.92578E-01
F	11	
1	3.0219590E+02	3.92583E-04
2	1.0324860E+02	4.40720E-03
3	4.3730010E+01	3.72966E-02
4	2.0118100E+01	1.20996E-01
5	9.7628810E+00	2.23413E-01
6	4.7887770E+00	3.13922E-01
7	2.3145640E+00	3.20942E-01
8	1.0768650E+00	2.46199E-01
9	4.6899160E-01	1.26985E-01
10	1.9078280E-01	3.22680E-02
11	6.9253500E-02	1.74564E-03
F	11	

1	3.0219590E+02	-4.13631E-04
2	1.0324860E+02	-4.74911E-03
3	4.3730010E+01	-4.00003E-02
4	2.0118100E+01	-1.30621E-01
5	9.7628810E+00	-2.34233E-01
6	4.7887770E+00	-2.60296E-01
7	2.3145640E+00	-8.00803E-02
8	1.0768650E+00	4.00731E-01
9	4.6899160E-01	4.53396E-01
10	1.9078280E-01	1.91477E-01
11	6.9253500E-02	2.69469E-02
F	11	
1	3.0219590E+02	3.20702E-04
2	1.0324860E+02	4.90352E-03
3	4.3730010E+01	3.57972E-02
4	2.0118100E+01	1.29824E-01
5	9.7628810E+00	1.95222E-01
6	4.7887770E+00	2.06222E-01
7	2.3145640E+00	-2.34970E-01
8	1.0768650E+00	-6.55767E-01
9	4.6899160E-01	3.54950E-01
10	1.9078280E-01	5.62386E-01
11	6.9253500E-02	1.33202E-01
F	11	
1	3.0219590E+02	-4.21756E-04
2	1.0324860E+02	-7.49303E-03
3	4.3730010E+01	-5.14372E-02
4	2.0118100E+01	-1.96694E-01
5	9.7628810E+00	-2.58204E-01
6	4.7887770E+00	-1.74682E-01
7	2.3145640E+00	9.57619E-01
8	1.0768650E+00	-2.83255E-01
9	4.6899160E-01	-7.53067E-01
10	1.9078280E-01	6.27149E-01
11	6.9253500E-02	2.77603E-01
G	3	
1	5.095277	1.000000E+00
2	1.309201	1.000000E+00
3	2.08E-01	1.000000E+00
H	1	
1	1.801534	1.000000E+00

The following basis set for Am(III) was constructed by re-contracting the cc-pVTZ-DK3 set in the presence of the ECP60MWB ECP using the procedure outlined in Ref. ¹¹.

S	33	
1	5.6292160E+07	1.05308E-09
2	1.4983125E+07	6.06649E-09
3	5.1217092E+06	4.83047E-09
4	1.9449982E+06	8.41915E-08
5	8.1034752E+05	-2.25535E-08

6	3.5799276E+05	7.74007E-07
7	1.6678096E+05	-6.05584E-07
8	8.0828430E+04	5.61761E-06
9	4.0578332E+04	-6.05969E-06
10	2.0958427E+04	3.41772E-05
11	1.1104413E+04	-4.25325E-05
12	6.0105724E+03	1.77257E-04
13	3.3098710E+03	-2.32261E-04
14	1.8445087E+03	7.83233E-04
15	1.0356408E+03	-1.08898E-03
16	5.8313620E+02	3.20071E-03
17	3.3298456E+02	-5.66761E-03
18	1.9220616E+02	1.46444E-02
19	1.1212845E+02	-3.69071E-02
20	6.7150160E+01	1.14293E-01
21	4.0441727E+01	-3.90767E-01
22	2.4492476E+01	9.54236E-01
23	1.4408020E+01	-8.16126E-01
24	8.7069655E+00	-8.35767E-01
25	5.3198651E+00	4.37052E-01
26	3.0565776E+00	8.90054E-01
27	1.7499853E+00	3.66790E-01
28	9.2999162E-01	4.09146E-02
29	4.9168519E-01	2.69875E-02
30	2.5123075E-01	6.74376E-03
31	7.8969540E-02	1.45757E-03
32	3.8585630E-02	7.61791E-04
33	1.8332100E-02	3.92298E-04
S	33	
1	5.6292160E+07	-8.15468E-10
2	1.4983125E+07	-3.38284E-09
3	5.1217092E+06	-6.93203E-09
4	1.9449982E+06	-4.25977E-08
5	8.1034752E+05	-3.64846E-08
6	3.5799276E+05	-3.60584E-07
7	1.6678096E+05	-8.17416E-08
8	8.0828430E+04	-2.44687E-06
9	4.0578332E+04	4.88603E-07
10	2.0958427E+04	-1.41267E-05
11	1.1104413E+04	7.00668E-06
12	6.0105724E+03	-7.04673E-05
13	3.3098710E+03	4.83496E-05
14	1.8445087E+03	-3.03091E-04
15	1.0356408E+03	2.68083E-04
16	5.8313620E+02	-1.19574E-03
17	3.3298456E+02	1.76376E-03
18	1.9220616E+02	-5.39974E-03
19	1.1212845E+02	1.43476E-02
20	6.7150160E+01	-5.11121E-02
21	4.0441727E+01	2.00417E-01
22	2.4492476E+01	-5.44073E-01

23	1.4408020E+01	5.38329E-01
24	8.7069655E+00	4.82913E-01
25	5.3198651E+00	-2.98264E-01
26	3.0565776E+00	-8.92834E-01
27	1.7499853E+00	-4.35200E-01
28	9.2999162E-01	4.96046E-01
29	4.9168519E-01	6.85027E-01
30	2.5123075E-01	2.08798E-01
31	7.8969540E-02	8.40394E-02
32	3.8585630E-02	9.45956E-02
33	1.8332100E-02	2.86397E-02
S	33	
1	5.6292160E+07	3.78611E-10
2	1.4983125E+07	1.57884E-09
3	5.1217092E+06	3.19845E-09
4	1.9449982E+06	1.99191E-08
5	8.1034752E+05	1.66012E-08
6	3.5799276E+05	1.68911E-07
7	1.6678096E+05	3.45023E-08
8	8.0828430E+04	1.14797E-06
9	4.0578332E+04	-2.53108E-07
10	2.0958427E+04	6.63586E-06
11	1.1104413E+04	-3.41326E-06
12	6.0105724E+03	3.31274E-05
13	3.3098710E+03	-2.32275E-05
14	1.8445087E+03	1.42473E-04
15	1.0356408E+03	-1.27381E-04
16	5.8313620E+02	5.60765E-04
17	3.3298456E+02	-8.24913E-04
18	1.9220616E+02	2.50360E-03
19	1.1212845E+02	-6.57548E-03
20	6.7150160E+01	2.32385E-02
21	4.0441727E+01	-9.11770E-02
22	2.4492476E+01	2.49731E-01
23	1.4408020E+01	-2.54436E-01
24	8.7069655E+00	-2.10879E-01
25	5.3198651E+00	1.25393E-01
26	3.0565776E+00	4.59923E-01
27	1.7499853E+00	2.05780E-01
28	9.2999162E-01	-2.72805E-01
29	4.9168519E-01	-5.45049E-01
30	2.5123075E-01	-2.45897E-01
31	7.8969540E-02	4.56133E-01
32	3.8585630E-02	5.86949E-01
33	1.8332100E-02	1.70916E-01
S	33	
1	5.6292160E+07	7.47794E-10
2	1.4983125E+07	4.21412E-09
3	5.1217092E+06	3.65754E-09
4	1.9449982E+06	5.81742E-08
5	8.1034752E+05	-1.21700E-08

6	3.5799276E+05	5.32608E-07
7	1.6678096E+05	-3.90749E-07
8	8.0828430E+04	3.85339E-06
9	4.0578332E+04	-4.00216E-06
10	2.0958427E+04	2.33861E-05
11	1.1104413E+04	-2.83194E-05
12	6.0105724E+03	1.20989E-04
13	3.3098710E+03	-1.54805E-04
14	1.8445087E+03	5.31896E-04
15	1.0356408E+03	-7.19307E-04
16	5.8313620E+02	2.13372E-03
17	3.3298456E+02	-3.63009E-03
18	1.9220616E+02	9.15372E-03
19	1.1212845E+02	-2.16243E-02
20	6.7150160E+01	6.35840E-02
21	4.0441727E+01	-2.18408E-01
22	2.4492476E+01	5.79527E-01
23	1.4408020E+01	-6.54827E-01
24	8.7069655E+00	-2.87387E-01
25	5.3198651E+00	6.13374E-02
26	3.0565776E+00	1.59549E+00
27	1.7499853E+00	-3.92912E-02
28	9.2999162E-01	-1.70644E+00
29	4.9168519E-01	-7.20919E-01
30	2.5123075E-01	1.66401E+00
31	7.8969540E-02	8.08079E-01
32	3.8585630E-02	-9.24755E-01
33	1.8332100E-02	-2.88397E-01
S	33	
1	5.6292160E+07	-1.20118E-09
2	1.4983125E+07	-4.92746E-09
3	5.1217092E+06	-1.03455E-08
4	1.9449982E+06	-6.17931E-08
5	8.1034752E+05	-5.60167E-08
6	3.5799276E+05	-5.21075E-07
7	1.6678096E+05	-1.43620E-07
8	8.0828430E+04	-3.52410E-06
9	4.0578332E+04	5.42455E-07
10	2.0958427E+04	-2.02899E-05
11	1.1104413E+04	9.22128E-06
12	6.0105724E+03	-1.00972E-04
13	3.3098710E+03	6.54011E-05
14	1.8445087E+03	-4.32544E-04
15	1.0356408E+03	3.63674E-04
16	5.8313620E+02	-1.68058E-03
17	3.3298456E+02	2.36441E-03
18	1.9220616E+02	-7.20497E-03
19	1.1212845E+02	1.83051E-02
20	6.7150160E+01	-6.40658E-02
21	4.0441727E+01	2.55968E-01
22	2.4492476E+01	-7.33774E-01

23	1.4408020E+01	8.41493E-01
24	8.7069655E+00	5.37329E-01
25	5.3198651E+00	-3.57440E-01
26	3.0565776E+00	-2.53687E+00
27	1.7499853E+00	8.84058E-01
28	9.2999162E-01	4.30364E+00
29	4.9168519E-01	-4.08330E+00
30	2.5123075E-01	-1.74691E-01
31	7.8969540E-02	2.48601E+00
32	3.8585630E-02	-1.18113E+00
33	1.8332100E-02	-4.87779E-01
S	33	
1	5.6292160E+07	-1.31469E-09
2	1.4983125E+07	-1.06120E-08
3	5.1217092E+06	1.34038E-09
4	1.9449982E+06	-1.57317E-07
5	8.1034752E+05	1.52768E-07
6	3.5799276E+05	-1.51792E-06
7	1.6678096E+05	2.02754E-06
8	8.0828430E+04	-1.14074E-05
9	4.0578332E+04	1.72572E-05
10	2.0958427E+04	-7.10962E-05
11	1.1104413E+04	1.12579E-04
12	6.0105724E+03	-3.74091E-04
13	3.3098710E+03	5.87201E-04
14	1.8445087E+03	-1.65852E-03
15	1.0356408E+03	2.61035E-03
16	5.8313620E+02	-6.70638E-03
17	3.3298456E+02	1.21306E-02
18	1.9220616E+02	-2.81841E-02
19	1.1212845E+02	6.26936E-02
20	6.7150160E+01	-1.61779E-01
21	4.0441727E+01	4.93411E-01
22	2.4492476E+01	-1.29456E+00
23	1.4408020E+01	1.74483E+00
24	8.7069655E+00	-3.74667E-02
25	5.3198651E+00	4.95052E-01
26	3.0565776E+00	-7.45164E+00
27	1.7499853E+00	1.05539E+01
28	9.2999162E-01	-3.58121E+00
29	4.9168519E-01	-4.71010E+00
30	2.5123075E-01	5.59232E+00
31	7.8969540E-02	-2.61646E+00
32	3.8585630E-02	1.70798E-01
33	1.8332100E-02	8.42138E-01
P	29	
1	5.4618670E+07	1.47383E-10
2	1.6477889E+07	-7.99910E-10
3	5.3245498E+06	3.95676E-09
4	1.8375817E+06	-1.34332E-08
5	6.6811421E+05	6.22674E-08

6	2.5396964E+05	-1.47904E-07
7	1.0046027E+05	8.20203E-07
8	4.1267789E+04	-1.09001E-06
9	1.7606875E+04	9.94547E-06
10	7.8134986E+03	-3.70566E-06
11	3.6102128E+03	1.07997E-04
12	1.7351406E+03	2.57422E-05
13	8.6411398E+02	9.59908E-04
14	4.4372855E+02	4.41994E-04
15	2.3446224E+02	6.35705E-03
16	1.2680930E+02	9.86973E-04
17	7.0263594E+01	2.68426E-02
18	3.9388042E+01	-2.09108E-02
19	2.1876140E+01	1.07300E-01
20	1.2291127E+01	-1.33971E-01
21	6.8589925E+00	-2.34596E-01
22	3.7470795E+00	6.27284E-01
23	2.0046380E+00	4.86389E-01
24	9.9978700E-01	1.39686E-01
25	4.9997200E-01	1.21387E-02
26	2.4206600E-01	1.95967E-02
27	9.9764000E-02	-9.37707E-04
28	4.3155000E-02	1.23524E-03
29	1.8156000E-02	-3.46994E-04
P	29	
1	5.4618670E+07	-8.54375E-11
2	1.6477889E+07	4.49599E-10
3	5.3245498E+06	-2.31552E-09
4	1.8375817E+06	7.35523E-09
5	6.6811421E+05	-3.74182E-08
6	2.5396964E+05	7.50892E-08
7	1.0046027E+05	-5.14940E-07
8	4.1267789E+04	4.14140E-07
9	1.7606875E+04	-6.57076E-06
10	7.8134986E+03	-1.34723E-06
11	3.6102128E+03	-7.42997E-05
12	1.7351406E+03	-5.64533E-05
13	8.6411398E+02	-6.77540E-04
14	4.4372855E+02	-6.08344E-04
15	2.3446224E+02	-4.52075E-03
16	1.2680930E+02	-2.32555E-03
17	7.0263594E+01	-1.84182E-02
18	3.9388042E+01	9.36677E-03
19	2.1876140E+01	-7.25248E-02
20	1.2291127E+01	1.16635E-01
21	6.8589925E+00	6.24345E-02
22	3.7470795E+00	-4.68272E-01
23	2.0046380E+00	-3.22843E-01
24	9.9978700E-01	2.35076E-01
25	4.9997200E-01	5.92112E-01
26	2.4206600E-01	3.47833E-01

27	9.9764000E-02	5.69877E-02
28	4.3155000E-02	-3.10056E-03
29	1.8156000E-02	1.64517E-03
P	29	
1	5.4618670E+07	2.06148E-11
2	1.6477889E+07	-1.07513E-10
3	5.3245498E+06	5.60206E-10
4	1.8375817E+06	-1.74481E-09
5	6.6811421E+05	9.11910E-09
6	2.5396964E+05	-1.73842E-08
7	1.0046027E+05	1.26964E-07
8	4.1267789E+04	-8.49171E-08
9	1.7606875E+04	1.64087E-06
10	7.8134986E+03	5.65973E-07
11	3.6102128E+03	1.87324E-05
12	1.7351406E+03	1.64830E-05
13	8.6411398E+02	1.71809E-04
14	4.4372855E+02	1.71034E-04
15	2.3446224E+02	1.14811E-03
16	1.2680930E+02	6.81770E-04
17	7.0263594E+01	4.63860E-03
18	3.9388042E+01	-2.06623E-03
19	2.1876140E+01	1.81473E-02
20	1.2291127E+01	-3.02314E-02
21	6.8589925E+00	-1.19495E-02
22	3.7470795E+00	1.21440E-01
23	2.0046380E+00	8.11005E-02
24	9.9978700E-01	-8.37532E-02
25	4.9997200E-01	-2.04744E-01
26	2.4206600E-01	-1.60217E-01
27	9.9764000E-02	1.99954E-01
28	4.3155000E-02	6.21318E-01
29	1.8156000E-02	3.35737E-01
P	29	
1	5.4618670E+07	6.68641E-11
2	1.6477889E+07	-3.46616E-10
3	5.3245498E+06	1.82027E-09
4	1.8375817E+06	-5.59560E-09
5	6.6811421E+05	2.97755E-08
6	2.5396964E+05	-5.48021E-08
7	1.0046027E+05	4.17661E-07
8	4.1267789E+04	-2.42985E-07
9	1.7606875E+04	5.44096E-06
10	7.8134986E+03	2.36052E-06
11	3.6102128E+03	6.24673E-05
12	1.7351406E+03	5.97249E-05
13	8.6411398E+02	5.74936E-04
14	4.4372855E+02	6.07362E-04
15	2.3446224E+02	3.84736E-03
16	1.2680930E+02	2.46104E-03
17	7.0263594E+01	1.55199E-02

18	3.9388042E+01	-6.63759E-03
19	2.1876140E+01	6.21917E-02
20	1.2291127E+01	-1.08834E-01
21	6.8589925E+00	-2.86222E-02
22	3.7470795E+00	4.29717E-01
23	2.0046380E+00	3.08810E-01
24	9.9978700E-01	-6.70268E-01
25	4.9997200E-01	-5.21875E-01
26	2.4206600E-01	3.97063E-01
27	9.9764000E-02	6.44214E-01
28	4.3155000E-02	1.90093E-01
29	1.8156000E-02	3.76205E-03
P	29	
1	5.4618670E+07	6.64365E-11
2	1.6477889E+07	-3.15129E-10
3	5.3245498E+06	1.85371E-09
4	1.8375817E+06	-4.66338E-09
5	6.6811421E+05	3.23242E-08
6	2.5396964E+05	-3.23514E-08
7	1.0046027E+05	4.96770E-07
8	4.1267789E+04	2.10555E-07
9	1.7606875E+04	7.07329E-06
10	7.8134986E+03	9.60928E-06
11	3.6102128E+03	8.62302E-05
12	1.7351406E+03	1.45528E-04
13	8.6411398E+02	8.21235E-04
14	4.4372855E+02	1.32863E-03
15	2.3446224E+02	5.54645E-03
16	1.2680930E+02	5.94948E-03
17	7.0263594E+01	2.15634E-02
18	3.9388042E+01	-2.85199E-03
19	2.1876140E+01	8.88106E-02
20	1.2291127E+01	-1.71583E-01
21	6.8589925E+00	-2.39963E-02
22	3.7470795E+00	8.07814E-01
23	2.0046380E+00	2.35566E-01
24	9.9978700E-01	-1.72865E+00
25	4.9997200E-01	4.62243E-01
26	2.4206600E-01	1.31407E+00
27	9.9764000E-02	-6.96803E-01
28	4.3155000E-02	-4.62068E-01
29	1.8156000E-02	8.97340E-03
P	29	
1	5.4618670E+07	-2.20188E-10
2	1.6477889E+07	1.42243E-09
3	5.3245498E+06	-5.55846E-09
4	1.8375817E+06	2.70322E-08
5	6.6811421E+05	-7.16823E-08
6	2.5396964E+05	3.92702E-07
7	1.0046027E+05	-5.88561E-07
8	4.1267789E+04	5.14028E-06

9	1.7606875E+04	-1.87136E-06
10	7.8134986E+03	6.19081E-05
11	3.6102128E+03	2.70815E-05
12	1.7351406E+03	6.29656E-04
13	8.6411398E+02	5.13020E-04
14	4.4372855E+02	4.95409E-03
15	2.3446224E+02	3.88827E-03
16	1.2680930E+02	2.55042E-02
17	7.0263594E+01	7.46952E-03
18	3.9388042E+01	5.98408E-02
19	2.1876140E+01	3.58593E-02
20	1.2291127E+01	-1.31465E-01
21	6.8589925E+00	-1.79060E-01
22	3.7470795E+00	2.21134E+00
23	2.0046380E+00	-2.23959E+00
24	9.9978700E-01	-9.54654E-01
25	4.9997200E-01	3.29699E+00
26	2.4206600E-01	-2.30031E+00
27	9.9764000E-02	4.23798E-02
28	4.3155000E-02	6.84868E-01
29	1.8156000E-02	-3.00921E-02
D	2.000000E+01	
1	1.2260514E+05	-9.21291E-09
2	2.8764076E+04	1.02699E-07
3	9.2733196E+03	-4.43193E-07
4	3.5765898E+03	3.31462E-06
5	1.5572799E+03	-5.55689E-06
6	7.3850180E+02	5.38734E-05
7	3.7201662E+02	-1.85554E-05
8	1.9609261E+02	5.60674E-04
9	1.0647837E+02	1.96355E-04
10	5.9214914E+01	3.75916E-03
11	3.3142124E+01	8.24353E-04
12	1.8355967E+01	2.82117E-02
13	1.0228860E+01	-1.12953E-01
14	5.6212585E+00	2.03166E-01
15	3.0041933E+00	5.16349E-01
16	1.5539126E+00	3.51533E-01
17	7.5505798E-01	9.33844E-02
18	3.2519923E-01	3.96772E-03
19	1.3082626E-01	8.07794E-04
20	4.9184900E-02	-2.10760E-04
D	20	
1	1.2260514E+05	1.23940E-09
2	2.8764076E+04	-1.71073E-08
3	9.2733196E+03	4.32339E-08
4	3.5765898E+03	-6.42452E-07
5	1.5572799E+03	-7.51176E-08
6	7.3850180E+02	-1.20382E-05
7	3.7201662E+02	-1.42227E-05
8	1.9609261E+02	-1.40499E-04

9	1.0647837E+02	-2.12494E-04
10	5.9214914E+01	-9.87048E-04
11	3.3142124E+01	-1.12281E-03
12	1.8355967E+01	-7.58698E-03
13	1.0228860E+01	3.56060E-02
14	5.6212585E+00	-8.20403E-02
15	3.0041933E+00	-1.81801E-01
16	1.5539126E+00	-8.77519E-02
17	7.5505798E-01	1.97837E-01
18	3.2519923E-01	4.53612E-01
19	1.3082626E-01	4.28968E-01
20	4.9184900E-02	1.62621E-01
D	20	
1	1.2260514E+05	-7.74521E-09
2	2.8764076E+04	6.32292E-08
3	9.2733196E+03	-4.89469E-07
4	3.5765898E+03	1.42188E-06
5	1.5572799E+03	-1.05610E-05
6	7.3850180E+02	1.18469E-05
7	3.7201662E+02	-1.33578E-04
8	1.9609261E+02	1.14166E-05
9	1.0647837E+02	-1.11790E-03
10	5.9214914E+01	-3.50058E-04
11	3.3142124E+01	-5.53030E-03
12	1.8355967E+01	-7.63359E-03
13	1.0228860E+01	5.61330E-02
14	5.6212585E+00	-1.45160E-01
15	3.0041933E+00	-3.87993E-01
16	1.5539126E+00	-1.32739E-01
17	7.5505798E-01	9.36297E-01
18	3.2519923E-01	1.43642E-01
19	1.3082626E-01	-6.34433E-01
20	4.9184900E-02	-2.37128E-01
D	20	
1	1.2260514E+05	1.49405E-07
2	2.8764076E+04	-1.40220E-06
3	9.2733196E+03	8.49709E-06
4	3.5765898E+03	-3.80234E-05
5	1.5572799E+03	1.55641E-04
6	7.3850180E+02	-4.88622E-04
7	3.7201662E+02	1.61784E-03
8	1.9609261E+02	-3.80220E-03
9	1.0647837E+02	1.09885E-02
10	5.9214914E+01	-1.98915E-02
11	3.3142124E+01	5.04363E-02
12	1.8355967E+01	-7.14950E-02
13	1.0228860E+01	5.81181E-02
14	5.6212585E+00	2.28475E-02
15	3.0041933E+00	1.09192E+00
16	1.5539126E+00	-1.18406E+00
17	7.5505798E-01	-5.32669E-01

18	3.2519923E-01	1.39446E+00
19	1.3082626E-01	-5.31896E-01
20	4.9184900E-02	-3.51929E-01
D	20	
1	1.2260514E+05	7.52509E-08
2	2.8764076E+04	-6.91409E-07
3	9.2733196E+03	4.33368E-06
4	3.5765898E+03	-1.80976E-05
5	1.5572799E+03	8.07774E-05
6	7.3850180E+02	-2.21581E-04
7	3.7201662E+02	8.79732E-04
8	1.9609261E+02	-1.63565E-03
9	1.0647837E+02	6.51045E-03
10	5.9214914E+01	-8.85295E-03
11	3.3142124E+01	3.42648E-02
12	1.8355967E+01	-3.36142E-02
13	1.0228860E+01	-6.00405E-02
14	5.6212585E+00	4.07707E-01
15	3.0041933E+00	1.07526E+00
16	1.5539126E+00	-2.84362E+00
17	7.5505798E-01	2.52407E+00
18	3.2519923E-01	-9.44330E-01
19	1.3082626E-01	-4.19834E-01
20	4.9184900E-02	7.54450E-01
F	13	
1	1.1664753E+03	-5.82198E-07
2	3.9242232E+02	2.47412E-05
3	1.6616422E+02	6.60030E-05
4	7.8013407E+01	8.60141E-04
5	3.8855696E+01	2.71694E-03
6	1.9750591E+01	1.31660E-02
7	1.0197502E+01	2.29065E-02
8	5.2790447E+00	1.57996E-01
9	2.6864586E+00	3.36239E-01
10	1.3377135E+00	3.57800E-01
11	6.3872673E-01	2.70242E-01
12	2.8613327E-01	1.32916E-01
13	1.1398101E-01	3.19534E-02
F	13	
1	1.1664753E+03	-2.21665E-06
2	3.9242232E+02	-1.07723E-05
3	1.6616422E+02	-1.71760E-04
4	7.8013407E+01	-7.61633E-04
5	3.8855696E+01	-4.34498E-03
6	1.9750591E+01	-1.39317E-02
7	1.0197502E+01	-3.61143E-02
8	5.2790447E+00	-2.01422E-01
9	2.6864586E+00	-3.85592E-01
10	1.3377135E+00	-1.39362E-01
11	6.3872673E-01	4.20366E-01
12	2.8613327E-01	4.57391E-01

13	1.1398101E-01	1.88996E-01
F	13	
1	1.1664753E+03	1.11890E-05
2	3.9242232E+02	-4.60261E-05
3	1.6616422E+02	4.63349E-04
4	7.8013407E+01	-2.16965E-05
5	3.8855696E+01	7.82615E-03
6	1.9750591E+01	8.88371E-03
7	1.0197502E+01	6.09089E-02
8	5.2790447E+00	2.11571E-01
9	2.6864586E+00	5.36344E-01
10	1.3377135E+00	-5.46283E-01
11	6.3872673E-01	-6.01100E-01
12	2.8613327E-01	5.36313E-01
13	1.1398101E-01	4.50855E-01
F	13	
1	1.1664753E+03	6.53586E-06
2	3.9242232E+02	-8.09430E-05
3	1.6616422E+02	4.48488E-05
4	7.8013407E+01	-2.05959E-03
5	3.8855696E+01	-3.60984E-03
6	1.9750591E+01	-2.49570E-02
7	1.0197502E+01	-3.90996E-02
8	5.2790447E+00	-3.61246E-01
9	2.6864586E+00	-4.50388E-01
10	1.3377135E+00	1.48293E+00
11	6.3872673E-01	-9.44293E-01
12	2.8613327E-01	-3.71526E-01
13	1.1398101E-01	8.08517E-01
G	3	
1	2.971818E+00	1.000000E+00
2	9.632869E-01	1.000000E+00
3	2.231343E-01	1.000000E+00
H	1	
1	1.446907E+00	1.000000E+00

E. Cartesian Spatial Coordinates for all Optimized Structures

All coordinates are provided in Angstroms.

16	Eu(H ₂ PO ₂) ₃ RI-MP2 SC ECP	16	Am(H ₂ PO ₂) ₃ RI-MP2 SC ECP
Eu	-0.038382 -0.051961 -0.009571	Am	0.077422 -0.136904 0.067323
O	-0.637128 -1.981527 1.148478	O	-0.686534 -2.131767 1.121543
O	-1.462073 -1.538949 -1.160293	O	-1.543078 -1.436308 -1.110589
P	-1.479021 -2.553891 -0.006136	P	-1.637791 -2.520887 -0.024578
H	-2.786449 -2.834665 0.413098	H	-2.953050 -2.668259 0.435670
H	-0.985267 -3.799457 -0.420051	H	-1.317088 -3.786608 -0.535694
O	1.917842 0.618068 1.048176	O	2.078236 0.545737 1.167646
O	1.985941 -0.618650 -1.111031	O	2.167545 -0.451196 -1.122365
P	2.854055 0.048826 -0.034518	P	3.012800 0.152812 0.006789

H 3.772690 -0.854650 0.517376	H 4.000820 -0.742021 0.440939
H 3.663714 1.058542 -0.571778	H 3.744896 1.262454 -0.438355
O -1.485184 1.432029 1.123625	O -1.299413 1.459112 1.216889
O -0.463052 1.979408 -1.085773	O -0.574422 1.791225 -1.155245
P -1.367640 2.513020 0.039576	P -1.396415 2.391906 0.000226
H -0.860909 3.710600 0.563889	H -0.943942 3.681276 0.315245
H -2.629136 2.873256 -0.455068	H -2.729984 2.589430 -0.385448
16 Eu(H ₂ PS ₂) ₃ RI-MP2 SC ECP	16 Am(H ₂ PS ₂) ₃ RI-MP2 SC ECP
Eu 0.086553 -0.033594 -0.087550	Am 0.158549 -0.068694 -0.044570
S -2.210842 1.424245 -0.469741	S -2.172202 1.389818 -0.402697
S -1.470185 -1.682268 -1.657173	S -1.447748 -1.714847 -1.627284
P -2.837694 -0.232441 -1.425836	P -2.799691 -0.254717 -1.384276
H -3.366399 0.113378 -2.678582	H -3.316748 0.116520 -2.634888
H -3.969371 -0.744168 -0.772133	H -3.942052 -0.757960 -0.742747
S 0.748673 1.486853 2.111223	S 0.757025 1.472389 2.211218
S -0.635876 -1.604229 2.045531	S -0.652047 -1.613470 2.110907
P -0.110137 -0.005192 3.143561	P -0.194266 0.013359 3.203028
H -1.230256 0.473297 3.840640	H -1.366817 0.514461 3.789543
H 0.729193 -0.402953 4.195008	H 0.546051 -0.368178 4.332000
S 1.531774 1.703363 -1.666272	S 1.567501 1.720532 -1.650545
S 2.375748 -1.446276 -0.649819	S 2.451789 -1.458136 -0.793166
P 2.917300 0.251802 -1.586415	P 2.948576 0.266326 -1.703142
H 4.091388 0.748403 -0.999813	H 4.158258 0.739061 -1.173084
H 3.350132 -0.050221 -2.886541	H 3.303823 0.003538 -3.034215
16 Eu(H ₂ PSe ₂) ₃ RI-MP2 SC ECP	16 Am(H ₂ PSe ₂) ₃ RI-MP2 SC ECP
Eu 0.284129 0.093545 -0.254897	Am -0.273618 -0.146991 -0.297041
Se -2.227529 1.492928 -0.014710	Se -2.507919 1.586100 -0.801702
Se -1.366248 -1.363840 -2.099830	Se -1.993847 -1.947055 -1.782866
P -2.877617 -0.334146 -0.957360	P -3.258141 -0.201861 -1.750570
H -3.989594 -0.088824 -1.776999	H -3.646615 0.099067 -3.064178
H -3.410600 -1.204645 0.005250	H -4.488378 -0.534863 -1.165976
Se 0.908520 1.543509 2.136380	Se 0.699651 1.724000 1.715965
Se -0.703278 -1.701219 1.763242	Se -0.851785 -1.569695 2.143938
P -0.445912 0.078353 2.942762	P 0.470418 -0.046337 2.912589
H -1.696834 0.666213 3.180683	H 0.047149 0.313769 4.201095
H -0.040653 -0.277858 4.238220	H 1.728223 -0.612396 3.167314
Se 1.918175 1.958339 -1.687474	Se 1.428478 1.301413 -2.154754
Se 2.467605 -1.616394 -0.916569	Se 2.268159 -1.508128 0.022945
P 3.193437 0.220532 -1.779392	P 2.913484 0.305039 -0.950071
H 4.434096 0.534403 -1.206255	H 3.424757 1.199708 0.001333
H 3.552308 -0.000891 -3.116962	H 4.039983 0.038232 -1.741935
16 Eu(H ₂ PTe ₂) ₃ RI-MP2 SC ECP	16 Am(H ₂ PTe ₂) ₃ RI-MP2 SC ECP
Eu 0.096011 0.001077 0.451788	Am 0.004459 0.030401 -0.546051
Te -2.685391 1.209750 -0.008637	Te -2.456750 1.815420 -1.150019
Te -0.846931 -1.892720 -1.798449	Te -1.768205 -2.110965 -1.951291
P -2.360803 -0.057871 -2.003976	P -3.323813 -0.400615 -1.359318
H -1.905920 0.792059 -3.027632	H -4.385665 -0.399829 -2.278303
H -3.595591 -0.482135 -2.526154	H -3.986891 -0.764002 -0.174630

Te	0.398325	1.997233	2.754174	Te	1.250765	1.520483	1.823915
Te	-0.251400	-2.051925	2.680104	Te	-1.222380	-1.575142	1.784262
P	-0.163591	-0.011085	3.915545	P	-0.011062	-0.028435	3.152472
H	-1.380157	0.168836	4.591701	H	-0.858747	0.666476	4.032774
H	0.710929	-0.170287	5.001654	H	0.804629	-0.701006	4.078919
Te	0.997611	1.930299	-1.769052	Te	1.822767	2.213949	-1.847965
Te	2.841702	-1.247883	-0.091101	Te	2.420356	-1.792313	-1.133526
P	2.469998	0.067698	-2.047342	P	3.318664	0.412818	-1.379528
H	3.697614	0.493260	-2.584114	H	4.069920	0.725761	-0.234217
H	1.977593	-0.746306	-3.082421	H	4.321950	0.386998	-2.361407

16	Eu(H ₂ PO ₂) ₃ B3LYP SC ECP			16	Am(H ₂ PO ₂) ₃ B3LYP SC ECP		
Eu	0.005022	-0.000030	-0.000040	Am	-0.000364	0.000000	0.000000
O	-0.506674	-2.053317	1.091782	O	-0.500604	-2.113942	1.078320
O	-1.527322	-1.466775	-1.098811	O	-1.581501	-1.490397	-1.079902
P	-1.470563	-2.538556	-0.001000	P	-1.488845	-2.579485	-0.001124
H	-2.752400	-2.799062	0.529287	H	-2.755683	-2.855514	0.555092
H	-1.065243	-3.785217	-0.523586	H	-1.093107	-3.813630	-0.558222
O	2.038241	0.583580	1.098231	O	2.080802	0.630125	1.075447
O	2.038294	-0.583545	-1.098245	O	2.080802	-0.630125	-1.075447
P	2.939490	0.000037	0.000005	P	2.978073	-0.000000	0.000000
H	3.811567	-0.978968	0.522875	H	3.850084	-0.956041	0.562486
H	3.811540	0.979077	-0.522844	H	3.850084	0.956041	-0.562486
O	-1.527300	1.466713	1.098782	O	-1.581501	1.490397	1.079902
O	-0.506665	2.053278	-1.091811	O	-0.500604	2.113942	-1.078320
P	-1.470514	2.538526	0.001005	P	-1.488846	2.579485	0.001124
H	-1.065125	3.785151	0.523621	H	-1.093107	3.813630	0.558222
H	-2.752347	2.799109	-0.529252	H	-2.755683	2.855513	-0.555092
16	Eu(H ₂ PS ₂) ₃ B3LYP SC ECP			16	Am(H ₂ PS ₂) ₃ B3LYP SC ECP		
Eu	0.000000	-0.000000	0.027504	Am	-0.000000	0.000000	0.008395
S	-2.507687	1.303936	-0.407830	S	-2.514121	1.309787	-0.409805
S	-1.466112	-1.620725	-1.824270	S	-1.480706	-1.612402	-1.844742
P	-2.925949	-0.228032	-1.663741	P	-2.946184	-0.228547	-1.653673
H	-3.259746	0.274581	-2.939431	H	-3.309217	0.266211	-2.924591
H	-4.139071	-0.842258	-1.286430	H	-4.146963	-0.849427	-1.247981
S	0.674734	1.568542	2.323562	S	0.681889	1.566985	2.312023
S	-0.674734	-1.568542	2.323562	S	-0.681889	-1.566985	2.312023
P	0.000000	-0.000000	3.411117	P	0.000000	0.000000	3.398037
H	-1.001238	0.432550	4.306872	H	-1.001117	0.433977	4.293595
H	1.001239	-0.432550	4.306872	H	1.001118	-0.433977	4.293595
S	1.466112	1.620725	-1.824270	S	1.480706	1.612403	-1.844742
S	2.507688	-1.303936	-0.407830	S	2.514120	-1.309787	-0.409804
P	2.925949	0.228032	-1.663740	P	2.946184	0.228547	-1.653673
H	4.139071	0.842258	-1.286430	H	4.146964	0.849426	-1.247982
H	3.259746	-0.274581	-2.939430	H	3.309216	-0.266211	-2.924591
16	Eu(H ₂ PSe ₂) ₃ B3LYP SC ECP			16	Am(H ₂ PSe ₂) ₃ B3LYP SC ECP		
Eu	-0.001095	-0.000908	0.049243	Am	0.000000	-0.000000	0.011233

Se	-2.637069	1.397894	-0.368251	Se	-2.611415	1.424561	-0.385526
Se	-1.467156	-1.738304	-1.935994	Se	-1.492774	-1.739122	-1.934091
P	-3.041520	-0.236764	-1.760938	P	-3.067273	-0.239728	-1.725746
H	-3.351104	0.288945	-3.032934	H	-3.430179	0.251355	-2.997332
H	-4.262730	-0.858475	-1.426505	H	-4.271421	-0.855898	-1.325781
Se	0.761352	1.685832	2.431653	Se	0.744145	1.692616	2.378722
Se	-0.760518	-1.685581	2.434294	Se	-0.744144	-1.692616	2.378722
P	0.001296	0.000615	3.594798	P	-0.000000	-0.000000	3.542352
H	-0.988545	0.451073	4.493468	H	-0.996793	0.434899	4.441004
H	0.992417	-0.449005	4.492481	H	0.996793	-0.434898	4.441005
Se	1.467673	1.739612	-1.932584	Se	1.492774	1.739122	-1.934092
Se	2.633713	-1.400555	-0.369685	Se	2.611415	-1.424562	-0.385527
P	3.040534	0.236437	-1.758936	P	3.067274	0.239727	-1.725747
H	4.262048	0.856417	-1.422395	H	4.271421	0.855897	-1.325782
H	3.350705	-0.287233	-3.031630	H	3.430178	-0.251356	-2.997332
16 Eu(H ₂ PTe ₂) ₃ B3LYP SC ECP				16 Am(H ₂ PTe ₂) ₃ B3LYP SC ECP			
Eu	0.005126	0.001067	-0.035527	Am	0.000000	-0.000000	0.003070
Te	-2.852638	1.561691	-0.290529	Te	-2.781387	1.589352	-0.351828
Te	-1.596585	-1.876748	-2.200827	Te	-1.538308	-1.914978	-2.097158
P	-3.365237	-0.257083	-1.824041	P	-3.297795	-0.258245	-1.845235
H	-3.806682	0.276557	-3.053401	H	-3.686270	0.229940	-3.111143
H	-4.542513	-0.915455	-1.409540	H	-4.501518	-0.876297	-1.444339
Te	0.883098	1.876254	2.502144	Te	0.838440	1.880049	2.491294
Te	-0.890280	-1.874855	2.493229	Te	-0.838439	-1.880050	2.491295
P	-0.008407	0.000421	3.766356	P	-0.000000	0.000000	3.784362
H	-0.986331	0.464963	4.671627	H	-0.988959	0.434900	4.692735
H	0.962931	-0.467244	4.677058	H	0.988958	-0.434899	4.692736
Te	1.601779	1.875722	-2.206446	Te	1.538308	1.914978	-2.097157
Te	2.863683	-1.558637	-0.298806	Te	2.781388	-1.589352	-0.351828
P	3.372459	0.256208	-1.837292	P	3.297795	0.258245	-1.845236
H	4.551621	0.915391	-1.429489	H	4.501518	0.876296	-1.444341
H	3.807977	-0.278253	-3.068431	H	3.686268	-0.229941	-3.111144

16 Eu(H ₂ PO ₂) ₃ PBE SC ECP				16 Am(H ₂ PO ₂) ₃ PBE SC ECP			
Eu	0.009817	-0.000019	-0.000012	Am	-0.001169	0.000000	0.000000
O	-0.485425	-2.076013	1.092123	O	-0.489999	-2.093197	1.098179
O	-1.555450	-1.458754	-1.106876	O	-1.570530	-1.471655	-1.100046
P	-1.477945	-2.542161	-0.002607	P	-1.477380	-2.561404	-0.001425
H	-2.761998	-2.804042	0.561922	H	-2.760692	-2.840965	0.554982
H	-1.088949	-3.799252	-0.553397	H	-1.072159	-3.810121	-0.558635
O	2.052899	0.614072	1.101545	O	2.056779	0.630771	1.094741
O	2.052927	-0.614057	-1.101545	O	2.056779	-0.630771	-1.094741
P	2.953268	0.000023	0.000002	P	2.955213	0.000000	-0.000000
H	3.835239	-0.974668	0.555124	H	3.836959	-0.969302	0.563916
H	3.835209	0.974744	-0.555114	H	3.836959	0.969302	-0.563917
O	-1.555431	1.458725	1.106865	O	-1.570530	1.471656	1.100047
O	-0.485410	2.075983	-1.092137	O	-0.489999	2.093197	-1.098178
P	-1.477910	2.542142	0.002607	P	-1.477380	2.561404	0.001425

H	-1.088879	3.799217	0.553407	H	-1.072159	3.810122	0.558635
H	-2.761961	2.804061	-0.561909	H	-2.760692	2.840965	-0.554982
16 Eu(H ₂ PS ₂) ₃ PBE SC ECP				16 Am(H ₂ PS ₂) ₃ PBE SC ECP			
Eu	-0.000000	-0.000000	0.032236	Am	-0.000003	0.000000	0.010709
S	-2.523677	1.287271	-0.366036	S	-2.492499	1.293698	-0.346838
S	-1.435184	-1.608093	-1.854479	S	-1.415441	-1.590253	-1.858414
P	-2.901896	-0.226907	-1.656421	P	-2.893276	-0.225072	-1.625687
H	-3.244565	0.312958	-2.930712	H	-3.269778	0.302674	-2.895172
H	-4.120850	-0.875759	-1.301610	H	-4.097574	-0.879987	-1.234623
S	0.720963	1.558311	2.321627	S	0.729943	1.552939	2.265274
S	-0.720962	-1.558311	2.321627	S	-0.729945	-1.552937	2.265277
P	0.000000	0.000000	3.394677	P	0.000003	0.000000	3.341195
H	-0.993980	0.471039	4.302216	H	-0.995204	0.470130	4.247541
H	0.993981	-0.471039	4.302216	H	0.995219	-0.470132	4.247531
S	1.435184	1.608093	-1.854478	S	1.415439	1.590252	-1.858413
S	2.523677	-1.287271	-0.366035	S	2.492494	-1.293699	-0.346834
P	2.901896	0.226907	-1.656420	P	2.893274	0.225071	-1.625682
H	4.120850	0.875759	-1.301609	H	4.097570	0.879987	-1.234614
H	3.244565	-0.312958	-2.930712	H	3.269780	-0.302675	-2.895166
16 Eu(H ₂ PSe ₂) ₃ PBE SC ECP				16 Am(H ₂ PSe ₂) ₃ PBE SC ECP			
Eu	-0.000904	-0.000526	0.051550	Am	0.000000	-0.000000	0.013587
Se	-2.629335	1.400208	-0.335984	Se	-2.589049	1.406869	-0.314294
Se	-1.427366	-1.738688	-1.941980	Se	-1.419248	-1.713881	-1.951066
P	-2.990376	-0.231550	-1.737895	P	-3.001339	-0.234743	-1.691380
H	-3.309256	0.312947	-3.015820	H	-3.379909	0.290799	-2.960752
H	-4.222288	-0.873014	-1.419309	H	-4.209499	-0.886304	-1.308788
Se	0.783725	1.689444	2.411775	Se	0.796741	1.677126	2.327479
Se	-0.783010	-1.689029	2.413911	Se	-0.796740	-1.677125	2.327479
P	0.001281	0.000476	3.548255	P	0.000000	0.000000	3.472634
H	-0.986627	0.470101	4.462052	H	-0.989555	0.471317	4.383733
H	0.990617	-0.468626	4.460773	H	0.989555	-0.471316	4.383733
Se	1.427399	1.739599	-1.939113	Se	1.419248	1.713880	-1.951066
Se	2.626696	-1.402484	-0.336545	Se	2.589049	-1.406870	-0.314295
P	2.989318	0.231238	-1.735832	P	3.001339	0.234742	-1.691381
H	4.221353	0.871569	-1.415464	H	4.209500	0.886303	-1.308790
H	3.308774	-0.311664	-3.014289	H	3.379908	-0.290800	-2.960753
16 Eu(H ₂ PTe ₂) ₃ PBE SC ECP				16 Am(H ₂ PTe ₂) ₃ PBE SC ECP			
Eu	0.006964	0.002067	-0.038309	Am	-0.000000	-0.000000	-0.001712
Te	-2.786754	1.586419	-0.250523	Te	-2.739553	1.584820	-0.281775
Te	-1.534688	-1.890436	-2.157351	Te	-1.467518	-1.897836	-2.097158
P	-3.268407	-0.246202	-1.764036	P	-3.217508	-0.252584	-1.787832
H	-3.720065	0.286371	-3.006053	H	-3.630406	0.256269	-3.053429
H	-4.460047	-0.908342	-1.349520	H	-4.425839	-0.895973	-1.391565
Te	0.864493	1.898962	2.422558	Te	0.877416	1.875610	2.411904
Te	-0.872114	-1.897802	2.410323	Te	-0.877415	-1.875611	2.411905
P	-0.010247	0.000010	3.649881	P	0.000000	0.000000	3.671186
H	-0.999480	0.458478	4.567353	H	-0.985336	0.459000	4.593159
H	0.970447	-0.461572	4.574882	H	0.985336	-0.458999	4.593160

Te	1.540704	1.889495	-2.166124	Te	1.467518	1.897836	-2.097157
Te	2.800960	-1.582044	-0.259464	Te	2.739553	-1.584821	-0.281775
P	3.276503	0.245496	-1.780118	P	3.217507	0.252584	-1.787833
H	4.470457	0.908520	-1.373761	H	4.425839	0.895973	-1.391567
H	3.721277	-0.289419	-3.023649	H	3.630405	-0.256269	-3.053429

16	Eu(H ₂ PO ₂) ₃ M06 SC ECP			16	Am(H ₂ PO ₂) ₃ M06 SC ECP		
Eu	0.032719	-0.000017	-0.000016	Am	0.030359	0.000000	-0.000000
O	-0.414691	-2.058422	1.035362	O	-0.421416	-2.111226	1.027011
O	-1.585667	-1.367816	-1.034987	O	-1.631382	-1.400609	-1.020690
P	-1.465820	-2.463261	0.011748	P	-1.487549	-2.504876	0.014537
H	-2.701198	-2.714257	0.634937	H	-2.711550	-2.766000	0.656355
H	-1.151228	-3.693501	-0.590926	H	-1.177779	-3.728144	-0.605313
O	2.043901	0.608459	1.080257	O	2.090997	0.614334	1.079986
O	2.043928	-0.608454	-1.080262	O	2.090997	-0.614334	-1.079986
P	2.926429	0.000017	0.000001	P	2.969893	0.000000	0.000000
H	3.795048	-0.960043	0.550155	H	3.838554	-0.958221	0.553591
H	3.795015	0.960109	-0.550150	H	3.838555	0.958221	-0.553590
O	-1.585640	1.367794	1.034979	O	-1.631382	1.400609	1.020690
O	-0.414660	2.058410	-1.035363	O	-0.421416	2.111226	-1.027012
P	-1.465785	2.463248	-0.011745	P	-1.487549	2.504875	-0.014537
H	-1.151189	3.693481	0.590941	H	-1.177779	3.728144	0.605312
H	-2.701161	2.714254	-0.634933	H	-2.711551	2.766000	-0.656354

16	Eu(H ₂ PS ₂) ₃ M06 SC ECP			16	Am(H ₂ PS ₂) ₃ M06 SC ECP		
Eu	0.000001	0.000000	0.070058	Am	0.000000	-0.000000	0.086451
S	-2.446834	1.255787	-0.378918	S	-2.456895	1.261388	-0.389951
S	-1.361880	-1.623919	-1.782072	S	-1.346857	-1.621490	-1.788773
P	-2.792076	-0.242162	-1.658969	P	-2.780318	-0.239943	-1.671542
H	-3.056926	0.286939	-2.937527	H	-3.039080	0.283864	-2.953492
H	-4.025347	-0.852851	-1.354904	H	-4.012339	-0.855802	-1.372710
S	0.779836	1.494676	2.322755	S	0.797859	1.490254	2.348880
S	-0.779836	-1.494676	2.322754	S	-0.797859	-1.490254	2.348880
P	-0.000000	0.000000	3.391673	P	-0.000000	0.000000	3.412035
H	-0.955724	0.521679	4.286813	H	-0.952957	0.527512	4.306389
H	0.955722	-0.521678	4.286814	H	0.952957	-0.527512	4.306389
S	1.361881	1.623920	-1.782072	S	1.346858	1.621490	-1.788773
S	2.446834	-1.255787	-0.378918	S	2.456895	-1.261389	-0.389951
P	2.792077	0.242161	-1.658969	P	2.780318	0.239942	-1.671542
H	4.025348	0.852850	-1.354905	H	4.012340	0.855801	-1.372711
H	3.056925	-0.286939	-2.937528	H	3.039079	-0.283865	-2.953493

16	Eu(H ₂ PSe ₂) ₃ M06 SC ECP			16	Am(H ₂ PSe ₂) ₃ M06 SC ECP		
Eu	-0.000743	0.000467	0.065436	Am	0.000001	-0.000001	0.084133
Se	-2.544960	1.397052	-0.236354	Se	-2.541408	1.408534	-0.263119
Se	-1.283902	-1.761135	-1.903159	Se	-1.275284	-1.770898	-1.886531
P	-2.815797	-0.234485	-1.664117	P	-2.803214	-0.231883	-1.677273
H	-3.085983	0.324925	-2.928894	H	-3.061887	0.307454	-2.953105
H	-4.046693	-0.861176	-1.383963	H	-4.036614	-0.854563	-1.398591

Se	0.865639	1.680484	2.314162	Se	0.864086	1.680390	2.335140
Se	-0.867861	-1.679051	2.314641	Se	-0.864082	-1.680391	2.335140
P	0.000389	0.000046	3.397952	P	-0.000000	0.000001	3.421537
H	-0.952202	0.518790	4.297577	H	-0.957017	0.514782	4.318686
H	0.956459	-0.519663	4.293304	H	0.957013	-0.514780	4.318691
Se	1.284588	1.761815	-1.902283	Se	1.275284	1.770898	-1.886531
Se	2.543341	-1.397041	-0.235057	Se	2.541410	-1.408536	-0.263121
P	2.815479	0.234238	-1.662860	P	2.803214	0.231882	-1.677274
H	4.046808	0.860079	-1.382680	H	4.036614	0.854562	-1.398593
H	3.085439	-0.325345	-2.927619	H	3.061886	-0.307454	-2.953108
16 Eu(H ₂ PTe ₂) ₃ M06 SC ECP				16 Am(H ₂ PTe ₂) ₃ M06 SC ECP			
Eu	0.622814	-0.691985	0.603247	Am	-0.008663	0.049923	-0.418376
Te	-1.891185	1.397739	0.140229	Te	-2.643425	1.811206	-0.442193
Te	-0.903061	-2.042052	-2.059589	Te	-1.573238	-1.729929	-2.484997
P	-2.313534	-0.092494	-1.810161	P	-3.269174	-0.344776	-1.396030
H	-2.302556	0.726941	-2.961290	H	-4.362422	-0.185759	-2.274977
H	-3.682069	-0.447508	-1.782867	H	-3.888436	-1.108466	-0.381551
Te	0.885444	1.737080	2.768567	Te	1.168071	1.801088	1.914671
Te	-0.493093	-2.317184	3.119176	Te	-0.997298	-1.832447	1.949745
P	-0.482114	0.020755	3.832901	P	-0.033760	0.065723	3.148640
H	-1.821615	0.472101	3.840185	H	-1.033331	0.667338	3.945395
H	-0.222276	0.049693	5.218971	H	0.795587	-0.447505	4.170257
Te	0.896164	1.951880	-1.565728	Te	1.775851	2.058544	-2.115559
Te	3.591620	-1.283421	-0.563584	Te	2.416308	-1.943614	-0.937276
P	2.568906	0.198022	-2.188916	P	3.290610	0.261352	-1.452336
H	3.578067	0.874172	-2.910696	H	4.050628	0.701678	-0.345858
H	1.968485	-0.553738	-3.224355	H	4.312686	0.175644	-2.423468

16 Eu(H ₂ PO ₂) ₃ wB97X SC ECP				16 Am(H ₂ PO ₂) ₃ wB97X SC ECP			
Eu	0.005927	-0.000029	-0.000041	Am	0.009178	0.000000	0.000000
O	-0.499135	-2.042243	1.080811	O	-0.502428	-2.102946	1.075630
O	-1.524006	-1.460038	-1.098431	O	-1.568598	-1.486173	-1.081276
P	-1.464957	-2.524758	-0.003051	P	-1.489320	-2.563240	0.001566
H	-2.741363	-2.778906	0.534180	H	-2.757565	-2.818009	0.558412
H	-1.061856	-3.770130	-0.520515	H	-1.102974	-3.803245	-0.542205
O	2.030171	0.580222	1.095160	O	2.083118	0.593427	1.090787
O	2.030221	-0.580187	-1.095169	O	2.083118	-0.593427	-1.090787
P	2.925939	0.000036	0.000007	P	2.976023	-0.000000	-0.000000
H	3.795085	-0.978467	0.518779	H	3.845166	-0.974088	0.527979
H	3.795058	0.978571	-0.518751	H	3.845166	0.974088	-0.527979
O	-1.523990	1.459976	1.098401	O	-1.568598	1.486173	1.081276
O	-0.499131	2.042203	-1.080842	O	-0.502428	2.102947	-1.075629
P	-1.464911	2.524728	0.003056	P	-1.489320	2.563240	-0.001566
H	-1.061738	3.770065	0.520550	H	-1.102975	3.803245	0.542205
H	-2.741313	2.778958	-0.534144	H	-2.757565	2.818008	-0.558413
16 Eu(H ₂ PS ₂) ₃ wB97X SC ECP				16 Am(H ₂ PS ₂) ₃ wB97X SC ECP			
Eu	0.000000	0.000000	0.028673	Am	-0.000000	-0.000000	0.012510

S	-2.448233	1.302582	-0.409818	S	-2.488378	1.302363	-0.413311
S	-1.441612	-1.628984	-1.759199	S	-1.466645	-1.605843	-1.814957
P	-2.871945	-0.229371	-1.634185	P	-2.913599	-0.227375	-1.639234
H	-3.182408	0.254819	-2.917185	H	-3.263362	0.260132	-2.910985
H	-4.089712	-0.818692	-1.251613	H	-4.111188	-0.841917	-1.232505
S	0.661145	1.556397	2.271676	S	0.678543	1.551441	2.292486
S	-0.661145	-1.556397	2.271676	S	-0.678543	-1.551441	2.292487
P	0.000000	-0.000000	3.350410	P	0.000000	0.000000	3.367895
H	-1.002733	0.426454	4.238826	H	-0.998689	0.436416	4.256345
H	1.002734	-0.426454	4.238825	H	0.998690	-0.436416	4.256345
S	1.441613	1.628984	-1.759199	S	1.466645	1.605842	-1.814957
S	2.448234	-1.302582	-0.409818	S	2.488378	-1.302364	-0.413311
P	2.871945	0.229370	-1.634184	P	2.913599	0.227375	-1.639234
H	4.089713	0.818691	-1.251613	H	4.111188	0.841916	-1.232506
H	3.182407	-0.254819	-2.917185	H	3.263362	-0.260133	-2.910985
16	Eu(H ₂ PSe ₂) ₃ wB97X SC ECP			16	Am(H ₂ PSe ₂) ₃ wB97X SC ECP		
Eu	-0.000930	-0.000721	0.051705	Am	-0.000000	0.000000	0.011892
Se	-2.571097	1.386963	-0.346764	Se	-2.583647	1.417883	-0.388029
Se	-1.419841	-1.726070	-1.880149	Se	-1.475483	-1.725168	-1.908694
P	-2.970556	-0.229598	-1.724669	P	-3.029495	-0.236211	-1.706011
H	-3.262626	0.290012	-2.997811	H	-3.388015	0.247171	-2.976414
H	-4.192354	-0.839927	-1.392623	H	-4.227396	-0.849600	-1.300555
Se	0.736740	1.675286	2.367610	Se	0.736756	1.676885	2.354980
Se	-0.735927	-1.675072	2.369819	Se	-0.736756	-1.676884	2.354980
P	0.001234	0.000507	3.519048	P	0.000000	-0.000000	3.502964
H	-0.992061	0.437534	4.412337	H	-0.994986	0.434824	4.395338
H	0.995739	-0.435962	4.411256	H	0.994987	-0.434824	4.395338
Se	1.419343	1.726345	-1.878008	Se	1.475483	1.725167	-1.908694
Se	2.568572	-1.389239	-0.347798	Se	2.583647	-1.417882	-0.388028
P	2.969599	0.229396	-1.722862	P	3.029495	0.236211	-1.706012
H	4.191165	0.838971	-1.388576	H	4.227397	0.849599	-1.300557
H	3.263002	-0.288423	-2.996429	H	3.388014	-0.247173	-2.976414*-
16	Eu(H ₂ PTe ₂) ₃ wB97X SC ECP			16	Am(H ₂ PTe ₂) ₃ wB97X SC ECP		
Eu	0.005105	0.002475	-0.022890	Am	-0.000000	-0.000000	0.003897
Te	-2.773649	1.541036	-0.278456	Te	-2.750664	1.580658	-0.359322
Te	-1.530608	-1.848852	-2.136588	Te	-1.520521	-1.895806	-2.065924
P	-3.292491	-0.247921	-1.800560	P	-3.262688	-0.253756	-1.828430
H	-3.716443	0.277736	-3.034089	H	-3.645340	0.225324	-3.093959
H	-4.467782	-0.900059	-1.388189	H	-4.460113	-0.868504	-1.422127
Te	0.860558	1.847436	2.441872	Te	0.822464	1.860241	2.466918
Te	-0.866927	-1.844123	2.428993	Te	-0.822463	-1.860241	2.466918
P	-0.008097	-0.000062	3.714033	P	0.000000	0.000000	3.751625
H	-0.988889	0.455840	4.612359	H	-0.988911	0.431376	4.653125
H	0.965823	-0.460774	4.617378	H	0.988911	-0.431375	4.653125
Te	1.534745	1.846188	-2.143899	Te	1.520521	1.895806	-2.065924
Te	2.785825	-1.535837	-0.283309	Te	2.750664	-1.580658	-0.359321
P	3.299419	0.246955	-1.813505	P	3.262688	0.253756	-1.828431
H	4.476165	0.901433	-1.409127	H	4.460113	0.868503	-1.422129
H	3.717249	-0.281472	-3.047936	H	3.645339	-0.225325	-3.093959

<p>16 Eu(H₂PO₂)₃ B5050LYP SC ECP</p> <p>Eu 0.004092 -0.000026 -0.000032 O -0.510961 -2.040282 1.075797 O -1.513005 -1.463810 -1.081702 P -1.461382 -2.523887 -0.000801 H -2.732185 -2.781014 0.521684 H -1.058032 -3.758742 -0.516578 O 2.028238 0.573329 1.081552 O 2.028283 -0.573301 -1.081561 P 2.921300 0.000033 0.000005 H 3.784509 -0.971244 0.515498 H 3.784481 0.971341 -0.515474 O -1.512983 1.463760 1.081680 O -0.510951 2.040246 -1.075821 P -1.461337 2.523860 0.000805 H -1.057929 3.758687 0.516604 H -2.732137 2.781051 -0.521656</p>	<p>16 Am(H₂PO₂)₃ B5050LYP SC ECP</p> <p>Am -0.000920 -0.000000 0.000000 O -0.510089 -2.104783 1.063231 O -1.568834 -1.494221 -1.064155 P -1.482977 -2.570251 -0.000973 H -2.739998 -2.843371 0.546819 H -1.087331 -3.793623 -0.549915 O 2.076816 0.616904 1.060313 O 2.076816 -0.616903 -1.060313 P 2.966191 -0.000000 0.000000 H 3.829778 -0.950033 0.553819 H 3.829778 0.950032 -0.553819 O -1.568834 1.494221 1.064155 O -0.510089 2.104783 -1.063231 P -1.482977 2.570251 0.000973 H -1.087332 3.793623 0.549915 H -2.739998 2.843370 -0.546819</p>
<p>16 Eu(H₂PS₂)₃ B5050LYP SC ECP</p> <p>Eu -0.000000 0.000000 0.027506 S -2.433686 1.337681 -0.474722 S -1.479153 -1.649216 -1.726197 P -2.891845 -0.226996 -1.644757 H -3.199925 0.211895 -2.935679 H -4.109788 -0.780137 -1.239453 S 0.592292 1.581407 2.290210 S -0.592291 -1.581406 2.290210 P 0.000000 0.000000 3.374006 H -1.015602 0.376289 4.257884 H 1.015603 -0.376289 4.257883 S 1.479153 1.649216 -1.726197 S 2.433685 -1.337681 -0.474721 P 2.891845 0.226996 -1.644757 H 4.109788 0.780137 -1.239452 H 3.199925 -0.211895 -2.935678</p>	<p>16 Am(H₂PS₂)₃ B5050LYP SC ECP</p> <p>Am -0.000000 0.000000 0.009373 S -2.488587 1.318140 -0.458914 S -1.508733 -1.626831 -1.794481 P -2.941587 -0.230018 -1.652769 H -3.283310 0.231896 -2.926770 H -4.141174 -0.813656 -1.236264 S 0.633083 1.567349 2.314869 S -0.633082 -1.567349 2.314869 P 0.000000 0.000000 3.395828 H -1.005016 0.402884 4.279770 H 1.005017 -0.402883 4.279769 S 1.508733 1.626830 -1.794481 S 2.488587 -1.318140 -0.458914 P 2.941586 0.230018 -1.652769 H 4.141174 0.813656 -1.236264 H 3.283310 -0.231896 -2.926770</p>
<p>16 Eu(H₂PSe₂)₃ B5050LYP SC ECP</p> <p>Eu -0.000606 -0.000316 0.043481 Se -2.529747 1.443773 -0.434226 Se -1.471147 -1.769197 -1.811604 P -2.990253 -0.232302 -1.722404 H -3.279969 0.219937 -3.013010 H -4.217063 -0.788211 -1.348714 Se 0.651983 1.707410 2.363290 Se -0.651549 -1.707216 2.364433 P 0.000764 0.000290 3.521635 H -1.009852 0.380476 4.409517 H 1.012187 -0.379704 4.408678</p>	<p>16 Am(H₂PSe₂)₃ B5050LYP SC ECP</p> <p>Am 0.000000 -0.000000 0.009482 Se -2.577863 1.432133 -0.429429 Se -1.516255 -1.751540 -1.881145 P -3.053482 -0.240104 -1.716838 H -3.399288 0.221027 -2.990215 H -4.255583 -0.821662 -1.304204 Se 0.692084 1.693729 2.370976 Se -0.692084 -1.693729 2.370977 P 0.000000 0.000000 3.524296 H -1.001445 0.403958 4.412007 H 1.001446 -0.403958 4.412007</p>

Se	1.470777	1.769214	-1.810590	Se	1.516254	1.751539	-1.881146
Se	2.528245	-1.444799	-0.434636	Se	2.577863	-1.432133	-0.429429
P	2.989674	0.232144	-1.721339	P	3.053482	0.240104	-1.716838
H	4.216252	0.787709	-1.346376	H	4.255583	0.821662	-1.304204
H	3.280305	-0.219208	-3.012050	H	3.399288	-0.221028	-2.990215
16 Eu(H ₂ PTe ₂) ₃ B5050LYP SC ECP				16 Am(H ₂ PTe ₂) ₃ B5050LYP SC ECP			
Eu	0.003938	0.005201	0.031466	Am	-0.000000	0.000000	-0.003088
Te	-2.693371	1.617206	-0.421294	Te	-2.734091	1.587147	-0.393206
Te	-1.524943	-1.937986	-1.965990	Te	-1.586217	-1.939025	-2.033842
P	-3.236897	-0.249118	-1.844168	P	-3.295654	-0.257357	-1.839990
H	-3.568471	0.191643	-3.129370	H	-3.657882	0.211177	-3.106599
H	-4.455117	-0.808996	-1.446590	H	-4.502583	-0.828522	-1.425295
Te	0.751126	1.881916	2.479778	Te	0.732047	1.899936	2.480870
Te	-0.755652	-1.878105	2.468102	Te	-0.732047	-1.899935	2.480870
P	-0.005767	-0.000568	3.777712	P	-0.000000	0.000000	3.768703
H	-1.008895	0.389178	4.671047	H	-1.005966	0.378309	4.663298
H	0.993087	-0.394143	4.674141	H	1.005966	-0.378308	4.663299
Te	1.536456	1.944271	-1.963738	Te	1.586217	1.939025	-2.033842
Te	2.699236	-1.611338	-0.418326	Te	2.734090	-1.587148	-0.393206
P	3.241088	0.247338	-1.851469	P	3.295654	0.257356	-1.839990
H	4.465621	0.802524	-1.466909	H	4.502583	0.828522	-1.425296
H	3.558561	-0.199024	-3.138307	H	3.657881	-0.211177	-3.106600

16 Eu(H ₂ PO ₂) ₃ PBE50 SC ECP				16 Am(H ₂ PO ₂) ₃ PBE50 SC ECP			
Eu	0.009176	-0.000012	-0.000005	Am	-0.000298	0.000000	0.000000
O	-0.508936	-2.017958	1.077832	O	-0.501687	-2.084634	1.065440
O	-1.494324	-1.447539	-1.090429	O	-1.555367	-1.475836	-1.067318
P	-1.452981	-2.498925	-0.003225	P	-1.470125	-2.547069	-0.001631
H	-2.732459	-2.747806	0.513373	H	-2.732454	-2.819768	0.545283
H	-1.051494	-3.743076	-0.509188	H	-1.071807	-3.774778	-0.549911
O	2.014296	0.571458	1.083503	O	2.055207	0.617760	1.060965
O	2.014310	-0.571449	-1.083501	O	2.055207	-0.617760	-1.060965
P	2.903189	0.000015	0.000002	P	2.940257	0.000000	-0.000000
H	3.769662	-0.975107	0.514170	H	3.806255	-0.952672	0.556495
H	3.769641	0.975155	-0.514166	H	3.806255	0.952672	-0.556496
O	-1.494311	1.447525	1.090425	O	-1.555367	1.475836	1.067318
O	-0.508924	2.017936	-1.077838	O	-0.501687	2.084634	-1.065440
P	-1.452958	2.498913	0.003224	P	-1.470125	2.547069	0.001631
H	-1.051451	3.743057	0.509189	H	-1.071807	3.774779	0.549911
H	-2.732435	2.747815	-0.513367	H	-2.732454	2.819768	-0.545283
16 Eu(H ₂ PS ₂) ₃ PBE50 SC ECP				16 Am(H ₂ PS ₂) ₃ PBE50 SC ECP			
Eu	0.000000	0.000000	0.028804	Am	-0.000002	-0.000000	0.012164
S	-2.408211	1.329232	-0.448392	S	-2.462468	1.306067	-0.423821
S	-1.445044	-1.639446	-1.714490	S	-1.464855	-1.607365	-1.788554
P	-2.849354	-0.224021	-1.622926	P	-2.895133	-0.224835	-1.629070
H	-3.154977	0.223955	-2.915604	H	-3.238761	0.250618	-2.902367
H	-4.070940	-0.783501	-1.223672	H	-4.095547	-0.822775	-1.220695

S	0.600308	1.573992	2.258330	S	0.644829	1.556692	2.278050
S	-0.600308	-1.573992	2.258330	S	-0.644828	-1.556692	2.278052
P	0.000000	0.000000	3.329291	P	0.000003	-0.000000	3.347585
H	-1.016554	0.382420	4.215749	H	-1.004578	0.412209	4.234618
H	1.016554	-0.382420	4.215749	H	1.004587	-0.412210	4.234614
S	1.445044	1.639446	-1.714489	S	1.464853	1.607365	-1.788553
S	2.408210	-1.329232	-0.448392	S	2.462464	-1.306069	-0.423819
P	2.849354	0.224021	-1.622926	P	2.895132	0.224834	-1.629066
H	4.070940	0.783500	-1.223672	H	4.095545	0.822774	-1.220689
H	3.154977	-0.223955	-2.915604	H	3.238762	-0.250618	-2.902363

16	Eu(H ₂ PSe ₂) ₃ PBE50 SC ECP			16	Am(H ₂ PSe ₂) ₃ PBE50 SC ECP		
Eu	-0.000599	-0.000221	0.049006	Am	0.000000	-0.000000	0.015935
Se	-2.504265	1.431427	-0.412244	Se	-2.551332	1.418345	-0.402330
Se	-1.436718	-1.757606	-1.796027	Se	-1.471420	-1.731555	-1.869219
P	-2.943689	-0.229506	-1.703491	P	-3.003642	-0.236060	-1.696315
H	-3.225562	0.231605	-2.996933	H	-3.346089	0.235231	-2.971177
H	-4.175871	-0.789933	-1.339670	H	-4.207444	-0.829889	-1.293048
Se	0.660212	1.695660	2.337538	Se	0.709850	1.675554	2.340059
Se	-0.659938	-1.695374	2.338493	Se	-0.709849	-1.675553	2.340059
P	0.000757	0.000246	3.481141	P	-0.000000	0.000000	3.481570
H	-1.010633	0.387310	4.371346	H	-0.999276	0.418119	4.371320
H	1.013083	-0.386793	4.370287	H	0.999276	-0.418118	4.371321
Se	1.436283	1.757539	-1.795151	Se	1.471421	1.731555	-1.869220
Se	2.502866	-1.432213	-0.412319	Se	2.551333	-1.418346	-0.402331
P	2.943131	0.229352	-1.702433	P	3.003642	0.236059	-1.696316
H	4.175088	0.789563	-1.337517	H	4.207445	0.829888	-1.293050
H	3.225854	-0.231056	-2.995942	H	3.346088	-0.235231	-2.971178

16	Eu(H ₂ PTe ₂) ₃ PBE50 SC ECP			16	Am(H ₂ PTe ₂) ₃ PBE50 SC ECP		
Eu	0.008171	0.019601	0.021671	Am	0.000000	-0.000001	0.019427
Te	-2.645184	1.623224	-0.418385	Te	-2.703037	1.551365	-0.280138
Te	-1.481054	-1.920269	-1.938925	Te	-1.536048	-1.902516	-2.003491
P	-3.178848	-0.250039	-1.797692	P	-3.202127	-0.205136	-1.821792
H	-3.536147	0.175926	-3.085145	H	-3.490414	0.320548	-3.089597
H	-4.389443	-0.815822	-1.372764	H	-4.440284	-0.777404	-1.496762
Te	0.750055	1.872916	2.436083	Te	0.484972	1.968793	2.450468
Te	-0.770073	-1.857447	2.400474	Te	-0.484970	-1.968794	2.450469
P	-0.014209	-0.002387	3.698804	P	-0.000001	0.000000	3.708477
H	-1.017364	0.388140	4.597806	H	-1.049092	0.247448	4.605403
H	0.985428	-0.408320	4.594832	H	1.049088	-0.247446	4.605406
Te	1.519948	1.943758	-1.932126	Te	1.536050	1.902517	-2.003488
Te	2.653206	-1.602206	-0.400088	Te	2.703037	-1.551367	-0.280142
P	3.189806	0.243781	-1.814149	P	3.202127	0.205136	-1.821794
H	4.421404	0.792279	-1.428649	H	4.440285	0.777402	-1.496764
H	3.504312	-0.203134	-3.105658	H	3.490411	-0.320547	-3.089600

16	Eu(H ₂ PO ₂) ₃ B2PLYP SC ECP			16	Am(H ₂ PO ₂) ₃ B2PLYP SC ECP		
Eu	-0.034894	0.000725	0.010706	Am	0.062584	0.204810	-0.083097

O	-0.518945	-2.034768	1.103576	O	-0.380608	-1.843334	1.090131
O	-1.506965	-1.481668	-1.112926	O	-1.416535	-1.390720	-1.137628
P	-1.434500	-2.554166	-0.016694	P	-1.314010	-2.408335	0.006876
H	-2.713975	-2.867901	0.473286	H	-2.583234	-2.703067	0.535258
H	-0.963466	-3.775218	-0.527613	H	-0.850760	-3.651686	-0.457524
O	1.982576	0.659475	1.057005	O	2.212533	0.614033	1.017919
O	1.971917	-0.664931	-1.049691	O	2.032737	-0.658108	-1.116678
P	2.878212	-0.002152	-0.001303	P	2.997756	-0.218572	-0.000642
H	3.748161	-0.936217	0.585172	H	3.596744	-1.337924	0.603440
H	3.740911	0.933160	-0.596926	H	4.085353	0.495516	-0.532114
O	-1.514242	1.489942	1.117853	O	-1.640561	1.458437	1.053380
O	-0.511725	2.031902	-1.094455	O	-0.670277	2.283074	-1.085005
P	-1.436652	2.556087	0.015507	P	-1.696784	2.590286	0.014450
H	-0.973041	3.781949	0.522131	H	-1.445244	3.838291	0.609375
H	-2.713369	2.863784	-0.485630	H	-2.989692	2.727297	-0.518143
16	Eu(H2PS2)3 B2PLYP SC ECP			16	Am(H2PS2)3 B2PLYP SC ECP		
Eu	0.002977	-0.003025	-0.025807	Am	0.000095	0.001053	0.013836
S	-2.450527	1.297860	-0.331074	S	-2.498098	1.279256	-0.344942
S	-1.455273	-1.596598	-1.828837	S	-1.425727	-1.577815	-1.873084
P	-2.907948	-0.220290	-1.581260	P	-2.900602	-0.222774	-1.630755
H	-3.304374	0.282091	-2.833089	H	-3.274640	0.299568	-2.881388
H	-4.090458	-0.843223	-1.146909	H	-4.084492	-0.869615	-1.236617
S	0.677530	1.567758	2.195460	S	0.721604	1.550591	2.274705
S	-0.667540	-1.576931	2.193713	S	-0.721809	-1.550609	2.274036
P	-0.004700	-0.001159	3.270540	P	-0.000214	-0.000299	3.349013
H	-1.014555	0.426736	4.148995	H	-0.987566	0.455761	4.239193
H	0.988167	-0.421857	4.171749	H	0.987325	-0.456420	4.238953
S	1.452123	1.591623	-1.841121	S	1.427168	1.579194	-1.873031
S	2.460556	-1.296753	-0.341537	S	2.497564	-1.278173	-0.343730
P	2.911453	0.222458	-1.592611	P	2.900620	0.222673	-1.630825
H	4.091375	0.850703	-1.158464	H	4.085472	0.868468	-1.237907
H	3.311195	-0.279394	-2.843663	H	3.273297	-0.300859	-2.881372
16	Eu(H2PSe2)3 B2PLYP SC ECP			16	Am(H2PSe2)3 B2PLYP SC ECP		
Eu	-0.140092	-0.246071	-0.105623	Am	-0.233704	-0.149017	-0.049008
Se	-2.629866	1.221841	-0.176958	Se	-2.781241	1.251342	-0.278920
Se	-1.699597	-1.779630	-2.049965	Se	-1.625622	-1.660624	-2.199484
P	-3.150780	-0.196343	-1.726264	P	-3.175154	-0.183318	-1.858071
H	-3.395597	0.476498	-2.937350	H	-3.459083	0.491849	-3.058644
H	-4.416227	-0.754060	-1.474200	H	-4.402087	-0.825593	-1.617500
Se	0.606242	1.687036	1.889692	Se	0.357948	1.811391	2.035920
Se	-0.597634	-1.749864	2.389988	Se	-0.520999	-1.757835	2.438706
P	0.218872	0.058338	3.270396	P	0.313434	0.047475	3.302972
H	-0.613363	0.489406	4.318533	H	-0.350420	0.339376	4.507605
H	1.396760	-0.249222	3.974049	H	1.615740	-0.212750	3.764690
Se	1.372133	1.606183	-1.851743	Se	1.376699	1.585681	-1.827956
Se	2.427723	-1.558750	-0.290547	Se	2.384721	-1.418491	0.015640
P	2.979251	0.224808	-1.417001	P	2.947254	0.178985	-1.351074
H	4.013734	0.900545	-0.744491	H	4.065338	0.859855	-0.835665
H	3.628445	-0.130716	-2.612432	H	3.487180	-0.358328	-2.533130

16 Eu(H ₂ PTe ₂) ₃ B2PLYP SC ECP	16 Am(H ₂ PTe ₂) ₃ B2PLYP SC ECP
Eu 0.037644 0.036583 -0.170547	Am 0.048442 0.036414 -0.133571
Te -2.654862 1.567147 -0.165411	Te -2.680817 1.583394 -0.172393
Te -1.616943 -1.857520 -2.076261	Te -1.596442 -1.881999 -2.043713
P -3.334508 -0.235396 -1.618709	P -3.313462 -0.248704 -1.613365
H -3.871326 0.252407 -2.824137	H -3.826370 0.227158 -2.833601
H -4.471593 -0.868107 -1.082183	H -4.458864 -0.883248 -1.097706
Te 0.664430 1.964673 2.225821	Te 0.712104 1.964527 2.270392
Te -0.646337 -1.943097 2.119006	Te -0.680473 -1.950704 2.150096
P -0.050639 -0.003412 3.447562	P -0.078960 0.004620 3.459961
H -1.116499 0.313895 4.310418	H -1.163830 0.348746 4.286909
H 0.931758 -0.349672 4.394112	H 0.869285 -0.359521 4.433349
Te 1.681890 1.897010 -2.076994	Te 1.688573 1.923656 -2.056856
Te 2.713500 -1.520102 -0.164400	Te 2.765342 -1.549428 -0.211389
P 3.369145 0.222980 -1.693173	P 3.370182 0.229379 -1.719021
H 4.558518 0.828200 -1.247490	H 4.568957 0.832091 -1.295754
H 3.805825 -0.305594 -2.921530	H 3.776329 -0.276384 -2.967256

16 Eu(H ₂ PO ₂) ₃ B3LYP LC ECP	16 Am(H ₂ PO ₂) ₃ B3LYP LC ECP
Eu 0.002311 -0.000016 0.000004	Am 0.000551 0.000000 0.000000
O -0.602075 -2.033539 1.140774	O -0.654096 -2.077678 1.154826
O -1.461066 -1.536291 -1.140304	O -1.472587 -1.604981 -1.154273
P -1.482477 -2.563034 0.000436	P -1.510622 -2.615442 0.000365
H -2.799949 -2.808104 0.441622	H -2.836145 -2.857963 0.419116
H -1.039928 -3.828013 -0.440501	H -1.058925 -3.885034 -0.418275
O 2.065075 0.492926 1.142013	O 2.127139 0.470277 1.155507
O 2.065084 -0.492919 -1.142002	O 2.127139 -0.470277 -1.155507
P 2.964360 0.000018 0.000003	P 3.021145 0.000000 0.000000
H 3.837015 -1.018332 0.438043	H 3.894388 -1.027177 0.416562
H 3.836978 1.018397 -0.438044	H 3.894388 1.027177 -0.416562
O -1.461040 1.536283 1.140305	O -1.472587 1.604981 1.154273
O -0.602051 2.033509 -1.140778	O -0.654096 2.077678 -1.154826
P -1.482442 2.563020 -0.000440	P -1.510623 2.615442 -0.000365
H -1.039880 3.827996 0.440490	H -1.058925 3.885034 0.418275
H -2.799914 2.808102 -0.441622	H -2.836145 2.857963 -0.419116

16 Eu(H ₂ PS ₂) ₃ B3LYP LC ECP	16 Am(H ₂ PS ₂) ₃ B3LYP LC ECP
Eu 0.000000 0.000000 0.026132	Am 0.000000 0.000000 0.030102
S -2.436129 1.393776 -0.553226	S -2.489032 1.397261 -0.591737
S -1.536533 -1.700583 -1.691875	S -1.593226 -1.716155 -1.715986
P -2.926101 -0.227052 -1.663084	P -2.971589 -0.232033 -1.694018
H -3.234289 0.163370 -2.983146	H -3.272518 0.154218 -3.016778
H -4.167430 -0.741861 -1.234158	H -4.217115 -0.739429 -1.268986
S 0.520257 1.627990 2.326042	S 0.516661 1.635083 2.394861
S -0.520256 -1.627990 2.326042	S -0.516660 -1.635083 2.394861
P 0.000000 0.000000 3.412258	P 0.000000 0.000000 3.472994
H -1.039166 0.327567 4.308295	H -1.039831 0.324241 4.369138
H 1.039167 -0.327567 4.308295	H 1.039831 -0.324241 4.369138

S	1.536533	1.700583	-1.691875	S	1.593226	1.716155	-1.715986
S	2.436129	-1.393776	-0.553226	S	2.489032	-1.397261	-0.591737
P	2.926101	0.227053	-1.663084	P	2.971589	0.232033	-1.694018
H	4.167430	0.741861	-1.234157	H	4.217115	0.739429	-1.268986
H	3.234289	-0.163370	-2.983146	H	3.272517	-0.154218	-3.016778
16 Eu(H ₂ PSe ₂) ₃ B3LYP LC ECP				16 Am(H ₂ PSe ₂) ₃ B3LYP LC ECP			
Eu	-0.000155	0.000044	0.033158	Am	0.000000	0.000000	0.031339
Se	-2.543160	1.497964	-0.504327	Se	-2.601608	1.499514	-0.531785
Se	-1.530942	-1.817381	-1.798045	Se	-1.587419	-1.830090	-1.829859
P	-3.039176	-0.237287	-1.736581	P	-3.086915	-0.240866	-1.762239
H	-3.348462	0.173068	-3.050164	H	-3.394107	0.170739	-3.075659
H	-4.281033	-0.767443	-1.328786	H	-4.329190	-0.770853	-1.356359
Se	0.615268	1.745120	2.393528	Se	0.604421	1.756702	2.456095
Se	-0.614837	-1.744877	2.393803	Se	-0.604421	-1.756702	2.456095
P	0.000179	0.000233	3.556635	P	0.000000	0.000000	3.608259
H	-1.026397	0.354579	4.456713	H	-1.028796	0.347585	4.508049
H	1.026714	-0.354007	4.456801	H	1.028796	-0.347585	4.508049
Se	1.531528	1.817889	-1.796870	Se	1.587419	1.830089	-1.829860
Se	2.542340	-1.498624	-0.504927	Se	2.601608	-1.499514	-0.531785
P	3.039010	0.237032	-1.736326	P	3.086915	0.240865	-1.762240
H	4.281130	0.766444	-1.328368	H	4.329190	0.770852	-1.356360
H	3.347993	-0.172755	-3.050158	H	3.394106	-0.170740	-3.075659
16 Eu(H ₂ PTe ₂) ₃ B3LYP LC ECP				16 Am(H ₂ PTe ₂) ₃ B3LYP LC ECP			
Eu	-0.000026	-0.000022	0.041422	Am	0.000075	-0.000051	0.043459
Te	-2.715318	1.654778	-0.453029	Te	-2.778126	1.651085	-0.473144
Te	-1.556805	-1.989624	-1.951553	Te	-1.597378	-2.004110	-1.991415
P	-3.250868	-0.247410	-1.869898	P	-3.286051	-0.257000	-1.892924
H	-3.559709	0.180756	-3.178665	H	-3.594450	0.175909	-3.199926
H	-4.500001	-0.786355	-1.494453	H	-4.532885	-0.803147	-1.521370
Te	0.716280	1.925307	2.517405	Te	0.724636	1.934756	2.580718
Te	-0.716336	-1.925306	2.517428	Te	-0.724546	-1.934755	2.580783
P	0.000090	-0.000031	3.818331	P	-0.000090	0.000073	3.863655
H	-1.014712	0.366062	4.728156	H	-1.013895	0.369777	4.772675
H	1.015072	-0.366209	4.727919	H	1.013521	-0.369544	4.772927
Te	1.556612	1.989554	-1.951660	Te	1.597637	2.004289	-1.991073
Te	2.715332	-1.654727	-0.452839	Te	2.778106	-1.651358	-0.473582
P	3.250787	0.247452	-1.869757	P	3.286096	0.256947	-1.893044
H	4.499846	0.786521	-1.494240	H	4.533026	0.802880	-1.521500
H	3.559756	-0.180746	-3.178482	H	3.594325	-0.175755	-3.200155
16 Eu(H ₂ PO ₂) ₃ B5050LYP LC ECP				16 Am(H ₂ PO ₂) ₃ B5050LYP LC ECP			
Eu	0.001334	-0.000015	0.000005	Am	-0.000339	0.000000	0.000000
O	-0.594755	-2.053092	1.117660	O	-0.644249	-2.097852	1.130595
O	-1.481564	-1.539790	-1.116481	O	-1.494727	-1.607640	-1.130468
P	-1.485170	-2.569406	0.000548	P	-1.513126	-2.621773	0.000188
H	-2.778531	-2.819306	0.455370	H	-2.814164	-2.868670	0.435222
H	-1.056192	-3.814614	-0.455059	H	-1.075725	-3.871808	-0.434536

O	2.077048	0.510105	1.118115	O	2.138513	0.489182	1.131237
O	2.077055	-0.510099	-1.118105	O	2.138514	-0.489182	-1.131237
P	2.969915	0.000016	0.000002	P	3.026356	0.000000	0.000000
H	3.833478	-0.995473	0.453202	H	3.890469	-1.004185	0.433375
H	3.833445	0.995531	-0.453204	H	3.890469	1.004186	-0.433375
O	-1.481541	1.539783	1.116482	O	-1.494727	1.607640	1.130468
O	-0.594732	2.053066	-1.117663	O	-0.644249	2.097851	-1.130595
P	-1.485139	2.569394	-0.000551	P	-1.513126	2.621772	-0.000188
H	-1.056151	3.814600	0.455049	H	-1.075725	3.871808	0.434536
H	-2.778499	2.819302	-0.455371	H	-2.814164	2.868670	-0.435222
16	Eu(H ₂ PS ₂) ₃ B5050LYP LC ECP			16	Am(H ₂ PS ₂) ₃ B5050LYP LC ECP		
Eu	0.000000	0.000000	0.028417	Am	0.000000	0.000000	0.029955
S	-2.464337	1.373147	-0.560893	S	-2.516261	1.377850	-0.597389
S	-1.557799	-1.686617	-1.713037	S	-1.615519	-1.701054	-1.735630
P	-2.952176	-0.230794	-1.680591	P	-2.998761	-0.233654	-1.709537
H	-3.253865	0.165920	-2.981838	H	-3.293353	0.158614	-3.013603
H	-4.175747	-0.747992	-1.259870	H	-4.225967	-0.743959	-1.291462
S	0.536356	1.609524	2.357423	S	0.522188	1.620022	2.422332
S	-0.536356	-1.609524	2.357423	S	-0.522188	-1.620022	2.422332
P	0.000000	0.000000	3.446666	P	0.000000	0.000000	3.503948
H	-1.023986	0.337675	4.329308	H	-1.027154	0.327874	4.386380
H	1.023986	-0.337675	4.329308	H	1.027154	-0.327873	4.386380
S	1.557799	1.686617	-1.713037	S	1.615519	1.701054	-1.735630
S	2.464337	-1.373147	-0.560893	S	2.516261	-1.377851	-0.597389
P	2.952177	0.230794	-1.680591	P	2.998761	0.233654	-1.709538
H	4.175747	0.747992	-1.259870	H	4.225967	0.743959	-1.291463
H	3.253865	-0.165920	-2.981838	H	3.293353	-0.158614	-3.013603
16	Eu(H ₂ PSe ₂) ₃ B5050LYP LC ECP			16	Am(H ₂ PSe ₂) ₃ B5050LYP LC ECP		
Eu	-0.000299	-0.000045	0.038448	Am	0.000000	0.000000	0.032476
Se	-2.577108	1.476044	-0.511361	Se	-2.630292	1.482852	-0.548411
Se	-1.555284	-1.801797	-1.820934	Se	-1.615438	-1.817734	-1.848761
P	-3.071106	-0.238269	-1.761673	P	-3.121638	-0.243954	-1.783784
H	-3.366466	0.181486	-3.057144	H	-3.421974	0.169233	-3.080006
H	-4.296445	-0.771780	-1.367210	H	-4.345358	-0.774046	-1.380520
Se	0.616912	1.731224	2.433894	Se	0.610691	1.741143	2.491364
Se	-0.616884	-1.730996	2.434259	Se	-0.610691	-1.741143	2.491364
P	0.000384	0.000111	3.604175	P	0.000000	0.000000	3.651209
H	-1.014487	0.356336	4.490050	H	-1.016804	0.351839	4.536318
H	1.015823	-0.356156	4.489380	H	1.016804	-0.351838	4.536318
Se	1.555014	1.801700	-1.820664	Se	1.615438	1.817734	-1.848761
Se	2.576501	-1.476266	-0.511143	Se	2.630293	-1.482852	-0.548411
P	3.070832	0.238175	-1.761140	P	3.121638	0.243953	-1.783785
H	4.296051	0.771665	-1.366278	H	4.345358	0.774045	-1.380521
H	3.366562	-0.181432	-3.056575	H	3.421974	-0.169233	-3.080007
16	Eu(H ₂ PTe ₂) ₃ B5050LYP LC ECP			16	Am(H ₂ PTe ₂) ₃ B5050LYP LC ECP		
Eu	0.000235	0.000146	0.036277	Am	-0.000001	-0.000005	0.037704
Te	-2.757821	1.636671	-0.471015	Te	-2.816388	1.636249	-0.495380
Te	-1.596803	-1.974520	-1.986359	Te	-1.639661	-1.991479	-2.020453

P	-3.305272	-0.251955	-1.895078	P	-3.340792	-0.261449	-1.917163
H	-3.615455	0.180156	-3.184023	H	-3.650312	0.171824	-3.205677
H	-4.530751	-0.796811	-1.513376	H	-4.564933	-0.810062	-1.537228
Te	0.732667	1.906451	2.559371	Te	0.732488	1.919212	2.619558
Te	-0.733126	-1.906411	2.558931	Te	-0.732485	-1.919213	2.619566
P	-0.000274	-0.000122	3.871784	P	0.000002	0.000003	3.914948
H	-1.002312	0.376419	4.765348	H	-1.002723	0.375106	4.808050
H	1.001715	-0.376762	4.765361	H	1.002726	-0.375098	4.808051
Te	1.596713	1.974251	-1.987196	Te	1.639659	1.991479	-2.020444
Te	2.758476	-1.636152	-0.470481	Te	2.816387	-1.636255	-0.495385
P	3.305486	0.252010	-1.895340	P	3.340790	0.261449	-1.917161
H	4.530914	0.797222	-1.513983	H	4.564930	0.810060	-1.537223
H	3.615609	-0.180592	-3.184135	H	3.650311	-0.171820	-3.205676

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