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Computational study of An-X bonding (An = Th, U; X = p-block-based ligands) in pyrrolic macrocycle-supported complexes from the quantum theory of atoms in molecules and bond energy decomposition analysis

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Bond distances (Å)															
	PBE					PBE0					Experimental				
X ligand	Th-Ar1	Th-Ar2	Th-N2	Th-N1	Th-X	Th-Ar1	Th-Ar2	Th-N2	Th-N1	Th-X	Th-Ar1	Th-Ar2	Th-N2	Th-N1	Th-X
$(\mu\text{-H})_3BH$	2.725	2.808	2.414	2.406	2.611	2.709	2.762	2.402	2.396	2.605	-	-	-	-	-
$(\mu\text{-H})_2BH_2$	-	-	-	-	-	2.615	2.615	2.394	2.394	2.837					
$BO_2C_2H_4$	2.585	2.585	2.420	2.420	2.705	2.581	2.581	2.405	2.405	2.700	-	-	-	-	-
Me	2.620	2.667	2.417	2.425	2.485	2.641	2.645	2.405	2.413	2.475	-	-	-	-	-
$N(SiH_3)_2$*	2.713	2.710	2.443	2.431	2.280	2.689	2.690	2.418	2.426	2.272	2.687	2.692	2.482	2.464	2.275
OPh	2.669	2.669	2.438	2.438	2.120	2.651	2.651	2.422	2.422	2.106	-	-	-	-	-
	U-Ar1	U-Ar2	U-N2	U-N1	U-X	U-Ar1	U-Ar2	U-N2	U-N1	U-X	U-Ar1	U-Ar2	U-N2	U-N1	U-X
$(\mu\text{-H})_3BH$	3.536	2.380	2.412	2.408	2.533	3.450	2.477	2.429	2.420	2.549	-	-	-	-	-
$(\mu\text{-H})_2BH_2$	-	-	-	-	-	2.575	2.575	2.460	2.460	2.855	2.601	2.580	2.476	2.452	2.927
$BO_2C_2H_4$	2.462	2.462	2.466	2.466	2.650	2.508	2.508	2.467	2.467	2.677	-	-	-	-	-
Me	2.589	2.516	2.463	2.479	2.518	2.615	2.564	2.468	2.484	2.519	-	-	-	-	-
$N(SiH_3)_2$*	3.415	2.371	2.428	2.412	2.267	2.724	2.596	2.470	2.473	2.359	2.814	2.642	2.545	2.532	2.364
OPh*	2.584	2.584	2.494	2.494	2.148	2.620	2.620	2.486	2.486	2.159	2.618	2.745	2.496	2.537	2.364

Table S1. Key bond lengths for the $[LTh^{IV}X]^+$ and $LU^{III}X$ complexes and experimental data where available. *Note that for experimental data, $N(SiH_3)_2$ and OPh are instead $N(TMS)_2$ and DTBP respectively. Atom labelling as in figure 2 in the main text.

Bond angles (°)									
	PBE			PBE0			Experimental		
X ligand	Ar-Th-Ar	Interplanar	N-Th-N	Ar-Th-Ar	Interplanar	N-Th-N	Ar-Th-Ar	Interplanar	N-Th-N
$(\mu\text{-H})_3BH$	173.0	24.4	118.5	172.4	23.4	117.9	-	-	-
$(\mu\text{-H})_2BH_2$	-	-	-	179.3	9.2	119.9	-	-	-
$BO_2C_2H_4$	175.6	2.3	124.6	177.1	4.0	123.7	-	-	-
Me	178.1	13.0	121.6	177.8	12.6	121.2	-	-	-
$N(SiH_3)_2$*	174.2	17.2	117.1	174.2	16.8	117.0	169.4	21.3	115.5
OPh	177.5	10.8	119.2	177.6	10.8	119.3	-	-	-
	Ar-U-Ar	Interplanar	N-U-N	Ar-U-Ar	Interplanar	N-U-N	Ar-U-Ar	Interplanar	N-U-N
$(\mu\text{-H})_3BH$	175.4	43.3	122.0	172.8	43.3	120.1	-	-	-
$(\mu\text{-H})_2BH_2$	-	-	-	177.9	9.2	119.5	174.7	14.4	118.9
$BO_2C_2H_4$	175.1	0.9	124.5	177.6	3.3	121.7	-	-	-
Me	174.8	10.1	122.1	177.3	11.6	121.2	-	-	-
$N(SiH_3)_2$*	179.0	34.4	123.1	175.4	16.8	118.7	176.0	19.5	114.6
OPh*	175.9	8.9	119.7	176.0	10.6	119.4	174.2	17.3	116.9

Table S2. Key bond angles for the $[LTh^{IV}X]^+$ and $LU^{III}X$ complexes and experimental data where available. *Note that for experimental data, $N(SiH_3)_2$ and OPh are instead $N(TMS)_2$ and DTBP respectively.

Table S3. Mean absolute deviation analysis for PBE and PBE0 when compared to experimental average bond lengths of the actinide to pyrrole nitrogens.

Average An-N(py) bond distance (Å)

	LThN(TMS)$_2$	**LUBH$_4$**	**LUN(TMS)$_2$**	**LUDTBP**				
Experiment	2.473	2.464	2.539	2.517				
PBE	2.437	2.410	2.420	2.494				
PBE0	2.422	2.460	2.472	2.486	**Totals**		**Mean absolute deviations**	
|expt – PBE|	0.036	0.054	0.119	0.023	Σ|expt – PBE|	0.232	PBE	0.058
|expt – PBE0|	0.051	0.004	0.067	0.031	Σ|expt – PBE0|	0.153	PBE0	0.038

Table S4. Mean absolute deviation analysis for PBE and PBE0 when compared to experimental actinide to arene(1) centroid distances.

An-Ar(1) bond distance (Å)

	LThN(TMS)$_2$	**LUBH$_4$**	**LUN(TMS)$_2$**	**LUDTBP**				
Experiment	2.687	2.601	2.814	2.618				
PBE	2.713	3.536	3.415	2.584				
PBE0	2.689	2.575	2.596	2.620	**Totals**		**Mean absolute deviations**	
|expt – PBE|	0.026	0.935	0.601	0.034	Σ|expt – PBE|	1.596	PBE	0.399
|expt – PBE0|	0.002	0. 026	0.218	0.002	Σ|expt – PBE0|	0.248	PBE0	0.062

Table S5. Mean absolute deviation analysis for PBE and PBE0 when compared to experimental actinide to arene(2) centroid distances.

An-Ar(2) bond distance (Å)

	LThN(TMS)$_2$	**LUBH$_4$**	**LUN(TMS)$_2$**	**LUDTBP**				
Experiment	2.692	2.580	2.642	2.745				
PBE	2.710	2.380	2.371	2.584				
PBE0	2.690	2.575	2.724	2.620	**Totals**		**Mean absolute deviations**	
|expt – PBE|	0.018	0.200	0.271	0.161	Σ|expt – PBE|	0.650	PBE	0.163
|expt – PBE0|	0.002	0.005	0.082	0.125	Σ|expt – PBE0|	0.214	PBE0	0.054

Table S6. Mean absolute deviation analysis for PBE and PBE0 when compared to experimental bond lengths of the actinide to X ligand.

	An-X bond distance (Å)							
	LThN(TMS)$_2$	**LUBH$_4$**	**LUN(TMS)$_2$**	**LUDTBP**				
Experiment	2.275	2.927	2.364	2.364				
PBE	2.280	2.533	2.267	2.148				
PBE0	2.272	2.855	2.359	2.159	**Totals**		**Mean absolute deviations**	
|expt – PBE|	0.005	0.394	0.097	0.216	Σ|expt – PBE|	0.712	PBE	0.178
|expt – PBE0|	0.003	0.072	0.005	0.205	Σ|expt – PBE0|	0.285	PBE0	0.071

Table S7. Mean absolute deviation analysis for PBE and PBE0 when compared to experimental bond angles between arene(1) centroid to actinide to arene(2) centroid.

	Ar-An-Ar bond angle (°)							
	LThN(TMS)$_2$	**LUBH$_4$**	**LUN(TMS)$_2$**	**LUDTBP**				
Experiment	169.4	174.7	176.0	174.2				
PBE	174.2	175.4	179.0	175.9				
PBE0	174.2	177.9	175.4	176.0	**Totals**		**Mean absolute deviations**	
|expt – PBE|	4.8	0.7	3.0	1.7	Σ|expt – PBE|	10.2	PBE	2.55
|expt – PBE0|	4.8	3.2	0.6	1.8	Σ|expt – PBE0|	10.4	PBE0	2.60

Table S8. Mean absolute deviation analysis for PBE and PBE0 when compared to experimental bond angles between pyrrole nitrogen(1) to actinide to pyrrole nitrogen(2).

	N(py)-An-N(py) bond angle (°)							
	LThN(TMS)$_2$	**LUBH$_4$**	**LUN(TMS)$_2$**	**LUDTBP**				
Experiment	115.5	118.9	114.6	116.9				
PBE	117.1	122.0	123.1	119.7				
PBE0	117.0	119.9	118.7	119.4	**Totals**		**Mean absolute deviations**	
|expt – PBE|	1.6	3.1	8.5	2.8	Σ|expt – PBE|	16.0	PBE MAD	4.00
|expt – PBE0|	1.5	1.0	4.1	2.5	Σ|expt – PBE0|	9.1	PBE0 MAD	2.28

Table S9. Mean absolute deviation analysis for PBE and PBE0 when compared to experimental arene interplanar angles.

	Interplanar angle (°)							
	LThN(TMS)$_2$	**LUBH$_4$**	**LUN(TMS)$_2$**	**LUDTBP**				
Experiment	21.3	14.4	19.5	17.3				
PBE	17.2	43.3	34.4	8.9				
PBE0	16.8	9.2	16.8	10.6	**Totals**		**Mean absolute deviations**	
|expt – PBE|	4.1	28.9	14.9	8.4	Σ|expt – PBE|	56.3	PBE	14.1
|expt – PBE0|	4.5	5.2	2.7	6.7	Σ|expt – PBE0|	19.1	PBE0	4.78

Table S10. Bond distance and bond angle parameters for LTh^{III}X complexes using PBE0.

	Bond distances (Å)					**Angles (°)**		
X ligand	Th-Ar1	Th-Ar2	Th-N1	Th-N2	Th-X	Ar-Th-Ar	Interplanar	N-Th-N
BH_4	2.775	2.385	2.469	2.480	2.888	176.8	9.6	115.7
$BO_2C_2H_4$	2.482	2.482	2.482	2.482	2.652	171.1	6.3	126.5
Me	2.411	2.831	2.476	2.495	2.525	177.3	12.4	118.2
$N(SiH_3)_2$	2.401	3.055	2.492	2.459	2.341	175.7	21.7	116.3
OPh	2.576	2.576	2.487	2.487	2.168	178.3	7.9	120.1

Table S11. PBE0 SCF energies, ZPEs and thermal corrections for the [LTh^{IV}X]$^+$ complexes. All values in Hartrees.

Complex	**SCF energy**	**SCP+ZPE correction**	**SCF+ZPE+Thermal correction to enthalpy**
LThBH$_4$	-1469.96141	-1469.54202	-1469.51775
LThBO$_2$C$_2$H$_4$	-1696.53211	-1696.08264	-1696.05517
LThMe	-1482.60413	-1482.19022	-1482.16577
LThN(SiH$_3$)$_2$	-2079.88776	-2079.45206	-2079.42428
LThOPh	-1749.43247	-1748.95853	-1748.93004

Table S12. PBE0 SCF energies, ZPEs and thermal corrections for the $LTh^{III}X$ complexes. All values in Hartrees.

Complex	SCF energy	SCP+ZPE correction	SCF+ZPE+Thermal correction to enthalpy
$LThBH_4$	-1470.13391	-1469.71809	-1469.69351
$LThBO_2C_2H_4$	-1696.69507	-1696.24953	-1696.22204
LThMe	-1482.76330	-1482.35379	-1482.32867
$LThN(SiH_3)_2$	-2080.04932	-2079.61762	-2079.58848
LThOPh	-1749.57967	-1749.11181	-1749.08331

Table S13. PBE0 SCF energies, ZPEs thermal corrections for the $LU^{III}X$ complexes. All values in Hartrees.

Complex	SCF energy	SCP+ZPE correction	SCF+ZPE+Thermal correction to enthalpy
$LUBH_4$	-1539.39098	-1538.97309	-1538.94863
$LUBO_2C_2H_4$	-1765.94545	-1765.49821	-1765.47049
LUMe	-1552.01607	-1551.60395	-1551.57925
$LUN(SiH_3)_2$	-2149.29793	-2148.86416	-2148.83499
LUOPh	-1818.83801	-1818.36282	-1818.33703

Table S14. PBE0 energies of geometry optimised molecular ionic fragments in $[LAnX]^{n+}$ (n = 1 (Th(IV)), 0 (Th(III) and U(III)) with ZPE and thermal corrections. All values in Hartrees.

Fragment	SCF energy	SCF+ZPE correction	SCF+ZPE+Thermal correction to enthalpy
BH_4^-	-27.208	-27.175	-27.171
$BO_2C_2H_4^-$	-253.719	-253.653	-253.648
Me^-	-39.770	-39.742	-39.738
$N(SiH_3)_2^-$	-637.115	-637.063	-637.057
OPh^-	-306.636	-306.546	-306.540
LTh^{2+}	-1442.410	-1442.031	-1442.009
LTh^+	-1442.726	-1442.348	-1442.326
LU^+	-1511.975	-1511.596	-1511.575

Table S15. PBE0 electron density and energy density at An-X BCP and An-X delocalisation indices from QTAIM analysis at PBE0 optimised geometries.

X ligand	ρ (e bohr^{-3})			H (Hartrees bohr^{-3})			δ(An-X)		
	Th^{IV}-X	U^{III}-X	Th^{III}-X	Th^{IV}-X	U^{III}-X	Th^{III}-X	Th^{IV}-X	U^{III}-X	Th^{III}-X
BH_4	0.042	0.037	0.037	-0.021	-0.012	-0.015	0.527	0.480	0.465
$BO_2C_2H_4$	0.068	0.067	0.071	-0.021	-0.021	-0.023	0.561	0.570	0.515
Me	0.088	0.076	0.081	-0.031	-0.024	-0.028	0.679	0.593	0.605
$N(SiH_3)_2$	0.104	0.082	0.090	-0.039	-0.023	-0.029	0.807	0.599	0.653
OPh	0.116	0.105	0.121	-0.042	-0.030	-0.031	0.857	0.673	0.670

Table S16. PBE ΔE (eV) for $LAnX]^{n+}$ (n = 1 (Th(IV)), 0 (Th(III) and U(III)) at PBE0 geometries.

X ligand	$[LTh^{IV}X]^+$	$LTh^{III}X$	$LU^{III}X$
BH_4	-9.16	-5.37	-5.54
$BO_2C_2H_4$	-10.73	-6.83	-6.83
Me	-11.36	-7.23	-7.33
$N(SiH_3)_2$	-9.70	-5.62	-5.54
OPh	-10.30	-6.03	-6.05

Table S17. QTAIM metrics at PBE0-optimised geometries using the PBE functional.

X ligand	ρ (e bohr^{-3})			H (Hartrees bohr^{-3})			δ(An-X)		
	Th^{IV}-X	U^{III}-X	Th^{III}-X	Th^{IV}-X	U^{III}-X	Th^{III}-X	Th^{IV}-X	U^{III}-X	Th^{III}-X
BH_4	0.050	0.042	0.043	-0.021	-0.013	-0.015	0.366	0.365	0.465
$BO_2C_2H_4$	0.069	0.065	0.069	-0.021	-0.019	-0.022	0.569	0.574	0.504
Me	0.089	0.077	0.080	-0.032	-0.024	-0.026	0.678	0.634	0.621
$N(SiH_3)_2$	0.106	0.084	0.089	-0.041	-0.023	-0.029	0.804	0.661	0.688
OPh	0.127	0.100	0.103	-0.049	-0.025	-0.031	0.825	0.737	0.720

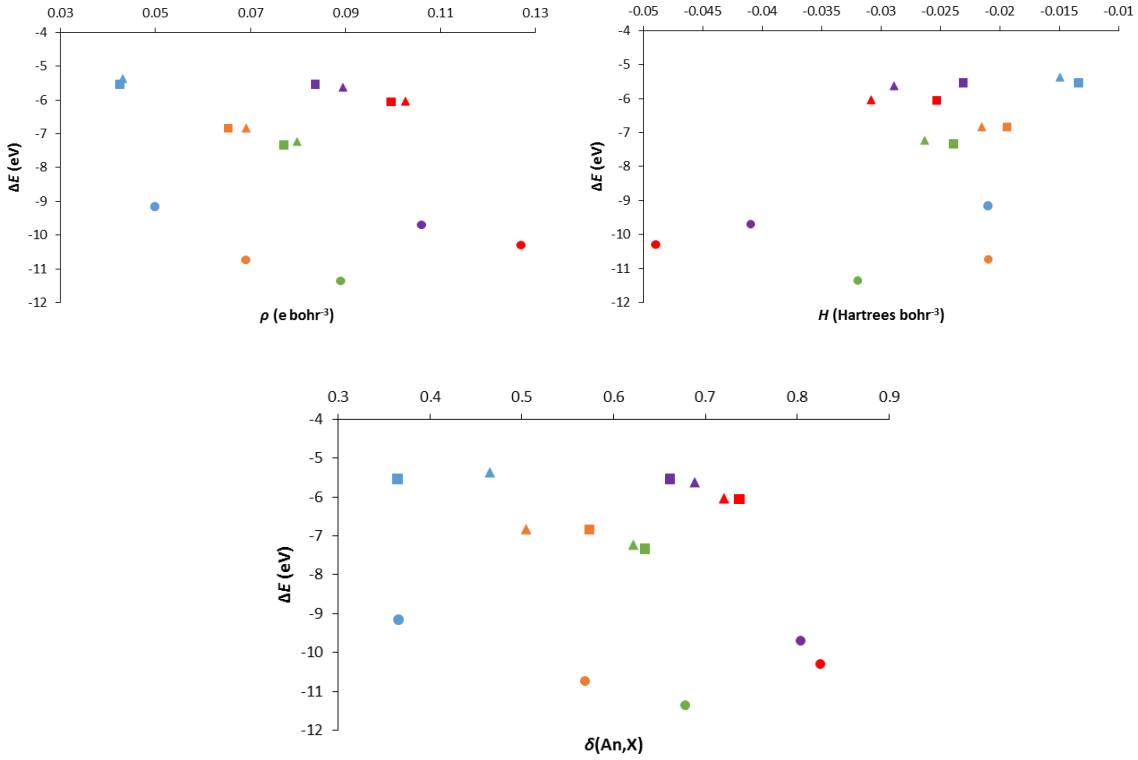

Fig.S.1. An-X Δ*E* vs, clockwise from top left, An-X electron densities, energy densities and delocalisation indices from single point PBE calculations on the PBE0-optimised $[LAnX]^{n+}$ (*n* = 1 (Th(IV)), 0 (Th(III) and U(III)). For the different actinides, circles = $LTh^{IV}X$, triangles = $LTh^{III}X$ and squares = $LU^{III}X$. For the different X ligands, blue = BH_4, orange = $BO_2C_2H_4$, green = Me, purple = $N(SiH_3)_2$ and red = OPh. R^2 for Δ*E* vs *ρ* = 0.060 (Th(IV)), 0.042 (Th(III)), 0.017 (U(III)); vs *H* = 0.004 (Th(IV)), 0.047 (Th(III)), 0.120 (U(III)); vs *δ*(An,X) = 0.121 (Th(IV)), 0.000 (Th(III)), 0.070 (U(III)).

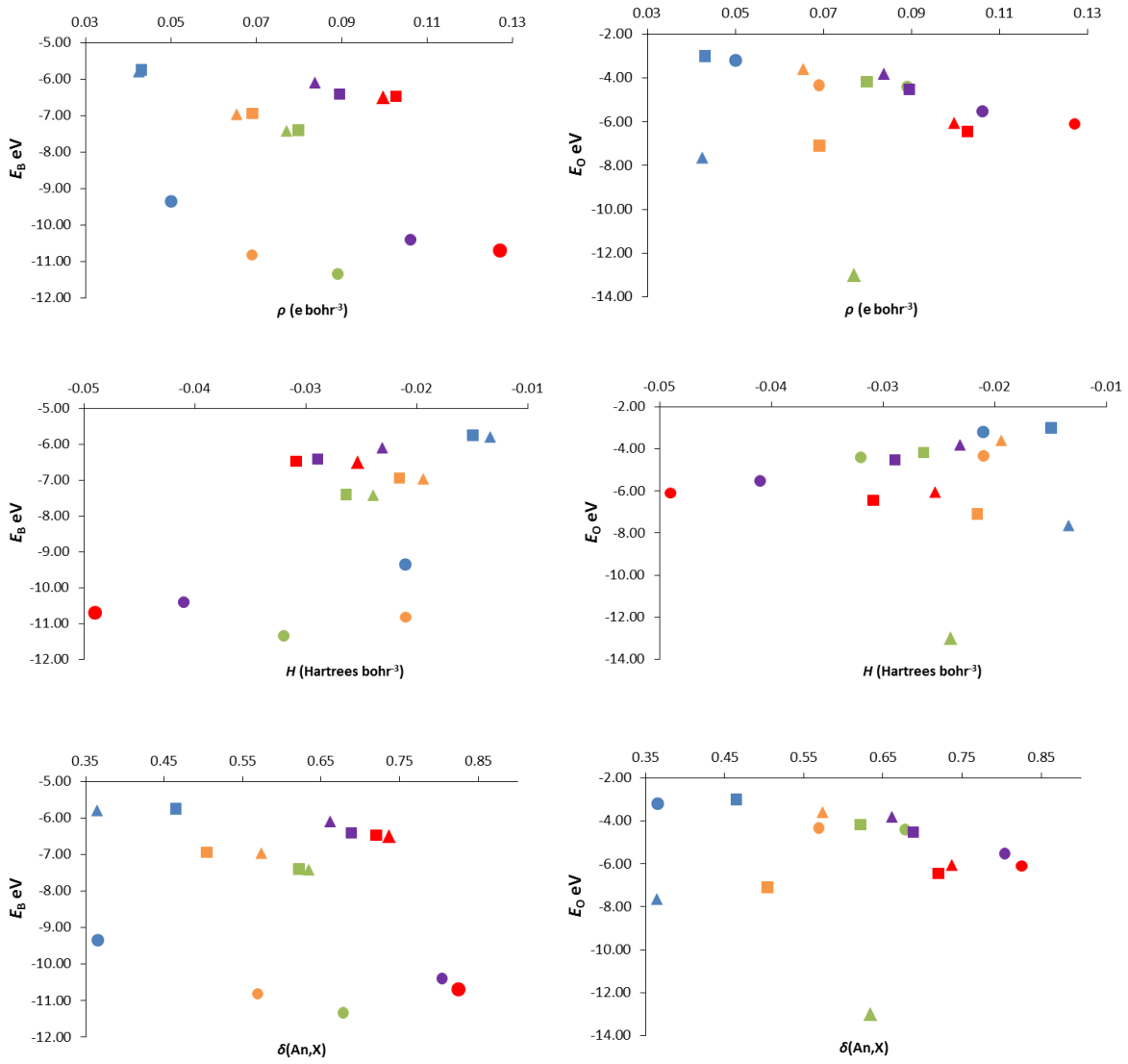

Fig.S.2. PBE//PBE0 ρ (top), H (middle) and An-X δ(An,X) (bottom) against E_B for $[LAnX]^{n+}$ (n = 1 (Th(IV)), 0 (Th(III) and U(III)). Th(IV) circles; Th(III) squares; U(III) triangles. BH_4 blue; $BO_2C_2H_4$ orange; Me green; $N(SiH_3)_2$ purple; OPh red.

Fig.S.3. PBE//PBE0 ρ (top), H (middle) and An-X δ(An,X) (bottom) against E_O for $[LAnX]^{n+}$ (n = 1 (Th(IV)), 0 (Th(III) and U(III)). Th(IV) circles; Th(III) squares; U(III) triangles. BH_4 blue; $BO_2C_2H_4$ orange; Me green; $N(SiH_3)_2$ purple; OPh red.

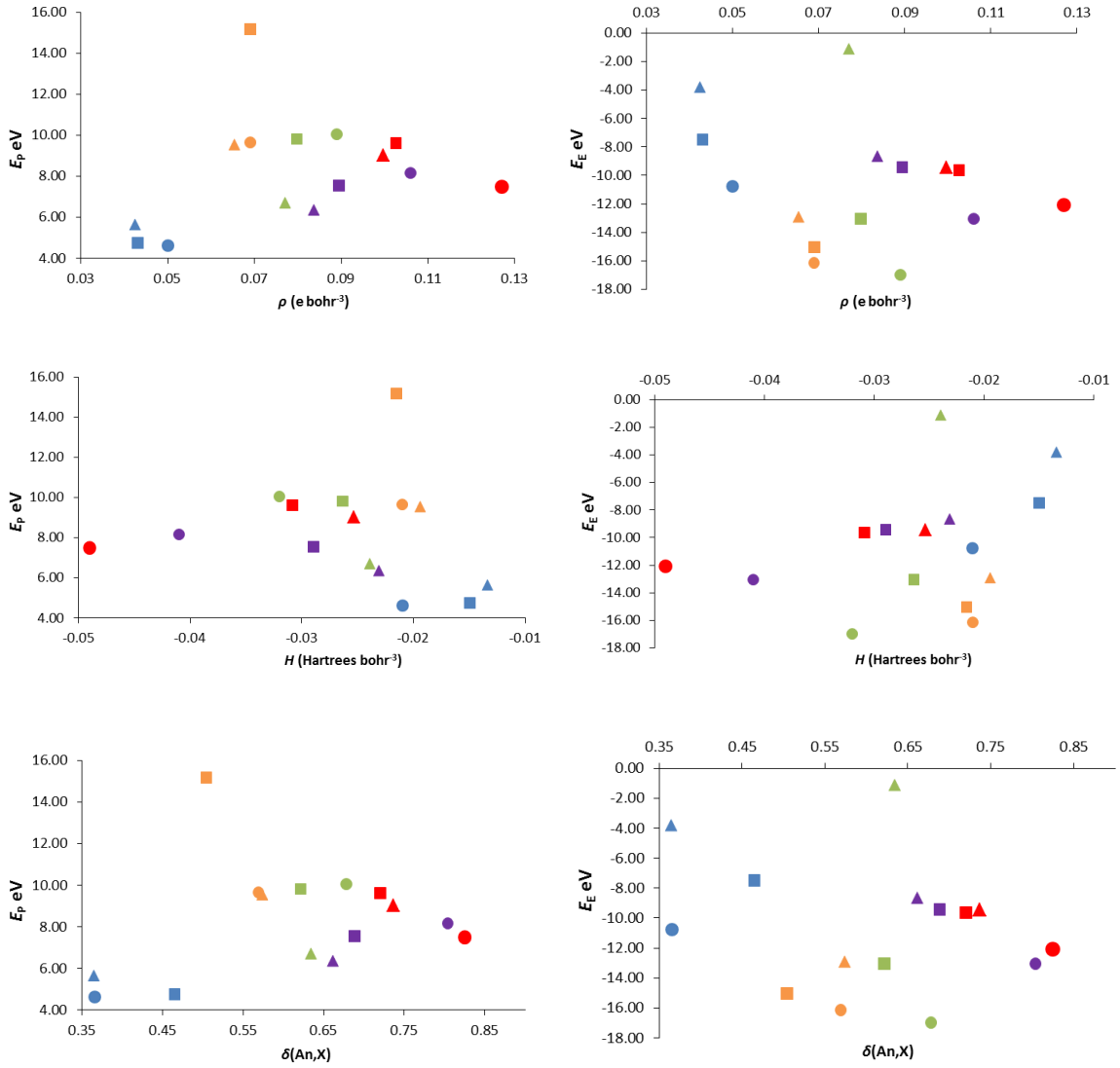

Fig.S.4. PBE//PBE0 ρ (top), H (middle) and An-X δ(An,X) (bottom) against E_P for $[LAnX]^{n+}$ (n = 1 (Th(IV)), 0 (Th(III) and U(III)).. Th(IV) circles; Th(III) squares; U(III) triangles. BH_4 blue; $BO_2C_2H_4$ orange; Me green; $N(SiH_3)_2$ purple; OPh red.

Fig.S.5. PBE//PBE0 ρ (top), H (middle) and An-X δ(An,X) (bottom) against E_E for $[LAnX]^{n+}$ (n = 1 (Th(IV)), 0 (Th(III) and U(III)).. Th(IV) circles; Th(III) squares; U(III) triangles. BH_4 blue; $BO_2C_2H_4$ orange; Me green; $N(SiH_3)_2$ purple; OPh red.

Table S18. PBE//PBE0 An-X* EDA energies (eV) for the $[LAnX^*]^{n+}$ complexes from ionic fragments.

X*	E_B			E_E			E_P			E_O		
	Th^{IV}-X*	Th^{III}-X*	U^{III}-X*	Th^{IV}-X*	Th^{III}-X*	U^{III}-X*	Th^{IV}-X*	Th^{III}-X*	U^{III}-X*	Th^{IV}-X*	Th^{III}-X*	U^{III}-X*
SiH_3	-9.51	-5.90	-5.84	-12.96	-10.01	-9.46	7.01	7.28	6.27	-3.56	-3.18	-2.65
PH_2	-9.71	-5.99	-6.09	-12.56	-9.44	-8.56	6.62	6.98	4.95	-3.77	-3.53	-2.49
SH	-9.92	-6.21	-2.72	-12.26	-8.72	-22.26	6.19	5.80	28.39	-3.85	-3.30	-8.80
Cl	-9.92	-6.21	-5.66	-11.79	-8.40	-8.71	5.64	5.66	6.60	-3.77	-3.46	-3.55

Table S19. PBE An-X* QTAIM metrics from PBE0-optimised geometries of $[LAnX^*]^{n+}$.

X*	ρ (e bohr^{-3})			H (Hartrees bohr^{-3})			δ(An-X)		
	Th^{IV}-X*	Th^{III}-X*	U^{III}-X*	Th^{IV}-X*	Th^{III}-X*	U^{III}-X*	Th^{IV}-X*	Th^{III}-X*	U^{III}-X*
SiH_3	0.052	0.049	0.107	-0.015	-0.013	-0.060	0.549	0.518	0.747
PH_2	0.060	0.054	0.142	-0.017	-0.014	-0.081	0.686	0.618	1.196
SH	0.068	0.060	0.202	-0.019	-0.015	-0.147	0.782	0.686	1.437
Cl	0.074	0.064	0.204	-0.021	-0.015	-0.137	0.775	0.667	1.463

Table S20. PBE//PBE0 An-X'' EDA energies (eV) for the $[LAnX'']^{n+}$ complexes from ionic fragments.

X''	E_B			E_E			E_P			E_O		
	Th^{IV}-X''	Th^{III}-X''	U^{III}-X''	Th^{IV}-X''	Th^{III}-X''	U^{III}-X''	Th^{IV}-X''	Th^{III}-X''	U^{III}-X''	Th^{IV}-X''	Th^{III}-X''	U^{III}-X''
CH_2Ph	-10.42	-6.08	-6.45	-13.45	-8.78	-11.28	7.90	6.58	7.32	-4.87	-3.88	-2.49
NHPh	-10.51	-4.21	-6.66	-13.73	-10.02	-9.34	8.77	7.41	6.80	-5.55	-4.21	-4.13
OPh	-10.69	-6.48	-6.51	-12.08	-9.65	-12.08	7.49	9.62	9.01	-6.10	-6.45	-6.10

Table S21. PBE An-X'' QTAIM metrics from PBE0-optimised geometries of $[LAnX'']^{n+}$ complexes from ionic fragments.

X''	ρ (e bohr^{-3})			H (Hartrees bohr^{-3})			δ(An-X)		
	Th^{IV}-X''	Th^{III}-X''	U^{III}-X''	Th^{IV}-X''	Th^{III}-X''	U^{III}-X''	Th^{IV}-X''	Th^{III}-X''	U^{III}-X''
CH_2Ph	0.086	0.067	0.081	-0.030	-0.020	-0.026	0.626	0.523	0.600
NHPh	0.109	0.101	0.098	-0.043	-0.036	-0.033	0.774	0.732	0.744
OPh	0.116	0.103	0.118	-0.045	-0.031	-0.041	0.857	0.720	0.887

Table S22. PBE//PBE0 An-X** EDA energies (eV) for the $[LAnX^{**}]^{n+}$ complexes from ionic fragments.

X**	E_B			E_E			E_P			E_O		
	Th^{IV}-X**	Th^{III}-X**	U^{III}-X**	Th^{IV}-X**	Th^{III}-X**	U^{III}-X**	Th^{IV}-X**	Th^{III}-X**	U^{III}-X**	Th^{IV}-X**	Th^{III}-X**	U^{III}-X**
SiH_2Ph	-9.34	-5.50	-3.75	-11.14	-8.30	-16.88	5.68	5.96	18.07	-3.87	-3.16	-4.94
PHPh	-9.45	-5.56	-5.60	-10.46	-7.64	11.44	5.25	5.56	-1.21	-4.24	-3.48	-15.83
SPh	-9.46	-5.61	-5.66	-10.16	-7.44	-10.04	4.98	5.44	7.65	-4.29	-3.62	-3.27

Table S23. PBE An-X** QTAIM metrics from PBE0-optimised geometries of $[LAnX^{**}]^{n+}$ complexes from ionic fragments.

X**	ρ (e bohr^{-3})			H (Hartrees bohr^{-3})			δ(An-X)		
	Th^{IV}-X**	Th^{III}-X**	U^{III}-X**	Th^{IV}-X**	Th^{III}-X**	U^{III}-X**	Th^{IV}-X**	Th^{III}-X**	U^{III}-X**
SiH_2Ph	0.050	0.044	0.105	-0.014	-0.011	-0.058	0.532	0.477	0.819
PHPh	0.058	0.051	0.049	-0.016	-0.012	-0.012	0.690	0.590	0.617
SPh	0.066	0.055	0.054	-0.018	-0.013	-0.012	0.763	0.632	0.669

Table S24. PBE//PBE0 An-X† EDA energies (eV) for the $[LAnX^{\dagger}]^{n+}$ complexes from ionic fragments.

X†	E_B		E_E		E_P		E_O	
	Th^{IV}-X†	Th^{III}-X†	Th^{IV}-X†	Th^{III}-X†	Th^{IV}-X†	Th^{III}-X†	Th^{IV}-X†	Th^{III}-X†
CPh_3	-9.71	-5.83	-3.83	-1.56	6.17	5.06	-5.87	-4.27
NPh_2	-10.00	-6.11	-12.23	-8.77	8.05	7.18	-5.83	-4.52
OPh	-10.69	-6.48	-12.08	-9.65	7.49	9.62	-6.10	-6.45
$SiPh_3$	-9.26	-5.26	-10.04	-7.20	5.05	5.06	-4.27	-3.12
PPh_2	-9.35	-5.22	-10.03	-7.28	5.32	5.56	-4.64	-3.51
SPh	-9.46	-5.61	-10.16	-7.44	4.98	5.44	-4.29	-3.62

Table S25. PBE An-X^{+} QTAIM metrics from PBE0-optimised geometries of $[LAnX^{+}]^{n+}$ complexes from ionic fragments.

X^{+}	ρ (e bohr^{-3})		H (Hartrees bohr^{-3})		δ(An-X)	
	Th^{IV}-X^{+}	Th^{III}-X^{+}	Th^{IV}-X^{+}	Th^{III}-X^{+}	Th^{IV}-X^{+}	Th^{III}-X^{+}
CPh$_3$	0.063	0.054	-0.018	-0.013	0.477	0.377
NPh$_2$	0.105	0.088	-0.040	-0.028	0.715	0.607
OPh	0.116	0.103	-0.045	-0.031	0.857	0.720
SiPh$_3$	0.047	0.040	-0.012	-0.009	0.504	0.442
PPh$_2$	0.058	0.049	-0.016	-0.011	0.692	0.521
SPh	0.066	0.055	-0.018	-0.013	0.763	0.632

PBE0 Cartesian coordinates (Å) and SCF energies (H) of all complexes studied.

[LTh^{IV}X]$^{+}$ complexes.

[LTh^{IV}(μ-H)$_3$BH]$^{+}$. SCF energy = -1469.95841

C -3.165537 0.296438 -0.683179
C -4.107254 -0.280408 -1.485041
H -5.099953 0.103012 -1.674509
C -3.537351 -1.463917 -2.011813
H -4.002217 -2.162939 -2.692494
C -2.267481 -1.548496 -1.519877
C -3.285235 1.568114 0.092058
C -1.944198 2.209863 0.257946
C -1.067880 2.286418 -0.843520
H -1.424444 1.974585 -1.820282
C 0.247522 2.697039 -0.689159
C 0.694103 3.081583 0.588659
H 1.731412 3.373073 0.719325
C -0.181351 3.103477 1.655235
H 0.159976 3.423704 2.633608
C -1.493247 2.646134 1.495164
H -2.155064 2.599576 2.353750
C 1.228618 2.604997 -1.808470
C 2.274502 1.591326 -1.477254
C 3.554274 1.532368 -1.947418
H 4.024751 2.254442 -2.599608
C 4.124418 0.338291 -1.446247
H 5.123336 -0.031949 -1.629095
C 3.172360 -0.270237 -0.680693
C 3.291249 -1.564719 0.057647
C 1.946888 -2.199141 0.215198
C 1.075451 -2.265984 -0.888122
H 1.437090 -1.953403 -1.862698
C -0.245159 -2.667788 -0.738540
C -0.698344 -3.046480 0.536507
H -1.739176 -3.326037 0.664573
C 0.169915 -3.065090 1.611672
H -0.179851 -3.376221 2.589406
C 1.485604 -2.623630 1.455168
H 2.146977 -2.588495 2.313774
C -1.224652 -2.564221 -1.858379
N -1.998895 -0.470195 -0.671494
N 1.999139 0.486492 -0.666135
Th 0.000923 -0.015382 0.567971
H -1.706877 -3.533429 -2.027496
H -0.695609 -2.308419 -2.784592
H -3.734160 1.411786 1.081038
H -3.957698 2.246181 -0.447341
H 0.701046 2.354490 -2.737103
H 1.708227 3.576726 -1.969907
H 3.955101 -2.231980 -0.505355
H 3.747909 -1.438125 1.047230
B -0.047297 -0.164325 3.168151
H -0.045878 -0.267857 4.357572
H 1.058000 -0.443721 2.667182
H -0.879495 -0.907964 2.620141
H -0.304997 0.969257 2.782921

[LTh^{IV}(μ-H)$_2$BH$_2$]$^{+}$. SCF energy = -1469.96141

C -3.139659 0.518549 -0.763243
C -4.128662 -0.021097 -1.534393
H -5.087981 0.430037 -1.745269
C -3.663998 -1.279281 -1.986599
H -4.191911 -1.975938 -2.622324
C -2.406781 -1.446351 -1.481903

C -3.168676 1.813185 -0.011995
C -1.778009 2.289660 0.254161
C -0.873998 2.400740 -0.817486
H -1.236080 2.226993 -1.826662
C 0.475442 2.662917 -0.607273
C 0.927642 2.853246 0.709623
H 1.983472 3.033119 0.884754
C 0.042024 2.792747 1.771814
H 0.395607 2.934617 2.785385
C -1.305331 2.488065 1.547522
H -1.978038 2.385445 2.391840
C 1.466005 2.585045 -1.721525
C 2.407221 1.446580 -1.481385
C 3.663941 1.278751 -1.987050
H 4.191713 1.975003 -2.623334
C 4.128347 0.020450 -1.534891
H 5.087289 -0.431199 -1.746384
C 3.139756 -0.518459 -0.762708
C 3.168824 -1.812679 -0.010803
C 1.778137 -2.289619 0.254547
C 0.874562 -2.400353 -0.817496
H 1.237046 -2.226252 -1.826472
C -0.474963 -2.662591 -0.607907
C -0.927699 -2.853301 0.708752
H -1.983618 -3.033133 0.883397
C -0.042498 -2.793197 1.771316
H -0.396503 -2.935365 2.784700
C 1.304955 -2.488497 1.547656
H 1.977327 -2.386080 2.392269
C -1.465118 -2.584304 -1.722534
N -2.043129 -0.342613 -0.706551
N 2.043658 0.343243 -0.705398
Th -0.000056 -0.000023 0.492679
H -2.035801 -3.518108 -1.781334
H -0.933367 -2.478505 -2.675895
H -3.707461 1.719499 0.938532
H -3.709059 2.560692 -0.605153
H 0.934626 2.480106 -2.675183
H 2.036976 3.518735 -1.779406
H 3.710070 -2.560194 -0.603149
H 3.706763 -1.718273 0.940143
B -0.000974 -0.000534 3.330130
H 0.998096 0.188699 2.575855
H -0.194378 0.995139 3.976551
H -0.999522 -0.189641 2.575243
H 0.192150 -0.996265 3.976563

[LTh^{IV}BO$_2$C$_2$H$_4$]$^+$. SCF energy = -1696.53211

C -2.166144 2.351574 -1.245219
C -3.271557 2.530731 -2.031070
H -3.723059 3.478624 -2.287744
C -3.710859 1.247190 -2.424628
H -4.562125 1.015445 -3.049109
C -2.845535 0.341294 -1.873985
C -1.365863 3.401754 -0.539491
C 0.000000 2.891734 -0.211387
C 0.837463 2.428540 -1.244969
H 0.506445 2.534066 -2.274221
C 2.047810 1.798759 -0.972301
C 2.439001 1.642606 0.368696
H 3.367336 1.125902 0.589597
C 1.638736 2.117627 1.396297
H 1.953446 2.010215 2.427574
C 0.413600 2.730004 1.105870
H -0.232501 3.040742 1.919636
C 2.845326 1.146687 -2.053731
C 2.845535 -0.341294 -1.873985
C 3.710859 -1.247190 -2.424628
H 4.562125 -1.015445 -3.049109
C 3.271557 -2.530731 -2.031070
H 3.723059 -3.478624 -2.287744
C 2.166144 -2.351574 -1.245219
C 1.365863 -3.401754 -0.539491
C 0.000000 -2.891734 -0.211387
C -0.837463 -2.428540 -1.244969
H -0.506445 -2.534066 -2.274221
C -2.047810 -1.798759 -0.972301
C -2.439001 -1.642606 0.368696
H -3.367336 -1.125902 0.589597
C -1.638736 -2.117627 1.396297
H -1.953446 -2.010215 2.427574
C -0.413600 -2.730004 1.105870
H 0.232501 -3.040742 1.919636
C -2.845326 -1.146687 -2.053731
N -1.871624 0.996103 -1.126288
N 1.871624 -0.996103 -1.126288
Th 0.000000 0.000000 0.007995
H -3.877532 -1.515162 -2.025669
H -2.435143 -1.434451 -3.029246
H -1.857130 3.731506 0.383875
H -1.284196 4.285530 -1.183447
H 2.435143 1.434451 -3.029246
H 3.877532 1.515162 -2.025669
H 1.284196 -4.285530 -1.183447
H 1.857130 -3.731506 0.383875
C -0.552257 0.527855 4.860336
C 0.552257 -0.527855 4.860336
H -1.511991 0.134754 5.211656
H -0.300918 1.413110 5.449173
H 0.300918 -1.413110 5.449173
H 1.511991 -0.134754 5.211656
B 0.000000 0.000000 2.705707
O -0.689896 0.904325 3.477675
O 0.689896 -0.904325 3.477675

[LTh^{IV}Me]$^+$. SCF energy = -1482.60413

C 3.186029 -0.438175 -0.711087
C 4.163727 0.122762 -1.485309
H 5.129824 -0.310342 -1.702977
C 3.669104 1.366948 -1.937910
H 4.177588 2.074722 -2.577260
C 2.405509 1.502290 -1.432637
C 3.227723 -1.751043 0.006128
C 1.843148 -2.264963 0.238888
C 0.944092 -2.360006 -0.839478
H 1.304400 -2.143174 -1.840872

C	-0.398828	-2.661551	-0.641599
C	-0.849473	-2.904574	0.667410
H	-1.901911	-3.112249	0.832120
C	0.034266	-2.869017	1.731057
H	-0.317710	-3.066202	2.737019
C	1.373390	-2.530870	1.519738
H	2.050924	-2.456349	2.363760
C	-1.391083	-2.577486	-1.754727
C	-2.371257	-1.477167	-1.489315
C	-3.629081	-1.336404	-2.007171
H	-4.130361	-2.037542	-2.659377
C	-4.129867	-0.097706	-1.545814
H	-5.094312	0.336487	-1.768534
C	-3.161811	0.455031	-0.753911
C	-3.213467	1.756063	-0.015924
C	-1.832276	2.266523	0.244224
C	-0.919972	2.379357	-0.822109
H	-1.268152	2.178846	-1.831137
C	0.420273	2.675337	-0.602823
C	0.854598	2.900428	0.715348
H	1.904537	3.107636	0.895615
C	-0.042105	2.849653	1.766408
H	0.298473	3.037997	2.778026
C	-1.378169	2.509496	1.535061
H	-2.063041	2.413885	2.371091
C	1.428305	2.604407	-1.701857
N	2.074391	0.397499	-0.651277
N	-2.050334	-0.380785	-0.692250
Th	-0.002436	-0.000144	0.510370
H	1.967898	3.555841	-1.773643
H	0.912471	2.462247	-2.659388
H	3.751117	-1.678824	0.967503
H	3.791574	-2.470256	-0.600121
H	-0.860709	-2.426229	-2.702888
H	-1.930600	-3.527366	-1.844548
H	-3.769228	2.485557	-0.617373
H	-3.749688	1.667258	0.936930
C	-0.150701	-0.083954	2.979075
H	-1.092265	-0.611121	3.213006
H	0.646363	-0.662351	3.463692
H	-0.198773	0.865223	3.520729

$[LTh^{IV}N(SiH_3)_2]^+$. SCF energy = -2079.88776

C	3.201504	-0.387352	-1.038006
C	4.244919	0.262172	-1.638050
H	5.208824	-0.166237	-1.874245
C	3.820357	1.587117	-1.882138
H	4.389019	2.377276	-2.351690
C	2.531380	1.680888	-1.434800
C	3.170617	-1.805902	-0.562492
C	1.764699	-2.307124	-0.501406
C	0.920793	-2.134030	-1.613698
H	1.339417	-1.727617	-2.529195
C	-0.437830	-2.406696	-1.540028
C	-0.965097	-2.899966	-0.332379
H	-2.031905	-3.086089	-0.260230
C	-0.133102	-3.148182	0.743722
H	-0.539992	-3.549465	1.665350
C	1.225525	-2.832819	0.666472
H	1.864272	-2.982018	1.530866
C	-1.362318	-2.045791	-2.654147
C	-2.306250	-0.974982	-2.208517
C	-3.542994	-0.694487	-2.719406
H	-4.044909	-1.241420	-3.504982
C	-4.016546	0.452726	-2.044299
H	-4.959464	0.957296	-2.201524
C	-3.054642	0.810597	-1.140885
C	-3.101751	1.949991	-0.171870
C	-1.720194	2.366010	0.215834
C	-0.762617	2.601517	-0.788626
H	-1.077174	2.571486	-1.827313
C	0.575410	2.800991	-0.480630
C	0.964667	2.803060	0.871528
H	2.014105	2.929865	1.117292
C	0.021012	2.652527	1.871060
H	0.322375	2.680354	2.912394
C	-1.315593	2.412377	1.543891
H	-2.041223	2.239655	2.332016
C	1.617169	2.859002	-1.547271
N	2.113201	0.467392	-0.892726
N	-1.970646	-0.060601	-1.211814
Th	0.000318	-0.033922	0.189003
H	2.204448	3.778883	-1.447559
H	1.128606	2.901595	-2.528496
H	3.636989	-1.919188	0.424219
H	3.754470	-2.425405	-1.254270
H	-0.774417	-1.731968	-3.525417
H	-1.938245	-2.925651	-2.962676
H	-3.624014	2.792953	-0.640703
H	-3.669633	1.697226	0.732222
Si	-1.792891	-0.860504	3.057402
H	-1.847915	-2.229590	3.648523
H	-2.244940	0.139922	4.068514
H	-2.725925	-0.806630	1.878894
Si	1.285780	-0.377880	3.208702
H	1.366661	0.699082	4.236490
H	1.761106	-1.668037	3.785763
H	2.207263	-0.005900	2.060678
N	-0.234208	-0.481068	2.403996

$[LTh^{IV}OPh]^+$. SCF energy = -1749.43247

C	2.792469	1.544544	1.458749
C	3.914805	1.360497	2.218233
H	4.662122	2.109142	2.440691
C	3.910474	0.012428	2.641869
H	4.647239	-0.475954	3.263956
C	2.778158	-0.562076	2.133951
C	2.374604	2.795072	0.747305
C	0.907748	2.781054	0.463117
C	0.000000	2.573182	1.517716
H	0.382064	2.517363	2.532876
C	-1.353310	2.369808	1.280100
C	-1.819349	2.414042	-0.046670
H	-2.871411	2.230979	-0.240891
C	-0.948460	2.678438	-1.088679
H	-1.312642	2.710138	-2.109727

C 0.416651 2.839436 -0.836795
H 1.102321 2.985124 -1.665211
C -2.281357 1.954412 2.373660
C -2.778158 0.562076 2.133951
C -3.910474 -0.012428 2.641869
H -4.647239 0.475954 3.263956
C -3.914805 -1.360497 2.218233
H -4.662122 -2.109142 2.440691
C -2.792469 -1.544544 1.458749
C -2.374604 -2.795072 0.747305
C -0.907748 -2.781054 0.463117
C 0.000000 -2.573182 1.517716
H -0.382064 -2.517363 2.532876
C 1.353310 -2.369808 1.280100
C 1.819349 -2.414042 -0.046670
H 2.871411 -2.230979 -0.240891
C 0.948460 -2.678438 -1.088679
H 1.312642 -2.710138 -2.109727
C -0.416651 -2.839436 -0.836795
H -1.102321 -2.985124 -1.665211
C 2.281357 -1.954412 2.373660
N 2.057460 0.364434 1.382864
N -2.057460 -0.364434 1.382864
Th 0.000000 0.000000 0.158171
H 3.137059 -2.638031 2.416098
H 1.764265 -2.037789 3.337415
H 2.922222 2.930134 -0.193510
H 2.619349 3.660449 1.375101
H -1.764265 2.037789 3.337415
H -3.137059 2.638031 2.416098
H -2.619349 -3.660449 1.375101
H -2.922222 -2.930134 -0.193510
O 0.000000 0.000000 -1.947826
C 0.000000 0.000000 -3.302078
C -1.198518 -0.135393 -3.994776
C 1.198518 0.135393 -3.994776
C -1.191230 -0.134582 -5.380883
H -2.126903 -0.241260 -3.442283
C 1.191230 0.134582 -5.380883
H 2.126903 0.241260 -3.442283
C 0.000000 0.000000 -6.078514
H -2.127173 -0.240593 -5.919291
H 2.127173 0.240593 -5.919291
H 0.000000 0.000000 -7.162530

$LTh^{III}X$ complexes.

$LTh^{III}(\mu\text{-}H)_2BH_2$. SCF energy = -1470.13391

C -3.127942 0.557746 -0.831643
C -4.140865 0.043448 -1.599903
H -5.081586 0.528237 -1.821987
C -3.721257 -1.239680 -2.020974
H -4.268980 -1.936270 -2.641194
C -2.467483 -1.434734 -1.501052
C -3.072741 1.858222 -0.094918
C -1.654772 2.234846 0.191268
C -0.729807 2.381920 -0.892186
H -1.094910 2.268513 -1.908605
C 0.617868 2.553728 -0.667020
C 1.094187 2.617558 0.678432
H 2.156070 2.717133 0.863442
C 0.158166 2.713493 1.736620
H 0.505372 2.861236 2.751291
C -1.185274 2.516951 1.499839
H -1.880307 2.502793 2.332973
C 1.612002 2.461488 -1.779143
C 2.497755 1.275110 -1.559639
C 3.755663 1.041313 -2.054796
H 4.320640 1.701665 -2.698196
C 4.151834 -0.226731 -1.572704
H 5.088424 -0.734150 -1.759724
C 3.121042 -0.693535 -0.795917
C 3.083956 -1.953820 0.011003
C 1.673669 -2.364186 0.288438
C 0.766443 -2.448794 -0.778795
H 1.130735 -2.278535 -1.787171
C -0.584234 -2.685863 -0.569744
C -1.040640 -2.862230 0.744487
H -2.100897 -3.012710 0.919439
C -0.156011 -2.810255 1.805274
H -0.512874 -2.925075 2.820780
C 1.197846 -2.544130 1.580404
H 1.870913 -2.448622 2.424943
C -1.562475 -2.609238 -1.695656
N -2.073970 -0.335974 -0.756037
N 2.078744 0.214205 -0.776826
Th -0.023208 0.135143 0.536171
H -2.161929 -3.526469 -1.735453
H -1.013028 -2.548756 -2.644002
H -3.623711 1.799045 0.853219
H -3.572695 2.635057 -0.690230
H 1.078568 2.399534 -2.736076
H 2.225641 3.370263 -1.812686
H 3.599567 -2.750745 -0.539798
H 3.616066 -1.840412 0.964398
B 0.004441 -0.042113 3.418626
H 0.994576 0.174625 2.664060
H -0.200978 0.940996 4.088861
H -0.996458 -0.251498 2.681788
H 0.233268 -1.041504 4.061424

$LTh^{III}BO_2C_2H_4$. SCF energy = -1696.69507

C 1.996192 2.177619 1.730327
C 2.888997 2.168911 2.773861
H 3.095889 2.992571 3.443495
C 3.502744 0.896759 2.770582
H 4.277399 0.543196 3.437314
C 2.951699 0.196945 1.725267
C 1.184822 3.323519 1.215772
C 0.000000 2.817288 0.460040
C -1.085356 2.251315 1.167367
H -1.106161 2.288686 2.251134
C -2.202410 1.759574 0.454516
C -2.155612 1.692989 -0.926851

H -2.992223 1.256518 -1.463161
C -1.014312 2.119060 -1.648807
H -1.046616 2.196257 -2.726719
C 0.028117 2.742251 -0.921359
H 0.893764 3.123408 -1.453783
C -3.341075 1.149592 1.204629
C -2.951699 -0.196945 1.725267
C -3.502744 -0.896759 2.770582
H -4.277399 -0.543196 3.437314
C -2.888997 -2.168911 2.773861
H -3.095889 -2.992571 3.443495
C -1.996192 -2.177619 1.730327
C -1.184822 -3.323519 1.215772
C 0.000000 -2.817288 0.460040
C 1.085356 -2.251315 1.167367
H 1.106161 -2.288686 2.251134
C 2.202410 -1.759574 0.454516
C 2.155612 -1.692989 -0.926851
H 2.992223 -1.256518 -1.463161
C 1.014312 -2.119060 -1.648807
H 1.046616 -2.196257 -2.726719
C -0.028117 -2.742251 -0.921359
H -0.893764 -3.123408 -1.453783
C 3.341075 -1.149592 1.204629
N 1.998142 0.959381 1.075195
N -1.998142 -0.959381 1.075195
Th 0.000000 0.000000 -0.042413
H 4.209274 -1.071594 0.536959
H 3.633628 -1.799311 2.036904
H 1.787390 3.959074 0.553479
H 0.856935 3.951407 2.051646
H -3.633628 1.799311 2.036904
H -4.209274 1.071594 0.536959
H -0.856935 -3.951407 2.051646
H -1.787390 -3.959074 0.553479
C 0.737849 0.196798 -4.846155
C -0.737849 -0.196798 -4.846155
H 1.384264 -0.629957 -5.169499
H 0.949622 1.066929 -5.474631
H -0.949622 -1.066929 -5.474631
H -1.384264 0.629957 -5.169499
B 0.000000 0.000000 -2.694062
O 1.024044 0.508305 -3.482609
O -1.024044 -0.508305 -3.482609

LTh^{III}Me. SCF energy = -1482.76330

C 3.152867 -0.574595 -0.806735
C 4.186328 -0.062277 -1.552087
H 5.115769 -0.564406 -1.783621
C 3.797035 1.237746 -1.945518
H 4.359177 1.933807 -2.553596
C 2.541304 1.444204 -1.430251
C 3.059138 -1.902872 -0.124909
C 1.634583 -2.263613 0.158429
C 0.697716 -2.411998 -0.894413
H 1.039987 -2.279194 -1.917796
C -0.651503 -2.561715 -0.650860
C -1.104699 -2.682242 0.712793
H -2.159888 -2.817668 0.912695
C -0.150028 -2.795380 1.733564
H -0.478600 -2.996505 2.747040
C 1.185789 -2.553911 1.489184
H 1.901024 -2.565337 2.304575
C -1.668186 -2.462252 -1.739391
C -2.538552 -1.263808 -1.521815
C -3.780885 -1.003742 -2.045115
H -4.348402 -1.656440 -2.694170
C -4.151787 0.280157 -1.588506
H -5.066793 0.813940 -1.807248
C -3.124551 0.729403 -0.795448
C -3.064368 2.014262 -0.031068
C -1.651457 2.411172 0.256762
C -0.713584 2.457626 -0.788153
H -1.051387 2.268145 -1.802565
C 0.630969 2.697240 -0.546463
C 1.053635 2.894647 0.776942
H 2.110497 3.040736 0.975253
C 0.138463 2.885704 1.810549
H 0.469397 3.033254 2.832126
C -1.210923 2.638039 1.551114
H -1.918311 2.591080 2.371569
C 1.642079 2.619804 -1.642401
N 2.122065 0.340226 -0.712663
N -2.110357 -0.207401 -0.739573
Th 0.016913 -0.149817 0.532692
H 2.239862 3.539002 -1.663772
H 1.120223 2.560773 -2.606597
H 3.614189 -1.898723 0.823270
H 3.542117 -2.666272 -0.750533
H -1.154609 -2.412433 -2.708260
H -2.293056 -3.364805 -1.759001
H -3.556905 2.800631 -0.617206
H -3.611856 1.948682 0.918590
C -0.117393 0.055272 3.046010
H -0.270317 -0.891872 3.574256
H 0.880769 0.412900 3.361360
H -0.838919 0.763250 3.473732

LTh^{III}N(SiH$_3$)$_2$. SCF energy = -2080.04932

C 3.329751 -0.810907 -0.419037
C 4.484931 -0.476122 -1.080504
H 5.448762 -0.951767 -0.960415
C 4.165682 0.605711 -1.930119
H 4.828655 1.122138 -2.611298
C 2.828968 0.864356 -1.754356
C 3.137640 -1.861302 0.630099
C 1.690004 -2.185543 0.814935
C 0.923835 -2.718030 -0.253146
H 1.420324 -2.926387 -1.197295
C -0.447549 -2.829516 -0.173076
C -1.101839 -2.494942 1.069611
H -2.177892 -2.588894 1.144053
C -0.315243 -2.230557 2.202866
H -0.795298 -2.088494 3.165551
C 1.045530 -2.037380 2.086835
H 1.636155 -1.769399 2.956241

C	-1.286843	-3.141005	-1.368042
C	-2.157236	-1.968890	-1.700475
C	-3.300713	-1.938032	-2.457691
H	-3.773391	-2.785691	-2.934378
C	-3.717624	-0.588795	-2.504141
H	-4.583657	-0.189331	-3.014522
C	-2.819116	0.132834	-1.757640
C	-2.887247	1.592289	-1.436225
C	-1.542950	2.194869	-1.161261
C	-0.448077	1.855445	-1.969776
H	-0.610737	1.204786	-2.824135
C	0.833682	2.312709	-1.692609
C	1.024192	3.148736	-0.585906
H	2.026888	3.486196	-0.343172
C	-0.054749	3.541226	0.183770
H	0.095721	4.200784	1.031763
C	-1.330272	3.056220	-0.093420
H	-2.162997	3.332332	0.545499
C	1.993385	1.845021	-2.510519
N	2.285633	0.005401	-0.816255
N	-1.836901	-0.699204	-1.253497
Th	0.034263	-0.139526	0.241139
H	2.618474	2.698045	-2.797192
H	1.611742	1.407007	-3.442908
H	3.548852	-1.530762	1.593562
H	3.707172	-2.759174	0.352201
H	-0.631576	-3.406086	-2.207647
H	-1.918911	-4.016587	-1.170559
H	-3.352545	2.112815	-2.283457
H	-3.536592	1.781033	-0.570672
Si	-2.356531	0.966188	2.770361
H	-2.584629	0.106208	3.977131
H	-2.770061	2.360335	3.140934
H	-3.272886	0.489717	1.686812
Si	0.668236	1.341859	3.056008
H	0.792357	2.803847	3.349525
H	0.936139	0.590250	4.321741
H	1.781641	0.991471	2.077940
N	-0.737037	0.888073	2.198605

LTh^{III}OPh. SCF energy = -1749.57967

C	2.843756	1.548779	1.492390
C	3.983812	1.366358	2.234603
H	4.728539	2.119026	2.455503
C	3.991954	0.012456	2.641965
H	4.736316	-0.481607	3.251408
C	2.849926	-0.556256	2.136580
C	2.384322	2.794155	0.800056
C	0.921066	2.727108	0.492334
C	0.000000	2.539220	1.522851
H	0.361279	2.508784	2.546993
C	-1.354610	2.295724	1.264164
C	-1.800664	2.355088	-0.083821
H	-2.852843	2.192907	-0.294416
C	-0.910962	2.586065	-1.106358
H	-1.256813	2.606241	-2.133939
C	0.465918	2.716267	-0.836255
H	1.169611	2.835188	-1.651689
C	-2.320420	1.938762	2.345464
C	-2.849926	0.556256	2.136580
C	-3.991954	-0.012456	2.641965
H	-4.736316	0.481607	3.251408
C	-3.983812	-1.366358	2.234603
H	-4.728539	-2.119026	2.455503
C	-2.843756	-1.548779	1.492390
C	-2.384322	-2.794155	0.800056
C	-0.921066	-2.727108	0.492334
C	0.000000	-2.539220	1.522851
H	-0.361279	-2.508784	2.546993
C	1.354610	-2.295724	1.264164
C	1.800664	-2.355088	-0.083821
H	2.852843	-2.192907	-0.294416
C	0.910962	-2.586065	-1.106358
H	1.256813	-2.606241	-2.133939
C	-0.465918	-2.716267	-0.836255
H	-1.169611	-2.835188	-1.651689
C	2.320420	-1.938762	2.345464
N	2.122304	0.371265	1.413319
N	-2.122304	-0.371265	1.413319
Th	0.000000	0.000000	0.170553
H	3.155871	-2.651403	2.361455
H	1.817940	-2.029314	3.317735
H	2.935255	2.961099	-0.134576
H	2.590773	3.662013	1.438753
H	-1.817940	2.029314	3.317735
H	-3.155871	2.651403	2.361455
H	-2.590773	-3.662013	1.438753
H	-2.935255	-2.961099	-0.134576
O	0.000000	0.000000	-1.997394
C	0.000000	0.000000	-3.328021
C	-1.198290	-0.115615	-4.037024
C	1.198290	0.115615	-4.037024
C	-1.191259	-0.115044	-5.422238
H	-2.127372	-0.206429	-3.482886
C	1.191259	0.115044	-5.422238
H	2.127372	0.206429	-3.482886
C	0.000000	0.000000	-6.124486
H	-2.130544	-0.206242	-5.959193
H	2.130544	0.206242	-5.959193
H	0.000000	0.000000	-7.208882

LU^{III}X complexes.

LU^{III}(μ-H$_3$)-BH. SCF energy = -1539.38749

C	-3.229309	-0.127702	-0.680737
C	-4.151412	-1.005099	-1.193139
H	-5.217193	-0.838945	-1.271980
C	-3.431616	-2.147257	-1.603237
H	-3.829649	-3.036238	-2.073605
C	-2.106806	-1.907927	-1.328710
C	-3.503141	1.252068	-0.151529
C	-2.239022	1.967398	0.197150
C	-1.327985	2.325693	-0.811114
H	-1.592487	2.139770	-1.847387

C -0.072944 2.847874 -0.505635
C 0.260346 3.057038 0.842866
H 1.245069 3.440279 1.088097
C -0.637205 2.739569 1.849416
H -0.366629 2.891118 2.888014
C -1.878824 2.177840 1.527945
H -2.563565 1.893032 2.319498
C 0.970379 3.045376 -1.557570
C 2.082284 2.053468 -1.377609
C 3.317294 2.051111 -1.975751
H 3.702853 2.801132 -2.652606
C 3.969615 0.874995 -1.540701
H 4.967804 0.549362 -1.800927
C 3.105425 0.225019 -0.692803
C 3.376260 -1.018369 0.085663
C 2.259111 -2.028418 0.121782
C 1.217497 -1.996827 -0.808257
H 1.272188 -1.284362 -1.630357
C 0.148969 -2.895054 -0.753881
C 0.156676 -3.877039 0.229764
H -0.665622 -4.583165 0.289601
C 1.214831 -3.959015 1.122656
H 1.220615 -4.737059 1.879208
C 2.245835 -3.036171 1.082670
H 3.047510 -3.087077 1.813258
C -0.961818 -2.774689 -1.753874
N -1.953661 -0.667474 -0.736977
N 1.926764 0.934172 -0.579668
U -0.088277 0.209211 0.548119
H -1.364574 -3.767148 -1.977082
H -0.535459 -2.393555 -2.693348
H -4.148532 1.213435 0.734093
H -4.048698 1.830570 -0.908731
H 0.504943 2.948090 -2.546364
H 1.371593 4.065007 -1.498274
H 4.269565 -1.492900 -0.339393
H 3.637838 -0.778178 1.126852
B 0.306424 -0.673279 2.906440
H 0.452462 -1.078734 4.025300
H 1.337410 -0.161995 2.431965
H -0.056804 -1.556260 2.110359
H -0.569667 0.212618 2.839000

$LU^{III}(\mu\text{-}H_2)\text{-}BH_2$. SCF energy = -1539.39098

C -3.160966 0.556951 -0.803702
C -4.156498 0.046565 -1.600186
H -5.099714 0.523371 -1.829937
C -3.711888 -1.221226 -2.038693
H -4.236779 -1.909643 -2.686958
C -2.464264 -1.408126 -1.495982
C -3.146949 1.850436 -0.051632
C -1.739844 2.274864 0.230181
C -0.821095 2.370527 -0.828896
H -1.172397 2.198609 -1.841792
C 0.527497 2.620260 -0.602223
C 0.966275 2.801714 0.717863
H 2.022655 2.961819 0.905527
C 0.068761 2.745195 1.769680
H 0.412601 2.864689 2.788801
C -1.278282 2.463732 1.528633
H -1.959675 2.360757 2.365627
C 1.529698 2.558337 -1.709657
C 2.464520 1.408231 -1.495819
C 3.712117 1.221172 -2.038536
H 4.237103 1.909521 -2.686796
C 4.156659 -0.046594 -1.599839
H 5.099878 -0.523452 -1.829474
C 3.161000 -0.556893 -0.803457
C 3.146928 -1.850159 -0.051038
C 1.739798 -2.274801 0.230390
C 0.821340 -2.370453 -0.828935
H 1.172889 -2.198340 -1.841710
C -0.527289 -2.620296 -0.602602
C -0.966314 -2.802126 0.717329
H -2.022717 -2.962365 0.904753
C -0.069035 -2.745821 1.769371
H -0.413214 -2.866107 2.788275
C 1.277976 -2.463984 1.528716
H 1.959220 -2.361117 2.365857
C -1.529320 -2.558067 -1.710142
N -2.100856 -0.322428 -0.722648
N 2.100913 0.322518 -0.722645
U 0.000037 0.000042 0.516033
H -2.102588 -3.492380 -1.747942
H -0.999981 -2.475270 -2.668136
H -3.692123 1.775206 0.898055
H -3.656753 2.620944 -0.643664
H 1.000458 2.475914 -2.667734
H 2.103043 3.492621 -1.747075
H 3.657153 -2.620750 -0.642603
H 3.691690 -1.774517 0.898855
B -0.001103 -0.000120 3.371146
H 0.980378 0.253250 2.624826
H -0.258872 0.979001 4.034825
H -0.981762 -0.253646 2.623919
H 0.256247 -0.978665 4.035807

$LU^{III}BO_2C_2H_4$. SCF energy = -1765.94545

C 2.174914 2.388586 1.280264
C 3.277541 2.587287 2.077237
H 3.709353 3.541620 2.346896
C 3.736098 1.306222 2.454178
H 4.585931 1.074757 3.082021
C 2.879706 0.398045 1.877002
C 1.337479 3.410943 0.580565
C 0.000000 2.839381 0.230866
C -0.841533 2.350399 1.251702
H -0.530871 2.460604 2.286043
C -2.044013 1.719173 0.954012
C -2.406576 1.551810 -0.392355
H -3.321821 1.019772 -0.628387
C -1.592094 2.032802 -1.407830
H -1.889355 1.924463 -2.443649
C -0.391140 2.677936 -1.090598
H 0.264417 3.004396 -1.890617
C -2.878960 1.092425 2.023900

C -2.879706 -0.398045 1.877002
C -3.736098 -1.306222 2.454178
H -4.585931 -1.074757 3.082021
C -3.277541 -2.587287 2.077237
H -3.709353 -3.541620 2.346896
C -2.174914 -2.388586 1.280264
C -1.337479 -3.410943 0.580565
C 0.000000 -2.839381 0.230866
C 0.841533 -2.350399 1.251702
H 0.530871 -2.460604 2.286043
C 2.044013 -1.719173 0.954012
C 2.406576 -1.551810 -0.392355
H 3.321821 -1.019772 -0.628387
C 1.592094 -2.032802 -1.407830
H 1.889355 -1.924463 -2.443649
C 0.391140 -2.677936 -1.090598
H -0.264417 -3.004396 -1.890617
C 2.878960 -1.092425 2.023900
N 1.908554 1.043332 1.142124
N -1.908554 -1.043332 1.142124
U 0.000000 0.000000 -0.022283
H 3.907019 -1.470945 1.961294
H 2.491492 -1.398496 3.004066
H 1.820106 3.770884 -0.337350
H 1.208526 4.286518 1.229396
H -2.491492 1.398496 3.004066
H -3.907019 1.470945 1.961294
H -1.208526 -4.286518 1.229396
H -1.820106 -3.770884 -0.337350
C 0.623182 0.440433 -4.867674
C -0.623182 -0.440433 -4.867674
H 1.513553 -0.098463 -5.215458
H 0.509098 1.344840 -5.472804
H -0.509098 -1.344840 -5.472804
H -1.513553 0.098463 -5.215458
B 0.000000 0.000000 -2.699181
O 0.804208 0.803110 -3.496372
O -0.804208 -0.803110 -3.496372

$LU^{III}Me$. SCF energy = -1552.01607

C 3.199347 -0.526770 -0.763347
C 4.189296 -0.015201 -1.569279
H 5.126554 -0.495801 -1.815536
C 3.743073 1.254671 -1.995452
H 4.259854 1.944235 -2.649176
C 2.500354 1.440199 -1.435940
C 3.178942 -1.836544 -0.041664
C 1.770924 -2.275280 0.217381
C 0.850130 -2.340288 -0.843112
H 1.198367 -2.131740 -1.850200
C -0.494957 -2.615620 -0.622995
C -0.930864 -2.838954 0.691748
H -1.985625 -3.015453 0.874306
C -0.030186 -2.814482 1.741148
H -0.372498 -2.981120 2.755293
C 1.313669 -2.522605 1.505182
H 2.004690 -2.456118 2.338769
C -1.498962 -2.548553 -1.729049
C -2.454890 -1.418224 -1.502534
C -3.696833 -1.235691 -2.064249
H -4.206764 -1.922544 -2.726164
C -4.153953 0.027062 -1.627516
H -5.092743 0.503931 -1.874990
C -3.171593 0.537524 -0.812069
C -3.158289 1.840207 -0.077039
C -1.752662 2.263940 0.218474
C -0.814148 2.357526 -0.826708
H -1.145924 2.182935 -1.845475
C 0.526869 2.624820 -0.574790
C 0.940455 2.812939 0.752655
H 1.992122 2.984147 0.956472
C 0.026012 2.750292 1.787859
H 0.353862 2.892341 2.810058
C -1.315392 2.463423 1.522041
H -2.017198 2.365291 2.343375
C 1.553440 2.579346 -1.660082
N 2.146232 0.355455 -0.662389
N -2.112677 -0.338692 -0.716507
U -0.008306 0.012020 0.525272
H 2.112294 3.523245 -1.683607
H 1.045406 2.491730 -2.629187
H 3.714595 -1.787264 0.915761
H 3.697517 -2.590279 -0.647723
H -0.970014 -2.439676 -2.684817
H -2.054094 -3.493113 -1.784746
H -3.656447 2.605008 -0.686331
H -3.716317 1.784685 0.867036
C -0.159384 -0.085488 3.038191
H -1.113478 -0.612912 3.226779
H 0.614893 -0.690121 3.532383
H -0.222219 0.845911 3.611830

$LU^{III}N(SiH_3)_2$. SCF energy = -2149.29793

C 3.105900 -1.066357 0.899493
C 4.083115 -1.997131 0.639283
H 5.007671 -2.121957 1.186657
C 3.649057 -2.735320 -0.483012
H 4.161436 -3.557042 -0.964604
C 2.424143 -2.222603 -0.837043
C 3.109517 -0.012964 1.961704
C 1.715853 0.395168 2.325887
C 0.752216 -0.587529 2.606574
H 1.059220 -1.628882 2.625120
C -0.583322 -0.261294 2.804870
C -0.964451 1.087719 2.740557
H -2.011750 1.346663 2.857100
C -0.016252 2.070913 2.528861
H -0.314174 3.112499 2.483904
C 1.316468 1.724923 2.308094
H 2.044599 2.499010 2.088407
C -1.622411 -1.322991 2.970030
C -2.542861 -1.358522 1.790928
C -3.813234 -1.882274 1.737976
H -4.366117 -2.301502 2.567662
C -4.230545 -1.788776 0.393258
H -5.177391 -2.106586 -0.021954

C -3.197778 -1.199077 -0.296319
C -3.149681 -0.845595 -1.749309
C -1.734286 -0.731438 -2.220472
C -0.832802 -1.786091 -1.994604
H -1.201156 -2.700993 -1.541328
C 0.520089 -1.658238 -2.285716
C 0.983525 -0.450549 -2.831684
H 2.044810 -0.331345 -3.023056
C 0.100125 0.578557 -3.105837
H 0.461807 1.509262 -3.527690
C -1.252481 0.442442 -2.789505
H -1.932801 1.269074 -2.965700
C 1.500768 -2.719584 -1.905791
N 2.067572 -1.183899 -0.000648
N -2.142360 -0.920325 0.545885
U -0.006206 0.156115 -0.081969
H 2.086449 -3.017835 -2.784033
H 0.950808 -3.611177 -1.577799
H 3.666209 0.879751 1.647065
H 3.625565 -0.403110 2.848345
H -1.121331 -2.289255 3.114677
H -2.205831 -1.134342 3.879212
H -3.671968 -1.619503 -2.326213
H -3.667890 0.099997 -1.956562
N 0.131165 2.449014 -0.617945
Si -1.376992 3.243557 -0.639515
H -1.515173 4.347965 0.366951
H -1.764032 3.818156 -1.972216
H -2.411447 2.200613 -0.293630
Si 1.660285 3.116009 -0.977689
H 1.784619 3.635753 -2.381283
H 2.073742 4.234336 -0.064638
H 2.680300 2.020103 -0.822787

LU^{III}OPh. SCF energy = -1818.83801

C 2.831556 1.536622 1.499048
C 3.960861 1.356253 2.262922
H 4.700861 2.109202 2.498643
C 3.962977 0.002608 2.662208
H 4.693981 -0.494719 3.285375
C 2.827906 -0.563231 2.130633
C 2.389359 2.790902 0.809733
C 0.924588 2.751523 0.508252
C 0.000000 2.537992 1.542860
H 0.364655 2.466292 2.563022
C -1.350698 2.341010 1.281718
C -1.796466 2.402587 -0.049432
H -2.846155 2.227582 -0.260956
C -0.905133 2.650086 -1.075151
H -1.248996 2.672987 -2.103186
C 0.456989 2.800493 -0.799850
H 1.158371 2.934751 -1.616506
C -2.308370 1.949150 2.360271
C -2.827906 0.563231 2.130633
C -3.962977 -0.002608 2.662208
H -4.693981 0.494719 3.285375
C -3.960861 -1.356253 2.262922
H -4.700861 -2.109202 2.498643
C -2.831556 -1.536622 1.499048
C -2.389359 -2.790902 0.809733
C -0.924588 -2.751523 0.508252
C 0.000000 -2.537992 1.542860
H -0.364655 -2.466292 2.563022
C 1.350698 -2.341010 1.281718
C 1.796466 -2.402587 -0.049432
H 2.846155 -2.227582 -0.260956
C 0.905133 -2.650086 -1.075151
H 1.248996 -2.672987 -2.103186
C -0.456989 -2.800493 -0.799850
H -1.158371 -2.934751 -1.616506
C 2.308370 -1.949150 2.360271
N 2.115134 0.363343 1.398191
N -2.115134 -0.363343 1.398191
U 0.000000 0.000000 0.143507
H 3.149027 -2.653556 2.386684
H 1.801928 -2.029108 3.331020
H 2.937442 2.954749 -0.127409
H 2.611829 3.651708 1.453001
H -1.801928 2.029108 3.331020
H -3.149027 2.653556 2.386684
H -2.611829 -3.651708 1.453001
H -2.937442 -2.954749 -0.127409
O 0.000000 0.000000 -2.015173
C 0.000000 0.000000 -3.342606
C -1.197164 -0.120167 -4.055955
C 1.197164 0.120167 -4.055955
C -1.190415 -0.119389 -5.441020
H -2.126239 -0.214854 -3.502005
C 1.190415 0.119389 -5.441020
H 2.126239 0.214854 -3.502005
C 0.000000 0.000000 -6.144353
H -2.129679 -0.213883 -5.977823
H 2.129679 0.213883 -5.977823
H 0.000000 0.000000 -7.228780

[LTh^{IV}X']$^{+}$ complexes.

[LTh^{IV}NH$_2$]$^{+}$ SCF energy = -1498.69114

C 3.163681 -0.464352 -0.753454
C 4.143942 0.089513 -1.530857
H 5.106400 -0.350121 -1.751828
C 3.659206 1.340283 -1.975999
H 4.171025 2.045479 -2.615572
C 2.399535 1.485029 -1.461962
C 3.206958 -1.769018 -0.019428
C 1.824752 -2.277364 0.239525
C 0.912154 -2.381284 -0.824646
H 1.260359 -2.171934 -1.831952
C -0.430397 -2.676404 -0.609619
C -0.865064 -2.911680 0.705165
H -1.915096 -3.118013 0.885462
C 0.033908 -2.872968 1.756694
H -0.310251 -3.077319 2.764892
C 1.370430 -2.532958 1.530011
H 2.060531 -2.454291 2.363534

C -1.432453 -2.600615 -1.714725
C -2.399411 -1.485183 -1.462021
C -3.659207 -1.340647 -1.975802
H -4.171052 -2.045938 -2.615248
C -4.143953 -0.089847 -1.530756
H -5.106460 0.349706 -1.751677
C -3.163592 0.464238 -0.753625
C -3.206923 1.769107 -0.019932
C -1.824775 2.277532 0.239155
C -0.911982 2.381309 -0.824856
H -1.260003 2.171880 -1.832207
C 0.430538 2.676418 -0.609609
C 0.864984 2.911809 0.705222
H 1.914986 3.118148 0.885685
C -0.034202 2.873331 1.756585
H 0.309751 3.077856 2.764823
C -1.370698 2.533373 1.529680
H -2.060987 2.454873 2.363067
C 1.432727 2.600604 -1.714600
N 2.061064 0.379377 -0.687805
N -2.061024 -0.379547 -0.687801
Th 0.000007 -0.000009 0.533448
H 1.983044 3.546130 -1.781998
H 0.908569 2.473277 -2.669766
H 3.742706 -1.683919 0.934099
H 3.760471 -2.499508 -0.621950
H -0.908229 -2.473163 -2.669842
H -1.982645 -3.546203 -1.782228
H -3.760349 2.499447 -0.622717
H -3.742818 1.684239 0.933530
N -0.000186 -0.000128 2.774110
H 0.135972 -0.797261 3.386346
H -0.136489 0.798148 3.384878

LTh^{IV}OH. SCF energy = -1518.58942

C -3.160738 0.446275 -0.752180
C -4.142015 -0.122428 -1.516199
H -5.109843 0.307944 -1.731921
C -3.650440 -1.371960 -1.956539
H -4.161050 -2.086275 -2.586889
C -2.385601 -1.502635 -1.453610
C -3.217736 1.758667 -0.032895
C -1.841857 2.279236 0.229489
C -0.928042 2.389673 -0.834629
H -1.272607 2.180442 -1.843030
C 0.409656 2.688698 -0.612848
C 0.839499 2.922988 0.706051
H 1.888864 3.131652 0.888497
C -0.061847 2.883919 1.754205
H 0.275433 3.074087 2.766773
C -1.395429 2.540165 1.519986
H -2.085164 2.451424 2.352706
C 1.416676 2.614084 -1.712444
C 2.385606 1.502655 -1.453604
C 3.650298 1.371762 -1.956889
H 4.160793 2.085897 -2.587537
C 4.141869 0.122257 -1.516499
H 5.109567 -0.308265 -1.732490
C 3.160714 -0.446237 -0.752128
C 3.217750 -1.758486 -0.032611
C 1.841885 -2.279254 0.229512
C 0.928153 -2.389561 -0.834700
H 1.272793 -2.180157 -1.843041
C -0.409539 -2.688619 -0.613064
C -0.839508 -2.923105 0.705783
H -1.888901 -3.131784 0.888057
C 0.061744 -2.884222 1.754007
H -0.275538 -3.074567 2.766539
C 1.395367 -2.540424 1.519919
H 2.085004 -2.451767 2.352727
C -1.416536 -2.613900 -1.712695
N -2.047893 -0.387892 -0.688403
N 2.048063 0.388084 -0.688100
Th -0.000027 0.000040 0.550357
H -1.965553 -3.560063 -1.780868
H -0.897277 -2.481794 -2.669860
H -3.760590 1.680864 0.917223
H -3.772399 2.477335 -0.648401
H 0.897413 2.482311 -2.669661
H 1.965778 3.560218 -1.780384
H 3.772700 -2.477185 -0.647823
H 3.760324 -1.680476 0.917654
O 0.000262 -0.000194 2.640223
H -0.000144 -0.000516 3.600815

LTh^{IV}F. SCF energy = -1542.62451

C 3.146656 -0.510984 -0.763642
C 4.140246 0.044927 -1.519973
H 5.097498 -0.405191 -1.742218
C 3.681423 1.314472 -1.938744
H 4.212507 2.026389 -2.554675
C 2.422036 1.472255 -1.431639
C 3.179133 -1.827591 -0.049277
C 1.794890 -2.305163 0.246009
C 0.867237 -2.427292 -0.804263
H 1.205776 -2.259514 -1.822676
C -0.475868 -2.688195 -0.560774
C -0.897141 -2.868331 0.769521
H -1.948925 -3.046876 0.969705
C 0.015014 -2.809035 1.809177
H -0.316551 -2.942610 2.832688
C 1.354295 -2.505974 1.550477
H 2.050800 -2.398851 2.375601
C -1.489280 -2.622151 -1.655696
C -2.422074 -1.472308 -1.431556
C -3.681349 -1.314404 -1.938897
H -4.212386 -2.026266 -2.554931
C -4.140135 -0.044825 -1.520184
H -5.097313 0.405376 -1.742585
C -3.146634 0.510992 -0.763670
C -3.179138 1.827553 -0.049237
C -1.794895 2.305208 0.245933
C -0.867314 2.427329 -0.804405
H -1.205921 2.259526 -1.822793
C 0.475816 2.688185 -0.561001
C 0.897184 2.868294 0.769265
H 1.948995 3.046761 0.969381
C -0.014903 2.809030 1.808980

H 0.316738 2.942571 2.832471
C -1.354213 2.506027 1.550367
H -2.050656 2.398886 2.375541
C 1.489176 2.622003 -1.655964
N 2.054673 0.351837 -0.686296
N -2.054744 -0.351939 -0.686131
Th -0.000003 0.000008 0.515840
H 2.067687 3.552491 -1.684675
H 0.973780 2.542366 -2.620907
H 3.747055 -1.766219 0.886956
H 3.695464 -2.562714 -0.678437
H -0.973930 -2.542706 -2.620678
H -2.067830 -3.552622 -1.684217
H -3.695609 2.562672 -0.678288
H -3.746941 1.766077 0.887063
F -0.000053 0.000035 2.606026

$LTh^{III}X'$ complexes.

$LTh^{III}NH_2$. SCF energy = -1498.84839

C 3.148857 -0.542490 -0.818645
C 4.170890 -0.015884 -1.570520
H 5.111945 -0.498916 -1.795932
C 3.753980 1.272104 -1.974991
H 4.302381 1.976207 -2.586440
C 2.493392 1.455974 -1.461493
C 3.083874 -1.863000 -0.117007
C 1.667789 -2.244799 0.175158
C 0.725363 -2.398816 -0.895152
H 1.071496 -2.272657 -1.916899
C -0.616338 -2.579251 -0.648337
C -1.071637 -2.665945 0.706154
H -2.128773 -2.781778 0.907147
C -0.111343 -2.787502 1.743197
H -0.444295 -2.991062 2.755300
C 1.223245 -2.572976 1.488408
H 1.944532 -2.597405 2.299842
C -1.633350 -2.488351 -1.740048
C -2.519463 -1.300034 -1.520288
C -3.768520 -1.060429 -2.039931
H -4.327052 -1.720817 -2.689146
C -4.160214 0.215760 -1.578350
H -5.087197 0.731980 -1.788893
C -3.136101 0.679490 -0.788008
C -3.095662 1.954619 -0.005286
C -1.689028 2.388989 0.263546
C -0.764413 2.434176 -0.790111
H -1.108274 2.208047 -1.794823
C 0.578825 2.709740 -0.571642
C 1.009160 2.960986 0.737632
H 2.063496 3.138973 0.922113
C 0.104083 2.958771 1.781498
H 0.447707 3.156294 2.790974
C -1.239433 2.659975 1.549177
H -1.939277 2.617500 2.377421
C 1.574963 2.616089 -1.681242
N 2.098404 0.349378 -0.735420
N -2.106943 -0.237374 -0.740539
Th 0.025252 -0.151566 0.567111
H 2.163429 3.539885 -1.733292
H 1.037300 2.530910 -2.634889
H 3.643542 -1.834429 0.828176
H 3.578115 -2.625394 -0.736474
H -1.117856 -2.430902 -2.707201
H -2.246908 -3.398113 -1.759127
H -3.619954 2.736602 -0.569602
H -3.623919 1.860308 0.953118
N -0.028172 0.086330 2.832937
H -0.272443 0.875607 3.421033
H 0.162795 -0.691440 3.456434

$LTh^{III}OH$. SCF energy = -1518.74566

C -3.146313 0.697783 -0.730279
C -4.266089 0.111845 -1.266327
H -5.240193 0.571031 -1.366166
C -3.891967 -1.190884 -1.662230
H -4.516501 -1.934747 -2.138773
C -2.560355 -1.334352 -1.358287
C -3.009548 2.088345 -0.178111
C -1.601838 2.412241 0.208730
C -0.600467 2.630394 -0.787222
H -0.892666 2.606428 -1.833668
C 0.733092 2.729788 -0.460754
C 1.114708 2.705040 0.926298
H 2.161405 2.782450 1.191146
C 0.106050 2.743373 1.917403
H 0.384118 2.832605 2.962428
C -1.218416 2.576539 1.576821
H -1.978795 2.537322 2.350791
C 1.804602 2.674900 -1.502762
C 2.596360 1.405868 -1.371637
C 3.812804 1.093865 -1.926231
H 4.414546 1.738984 -2.551526
C 4.108999 -0.230184 -1.530286
H 4.992999 -0.802741 -1.777393
C 3.068033 -0.655755 -0.739884
C 2.992006 -1.939788 0.021454
C 1.620588 -2.544687 0.151690
C 0.636092 -2.311994 -0.813465
H 0.900802 -1.742189 -1.702200
C -0.657095 -2.822695 -0.688265
C -0.955658 -3.612634 0.418716
H -1.959069 -4.009774 0.536718
C 0.025363 -3.897935 1.355063
H -0.210123 -4.532442 2.203823
C 1.296589 -3.359067 1.232395
H 2.048170 -3.562166 1.989564
C -1.685731 -2.490512 -1.726775
N -2.076285 -0.182219 -0.765580
N 2.115427 0.337549 -0.637352
Th -0.036003 0.247290 0.540251
H -2.328138 -3.359146 -1.902050
H -1.165310 -2.289738 -2.674366
H -3.658556 2.217627 0.697552

H -3.369486 2.809611 -0.925683
H 1.343238 2.755266 -2.495064
H 2.478918 3.534708 -1.396109
H 3.652494 -2.663773 -0.473408
H 3.400328 -1.818291 1.035757
O 0.061252 -0.612397 2.465579
H 0.087267 -0.992249 3.345597

$LTh^{III}F$. SCF energy = -1542.78658

C 3.149838 -0.606583 -0.785944
C 4.197484 -0.088164 -1.505656
H 5.135615 -0.584426 -1.713519
C 3.812566 1.211588 -1.904227
H 4.388243 1.913358 -2.492768
C 2.544336 1.413082 -1.419652
C 3.056663 -1.933005 -0.097691
C 1.636056 -2.282189 0.210175
C 0.690105 -2.455448 -0.842592
H 1.032234 -2.368527 -1.870353
C -0.655652 -2.591796 -0.587492
C -1.106372 -2.638813 0.777913
H -2.163740 -2.741995 0.985686
C -0.146562 -2.728758 1.810806
H -0.475155 -2.860235 2.835945
C 1.189044 -2.530446 1.546069
H 1.908087 -2.517988 2.359143
C -1.673305 -2.513817 -1.678559
C -2.527471 -1.296548 -1.498284
C -3.770244 -1.040828 -2.021654
H -4.345590 -1.705033 -2.651854
C -4.132226 0.255028 -1.591312
H -5.047843 0.786203 -1.813742
C -3.099680 0.717116 -0.812720
C -3.047950 2.006858 -0.053481
C -1.641917 2.425746 0.241237
C -0.697178 2.456787 -0.797006
H -1.025848 2.238396 -1.808795
C 0.644737 2.708180 -0.552038
C 1.053168 2.952121 0.767884
H 2.107034 3.112612 0.972081
C 0.127663 2.971835 1.793308
H 0.449657 3.148167 2.813391
C -1.214911 2.697024 1.533339
H -1.923438 2.650998 2.353200
C 1.658239 2.596503 -1.644318
N 2.110585 0.303638 -0.716394
N -2.088851 -0.222704 -0.744773
Th 0.017618 -0.150767 0.549461
H 2.271341 3.504705 -1.680623
H 1.135252 2.531232 -2.607688
H 3.630067 -1.928733 0.839327
H 3.521930 -2.702355 -0.729961
H -1.159715 -2.504038 -2.648401
H -2.311175 -3.406989 -1.665350
H -3.547388 2.785908 -0.643739
H -3.599404 1.938044 0.893587
F -0.221830 0.164479 2.635831

$LU^{III}X'$ complexes.

$LU^{III}NH_2$. SCF energy = -1568.09841

C 3.187865 -0.530106 -0.797174
C 4.175105 -0.015073 -1.605100
H 5.113821 -0.491674 -1.853910
C 3.724218 1.254693 -2.028147
H 4.237558 1.946251 -2.682584
C 2.482027 1.435299 -1.464470
C 3.172762 -1.834558 -0.064078
C 1.767251 -2.266103 0.221953
C 0.832943 -2.347528 -0.824059
H 1.168108 -2.154611 -1.838611
C -0.511438 -2.620195 -0.582987
C -0.929181 -2.827086 0.738441
H -1.981093 -3.000578 0.938496
C -0.015070 -2.785247 1.776928
H -0.351470 -2.947531 2.794226
C 1.326331 -2.492498 1.521987
H 2.032024 -2.417993 2.342701
C -1.529303 -2.572019 -1.678005
C -2.481948 -1.435302 -1.464601
C -3.724462 -1.255007 -2.027661
H -4.237857 -1.946627 -2.681986
C -4.175376 0.014737 -1.604562
H -5.114206 0.491240 -1.853130
C -3.187935 0.529904 -0.796945
C -3.172762 1.834711 -0.064380
C -1.767211 2.266010 0.221874
C -0.832836 2.347526 -0.824075
H -1.167896 2.154793 -1.838690
C 0.511543 2.620194 -0.582931
C 0.929241 2.826984 0.738502
H 1.981131 3.000473 0.938675
C 0.015065 2.785005 1.776925
H 0.351429 2.947211 2.794257
C -1.326304 2.492246 1.521937
H -2.032001 2.417608 2.342636
C 1.529276 2.571882 -1.678072
N 2.133798 0.347991 -0.694289
N -2.133658 -0.347899 -0.694561
U -0.000043 0.000107 0.538159
H 2.085766 3.516903 -1.709184
H 1.010744 2.483198 -2.641686
H 3.723216 -1.776636 0.884457
H 3.678631 -2.597142 -0.670009
H -1.010977 -2.483814 -2.641765
H -2.085873 -3.517022 -1.708569
H -3.678186 2.597135 -0.670877
H -3.723563 1.777378 0.883973
N 0.000560 0.000011 2.807663
H -0.259468 0.765125 3.420706
H 0.260421 -0.765099 3.420741

$LU^{III}OH$. SCF energy = -1587.99144

C 3.189021 -0.539061 -0.778200

C 4.202452 0.002338 -1.534008
H 5.156628 -0.458546 -1.751424
C 3.750563 1.270906 -1.956690
H 4.279448 1.979323 -2.580090
C 2.481608 1.425924 -1.447538
C 3.168089 -1.862630 -0.077821
C 1.764402 -2.276650 0.234207
C 0.820527 -2.409478 -0.800518
H 1.145420 -2.268658 -1.826554
C -0.521953 -2.657004 -0.531250
C -0.927354 -2.799662 0.805704
H -1.978538 -2.957826 1.021916
C -0.005238 -2.704169 1.834649
H -0.329748 -2.808494 2.863445
C 1.334440 -2.426971 1.550747
H 2.046817 -2.308401 2.360338
C -1.556348 -2.633905 -1.610362
C -2.490231 -1.476617 -1.419376
C -3.726438 -1.289311 -1.991628
H -4.246779 -1.985716 -2.635267
C -4.158599 -0.004329 -1.596239
H -5.089755 0.480990 -1.856570
C -3.168115 0.514827 -0.795099
C -3.166966 1.832338 -0.084661
C -1.777182 2.332436 0.172365
C -0.830826 2.339837 -0.864035
H -1.144098 2.038398 -1.859501
C 0.500280 2.667746 -0.633346
C 0.887729 3.027490 0.664763
H 1.931282 3.252474 0.860360
C -0.045588 3.084245 1.681934
H 0.262748 3.352204 2.685914
C -1.368243 2.721417 1.441337
H -2.079647 2.702007 2.259972
C 1.526217 2.546993 -1.716178
N 2.116946 0.323506 -0.705632
N -2.126430 -0.377058 -0.670511
U 0.013531 -0.063221 0.547471
H 2.087435 3.485090 -1.802399
H 1.010387 2.403504 -2.675134
H 3.745120 -1.839147 0.856167
H 3.643349 -2.618681 -0.715931
H -1.052643 -2.584135 -2.584350
H -2.126252 -3.571673 -1.600058
H -3.715487 2.562176 -0.694113
H -3.697860 1.774424 0.875184
O -0.045351 0.195748 2.652412
H 0.043001 -0.124380 3.551973

LU^{III}F. SCF energy = -1611.98194

C -1.143953 3.007828 -0.809190
C -2.104775 3.599435 -1.594994
H -2.166365 4.648921 -1.849686
C -2.994215 2.573994 -1.983302
H -3.869587 2.670947 -2.611194
C -2.519198 1.410995 -1.423954
C 0.000000 3.666335 -0.101843
C 1.076299 2.677494 0.222186
C 1.652382 1.908208 -0.803043
H 1.348598 2.093665 -1.829079
C 2.556312 0.887139 -0.527278
C 2.904309 0.639079 0.809615
H 3.579680 -0.179656 1.035074
C 2.376804 1.414507 1.827713
H 2.628275 1.201752 2.859757
C 1.455427 2.420184 1.535691
H 0.999245 2.982127 2.343732
C 3.053497 -0.022617 -1.605624
C 2.519198 -1.410995 -1.423954
C 2.994215 -2.573994 -1.983302
H 3.869587 -2.670947 -2.611194
C 2.104775 -3.599435 -1.594994
H 2.166365 -4.648921 -1.849686
C 1.143953 -3.007828 -0.809190
C 0.000000 -3.666335 -0.101843
C -1.076299 -2.677494 0.222186
C -1.652382 -1.908208 -0.803043
H -1.348598 -2.093665 -1.829079
C -2.556312 -0.887139 -0.527278
C -2.904309 -0.639079 0.809615
H -3.579680 0.179656 1.035074
C -2.376804 -1.414507 1.827713
H -2.628275 -1.201752 2.859757
C -1.455427 -2.420184 1.535691
H -0.999245 -2.982127 2.343732
C -3.053497 0.022617 -1.605624
N -1.377874 1.654980 -0.688899
N 1.377874 -1.654980 -0.688899
U 0.000000 0.000000 0.516464
H -4.150095 0.049460 -1.591904
H -2.763967 -0.391779 -2.580119
H -0.324789 4.150453 0.828592
H 0.408659 4.461784 -0.737995
H 2.763967 0.391779 -2.580119
H 4.150095 -0.049460 -1.591904
H -0.408659 -4.461784 -0.737995
H 0.324789 -4.150453 0.828592
F 0.000000 0.000000 2.649317

[LTh^{IV}X*]$^{+}$ complexes.

[LTh^{IV}SiH$_3$]$^{+}$. SCF energy = -1733.90618

C 3.200034 -0.505033 -0.765277
C 4.212343 0.046659 -1.498987
H 5.170700 -0.409054 -1.704050
C 3.768284 1.318922 -1.927030
H 4.317185 2.029282 -2.528958
C 2.498400 1.482351 -1.448723
C 3.186328 -1.831000 -0.071597
C 1.780273 -2.289915 0.141689
C 0.904089 -2.374860 -0.957931
H 1.296399 -2.193447 -1.954398
C -0.452684 -2.628888 -0.788068
C -0.943354 -2.827284 0.514727
H -2.005639 -2.995901 0.658914
C -0.087628 -2.785694 1.602933

H -0.469359 -2.956347 2.603476
C 1.270347 -2.500195 1.417630
H 1.923375 -2.423125 2.280484
C -1.413461 -2.527675 -1.927026
C -2.354816 -1.385779 -1.698388
C -3.588264 -1.191196 -2.253664
H -4.095573 -1.866290 -2.928252
C -4.060819 0.057757 -1.788007
H -5.003906 0.526252 -2.031433
C -3.102237 0.564548 -0.956539
C -3.140348 1.843619 -0.180601
C -1.753332 2.292295 0.149504
C -0.808488 2.435188 -0.886070
H -1.135294 2.304869 -1.913640
C 0.533086 2.678550 -0.615598
C 0.937119 2.815146 0.724854
H 1.987082 2.981095 0.943491
C 0.014101 2.721033 1.751282
H 0.327330 2.838070 2.781592
C -1.327125 2.436667 1.465189
H -2.035673 2.317140 2.278797
C 1.569072 2.631686 -1.689504
N 2.112040 0.364992 -0.709477
N -2.020319 -0.311058 -0.875612
Th 0.000276 -0.003687 0.358821
H 2.142949 3.565666 -1.693824
H 1.077997 2.558651 -2.667374
H 3.704672 -1.792915 0.894103
H 3.724908 -2.562792 -0.685510
H -0.855982 -2.412979 -2.864466
H -1.987403 -3.457588 -2.013272
H -3.644657 2.612013 -0.778746
H -3.717550 1.741112 0.746292
Si -0.349207 -0.178307 3.397729
H -1.728325 -0.771632 3.562529
H 0.559725 -1.118854 4.137141
H -0.376459 1.075949 4.221820

[LTh^{IV}PH$_2$]$^+$. SCF energy = -1785.18430

C 3.098842 -0.515489 -0.951756
C 4.046893 0.004676 -1.787466
H 4.996537 -0.449257 -2.033104
C 3.552894 1.245358 -2.253317
H 4.045793 1.926927 -2.932034
C 2.318326 1.419937 -1.693625
C 3.158753 -1.790337 -0.170698
C 1.778003 -2.274563 0.136538
C 0.842427 -2.400138 -0.907045
H 1.173946 -2.234320 -1.927910
C -0.499173 -2.669200 -0.653621
C -0.910509 -2.848526 0.677133
H -1.959826 -3.031526 0.884650
C 0.007173 -2.779649 1.712009
H -0.315105 -2.946446 2.732210
C 1.346715 -2.471262 1.444871
H 2.052787 -2.371335 2.262740
C -1.525906 -2.606994 -1.736700
C -2.474112 -1.478991 -1.471543
C -3.749444 -1.325910 -1.938006
H -4.290825 -2.030693 -2.553150
C -4.210862 -0.070402 -1.477567
H -5.178770 0.373195 -1.663659
C -3.201934 0.480598 -0.738714
C -3.204676 1.785824 -0.005741
C -1.805100 2.272534 0.192896
C -0.945240 2.368622 -0.916104
H -1.347480 2.173746 -1.906059
C 0.411098 2.639365 -0.766865
C 0.914974 2.856211 0.527334
H 1.976391 3.039713 0.658444
C 0.071392 2.819032 1.624425
H 0.469462 3.004353 2.615544
C -1.282816 2.503926 1.462204
H -1.928585 2.431484 2.330427
C 1.357206 2.545515 -1.918518
N 2.003917 0.340991 -0.869131
N -2.099996 -0.371547 -0.712171
Th -0.003714 0.001967 0.391163
H 1.915962 3.483143 -2.018839
H 0.788435 2.416473 -2.847366
H 3.715167 -1.668576 0.766553
H 3.694283 -2.546642 -0.757104
H -1.025737 -2.498790 -2.706751
H -2.085693 -3.548592 -1.773966
H -3.773627 2.522402 -0.585708
H -3.701584 1.706326 0.968824
P 0.499156 0.135449 3.214356
H 0.110168 -1.033099 3.915495
H -0.381780 1.025870 3.879126

[LTh^{IV}SH]$^+$. SCF energy = -1841.46361

C -3.153467 0.427456 -0.849104
C -4.129127 -0.144221 -1.615998
H -5.097003 0.283555 -1.836200
C -3.633973 -1.395192 -2.052786
H -4.143112 -2.111743 -2.681682
C -2.372456 -1.524676 -1.544764
C -3.204197 1.738568 -0.129055
C -1.822043 2.258657 0.102180
C -0.924513 2.336568 -0.977397
H -1.286501 2.106870 -1.975285
C 0.420668 2.635881 -0.785929
C 0.873452 2.898889 0.517521
H 1.926483 3.104690 0.680154
C -0.009425 2.883156 1.583744
H 0.345091 3.095030 2.585635
C -1.351345 2.540415 1.380957
H -2.023335 2.475204 2.229622
C 1.408813 2.528058 -1.900219
C 2.378124 1.424269 -1.613910
C 3.637808 1.264575 -2.118063
H 4.147185 1.946283 -2.784359
C 4.131657 0.037280 -1.617266
H 5.098299 -0.403327 -1.816650
C 3.157070 -0.490237 -0.818261
C 3.205869 -1.760132 -0.028236

C 1.822252 -2.265726 0.224572
C 0.929411 -2.399497 -0.854471
H 1.297157 -2.222216 -1.860845
C -0.415809 -2.687609 -0.654685
C -0.875783 -2.882437 0.659039
H -1.929198 -3.082716 0.825800
C 0.001906 -2.810910 1.725927
H -0.361261 -2.987524 2.731838
C 1.344741 -2.478859 1.513033
H 2.018828 -2.373936 2.356520
C -1.399521 -2.637623 -1.776452
N -2.039251 -0.406473 -0.780287
N 2.044720 0.348708 -0.790832
Th 0.000245 0.006329 0.416393
H -1.944298 -3.586694 -1.837605
H -0.863315 -2.519682 -2.725969
H -3.724518 1.656985 0.832924
H -3.773961 2.456067 -0.731778
H 0.875934 2.366102 -2.845100
H 1.956974 3.471239 -2.005362
H 3.776925 -2.509540 -0.589498
H 3.723131 -1.627182 0.929802
S -0.026996 0.267185 3.137012
H 0.231428 -0.957624 3.626025

$[LTh^{IV}Cl]^{+}$. SCF energy = -1902.89946

C 3.152542 -0.450872 -0.827912
C 4.128258 0.107979 -1.602759
H 5.098255 -0.321433 -1.810049
C 3.630797 1.347645 -2.067884
H 4.140065 2.052666 -2.709540
C 2.367512 1.484778 -1.568251
C 3.210722 -1.747145 -0.082665
C 1.831640 -2.266275 0.162599
C 0.934387 -2.374774 -0.916892
H 1.296441 -2.171856 -1.920429
C -0.407429 -2.670075 -0.715795
C -0.860543 -2.897381 0.596886
H -1.913547 -3.100827 0.763381
C 0.021779 -2.852400 1.660638
H -0.331617 -3.027318 2.669871
C 1.362582 -2.514908 1.446453
H 2.032681 -2.416936 2.293672
C -1.396846 -2.592405 -1.830316
C -2.367502 -1.484858 -1.568219
C -3.630785 -1.347726 -2.067858
H -4.140057 -2.052758 -2.709498
C -4.128241 -0.108049 -1.602760
H -5.098237 0.321363 -1.810060
C -3.152536 0.450799 -0.827898
C -3.210722 1.747073 -0.082656
C -1.831641 2.266227 0.162573
C -0.934382 2.374615 -0.916923
H -1.296427 2.171580 -1.920441
C 0.407421 2.669995 -0.715856
C 0.860517 2.897486 0.596800
H 1.913508 3.101023 0.763275
C -0.021813 2.852608 1.660553
H 0.331564 3.027693 2.669764
C -1.362600 2.515027 1.446402
H -2.032708 2.417161 2.293626
C 1.396834 2.592295 -1.830383
N 2.033239 0.381223 -0.779929
N -2.033221 -0.381280 -0.779928
Th 0.000005 0.000001 0.427689
H 1.943861 3.538438 -1.912074
H 0.865900 2.451590 -2.779727
H 3.735120 -1.645599 0.875202
H 3.780661 -2.473681 -0.674268
H -0.865919 -2.451763 -2.779672
H -1.943894 -3.538541 -1.911950
H -3.780678 2.473590 -0.674266
H -3.735107 1.645542 0.875221
Cl -0.000009 0.000140 3.046333

$LTh^{III}X^{*}$ complexes.

$LTh^{III}SiH_3$. SCF energy = -1734.07782

C 3.244916 -0.701113 -0.751690
C 4.275878 -0.232293 -1.526315
H 5.205355 -0.746253 -1.731156
C 3.887310 1.046286 -1.988617
H 4.454296 1.708092 -2.628878
C 2.633297 1.286063 -1.484255
C 3.159399 -1.989142 0.003358
C 1.731967 -2.347941 0.270754
C 0.828993 -2.481525 -0.799686
H 1.202925 -2.382185 -1.814618
C -0.526641 -2.694363 -0.583565
C -0.991988 -2.785421 0.737617
H -2.054702 -2.913119 0.914591
C -0.113971 -2.677736 1.799682
H -0.478784 -2.749487 2.817870
C 1.244482 -2.444801 1.565918
H 1.917031 -2.315185 2.407005
C -1.511319 -2.692336 -1.708974
C -2.446504 -1.530803 -1.576480
C -3.689885 -1.371300 -2.135655
H -4.219933 -2.100706 -2.732854
C -4.118871 -0.066274 -1.803247
H -5.054785 0.401506 -2.076518
C -3.120078 0.501250 -1.051008
C -3.102560 1.857763 -0.410160
C -1.707517 2.271115 -0.041167
C -0.730268 2.348921 -1.027701
H -1.016306 2.200898 -2.065084
C 0.645485 2.523785 -0.699365
C 0.968256 2.803176 0.656426
H 2.000052 3.021420 0.914853
C 0.015677 2.725810 1.641943
H 0.278006 2.923138 2.673008
C -1.334904 2.373087 1.314422
H -2.083994 2.313205 2.093519
C 1.725614 2.452068 -1.732223
N 2.216653 0.220814 -0.707527

N -2.074163 -0.389087 -0.893617
Th -0.008338 0.145382 0.334144
H 2.314611 3.378985 -1.740304
H 1.262867 2.378882 -2.725526
H 3.696435 -1.938991 0.959408
H 3.636774 -2.785650 -0.580984
H -0.966602 -2.666972 -2.661786
H -2.085577 -3.626713 -1.700136
H -3.538085 2.590366 -1.100205
H -3.724079 1.872279 0.493829
Si -0.375551 0.044399 3.381389
H -1.650414 -0.711926 3.699737
H 0.649731 -0.736229 4.178250
H -0.534749 1.310983 4.181506

LTh^{III}PH$_2$. SCF energy = -1785.35234

C 3.109071 -0.594954 -0.969465
C 4.117631 -0.101458 -1.758701
H 5.044149 -0.604849 -1.998584
C 3.713351 1.187200 -2.176812
H 4.260243 1.870184 -2.812771
C 2.473027 1.406276 -1.632423
C 3.040253 -1.890382 -0.225422
C 1.620122 -2.246443 0.083504
C 0.679031 -2.410543 -0.973561
H 1.025357 -2.310642 -1.998593
C -0.667195 -2.561180 -0.723939
C -1.117524 -2.626137 0.636347
H -2.175572 -2.725709 0.842216
C -0.166681 -2.712403 1.670603
H -0.498499 -2.887121 2.686496
C 1.174639 -2.501987 1.414764
H 1.891369 -2.503071 2.229082
C -1.684804 -2.475442 -1.813986
C -2.554059 -1.275895 -1.597396
C -3.811848 -1.029167 -2.087576
H -4.391103 -1.689791 -2.717930
C -4.184978 0.251544 -1.621652
H -5.113507 0.772295 -1.812475
C -3.141916 0.713084 -0.857954
C -3.074927 1.989165 -0.078508
C -1.655546 2.376158 0.186578
C -0.751615 2.445662 -0.886029
H -1.124475 2.283489 -1.892760
C 0.603558 2.664730 -0.684583
C 1.070646 2.824305 0.628988
H 2.134167 2.953766 0.799827
C 0.189910 2.790389 1.694386
H 0.560239 2.916209 2.705120
C -1.171872 2.553850 1.475619
H -1.849915 2.488768 2.318769
C 1.576884 2.589715 -1.814939
N 2.076512 0.318413 -0.876753
N -2.114908 -0.211674 -0.831150
Th 0.019298 -0.126831 0.420345
H 2.181088 3.504294 -1.849123
H 1.023503 2.541051 -2.761721
H 3.603122 -1.832945 0.715931
H 3.522515 -2.678755 -0.819850
H -1.172294 -2.433746 -2.783499
H -2.309143 -3.377947 -1.822220
H -3.576348 2.784374 -0.644711
H -3.605854 1.907389 0.878850
P 0.238020 0.099748 3.301746
H -0.577364 1.040522 3.991545
H -0.200965 -1.042912 4.017389

LTh^{III}SH. SCF energy = -1841.62692

C -3.253336 0.451954 -0.752952
C -4.313425 -0.148953 -1.385226
H -5.286787 0.290993 -1.554222
C -3.881885 -1.439014 -1.766669
H -4.447840 -2.185370 -2.307495
C -2.578312 -1.554429 -1.353606
C -3.206738 1.822704 -0.146253
C -1.792111 2.261764 0.079937
C -0.914109 2.342215 -0.988439
H -1.291635 2.166887 -1.992072
C 0.486276 2.497478 -0.791990
C 0.928879 2.834817 0.526487
H 1.975343 3.075717 0.684983
C 0.060211 2.796154 1.587335
H 0.413988 3.019169 2.586547
C -1.297269 2.400218 1.399322
H -1.963891 2.322956 2.247746
C 1.467163 2.421377 -1.918665
C 2.414095 1.279744 -1.719355
C 3.629903 1.042811 -2.308048
H 4.136636 1.691085 -3.009568
C 4.072809 -0.215201 -1.834851
H 4.994102 -0.721231 -2.090447
C 3.112287 -0.674595 -0.970231
C 3.117595 -1.931826 -0.161193
C 1.723500 -2.366318 0.170732
C 0.756550 -2.454313 -0.844816
H 1.058964 -2.270388 -1.871696
C -0.575050 -2.722809 -0.559332
C -0.949081 -2.934419 0.776311
H -1.993611 -3.116432 1.007627
C -0.001523 -2.898811 1.778599
H -0.296259 -3.078225 2.806895
C 1.328920 -2.592448 1.481316
H 2.055560 -2.504949 2.280538
C -1.628138 -2.677578 -1.617834
N -2.165524 -0.401722 -0.711337
N 2.073346 0.232424 -0.881635
Th -0.002539 0.166096 0.398285
H -2.181413 -3.624017 -1.635426
H -1.145890 -2.576642 -2.599216
H -3.743121 1.851089 0.810364
H -3.718154 2.529861 -0.810407
H 0.915938 2.310898 -2.862246
H 2.034131 3.358287 -2.006078
H 3.626525 -2.721486 -0.728379
H 3.678305 -1.809329 0.774526
S 0.599836 0.247130 3.121500
H 0.212200 -0.969676 3.545678

LTh^{III}Cl. SCF energy = -1903.06655

C 3.184761 -0.546239 -0.789621
C 4.229609 -0.025796 -1.509489
H 5.182646 -0.505129 -1.686460
C 3.818441 1.250363 -1.956909
H 4.385994 1.948062 -2.557835
C 2.538938 1.435150 -1.499237
C 3.105537 -1.851379 -0.065048
C 1.679432 -2.235818 0.163014
C 0.796339 -2.398791 -0.942991
H 1.190184 -2.276959 -1.948147
C -0.557387 -2.570110 -0.760906
C -1.074537 -2.660172 0.576237
H -2.139756 -2.779413 0.727341
C -0.170976 -2.764958 1.652728
H -0.549341 -2.931337 2.654233
C 1.173387 -2.532965 1.464033
H 1.846405 -2.523143 2.314942
C -1.521250 -2.485368 -1.898004
C -2.418018 -1.303292 -1.705907
C -3.653473 -1.067877 -2.252465
H -4.191710 -1.727931 -2.918611
C -4.066239 0.201669 -1.789055
H -4.991061 0.713174 -2.018840
C -3.069812 0.668448 -0.969284
C -3.064642 1.939440 -0.180029
C -1.668709 2.387270 0.116811
C -0.723270 2.427869 -0.921437
H -1.047707 2.203274 -1.932873
C 0.613232 2.697565 -0.675061
C 1.019473 2.945260 0.645627
H 2.071433 3.116684 0.850165
C 0.094580 2.950708 1.670261
H 0.412043 3.126942 2.691248
C -1.247122 2.661911 1.408263
H -1.953176 2.605853 2.228603
C 1.631247 2.592561 -1.761704
N 2.119997 0.338252 -0.765168
N -2.030996 -0.242922 -0.904286
Th 0.018491 -0.151861 0.460553
H 2.224254 3.513281 -1.812714
H 1.116120 2.494364 -2.726236
H 3.618262 -1.798076 0.904953
H 3.634352 -2.621683 -0.643625
H -0.963044 -2.420802 -2.840645
H -2.129431 -3.397395 -1.948587
H -3.589548 2.715009 -0.752194
H -3.609728 1.831042 0.766719
Cl -0.394212 0.083626 3.103883

LU^{III}X* complexes.

LU^{III}SiH$_3$. SCF energy = -1803.33184

C 3.214820 -0.555448 -0.818152
C 4.237437 -0.033629 -1.572891
H 5.176711 -0.519022 -1.800648
C 3.823190 1.255186 -1.975409
H 4.374365 1.958131 -2.585139
C 2.565401 1.443359 -1.454928
C 3.152454 -1.880911 -0.128850
C 1.728746 -2.277038 0.105028
C 0.834038 -2.334428 -0.981656
H 1.214745 -2.156805 -1.982720
C -0.521292 -2.573351 -0.791405
C -0.998295 -2.759501 0.516711
H -2.061507 -2.904362 0.675223
C -0.127388 -2.730402 1.593238
H -0.497263 -2.886673 2.600156
C 1.233070 -2.482434 1.385448
H 1.898217 -2.414824 2.239754
C -1.494981 -2.490175 -1.922479
C -2.421584 -1.332107 -1.717945
C -3.643643 -1.108692 -2.304468
H -4.154399 -1.771044 -2.990083
C -4.085716 0.153046 -1.847928
H -5.010225 0.652821 -2.103207
C -3.115399 0.624053 -0.997323
C -3.103590 1.897948 -0.214126
C -1.699747 2.278123 0.138208
C -0.737568 2.404750 -0.883277
H -1.052468 2.290227 -1.915866
C 0.601546 2.629049 -0.591230
C 0.990972 2.741907 0.754167
H 2.041040 2.882736 0.987173
C 0.054831 2.646379 1.767859
H 0.355937 2.734473 2.804049
C -1.287829 2.400574 1.459354
H -2.008105 2.283227 2.262719
C 1.649828 2.611120 -1.655792
N 2.168300 0.339167 -0.728129
N -2.074200 -0.276245 -0.899521
U -0.002974 -0.004922 0.380593
H 2.229148 3.542213 -1.624238
H 1.162970 2.576895 -2.638814
H 3.680720 -1.867725 0.833321
H 3.652136 -2.636943 -0.747516
H -0.941701 -2.402662 -2.866278
H -2.075421 -3.419033 -1.983301
H -3.566939 2.695606 -0.808349
H -3.692281 1.814984 0.708622
Si -0.333943 -0.193915 3.425363
H -1.717442 -0.772022 3.663900
H 0.540291 -1.148489 4.209756
H -0.354240 1.031201 4.312450

LU^{III}PH$_2$. SCF energy = -1853.89517

C 3.181152 -0.368317 -0.785828
C 4.157579 0.222805 -1.539361
H 5.142900 -0.178354 -1.730804
C 3.631648 1.446668 -2.009325
H 4.128260 2.169118 -2.641504
C 2.352369 1.538660 -1.534617
C 3.266287 -1.669933 -0.052411
C 1.902558 -2.241731 0.159365

C 1.017373 -2.338409 -0.929870
H 1.379587 -2.086284 -1.921730
C -0.315371 -2.680805 -0.750463
C -0.771398 -2.969783 0.548873
H -1.819506 -3.208517 0.698548
C 0.106323 -2.954342 1.617136
H -0.244390 -3.199508 2.613570
C 1.435885 -2.570795 1.426226
H 2.107823 -2.511170 2.276154
C -1.294523 -2.599128 -1.873308
C -2.300474 -1.527619 -1.597342
C -3.568148 -1.430891 -2.100200
H -4.051127 -2.148571 -2.748159
C -4.104200 -0.210140 -1.632723
H -5.085176 0.192441 -1.842528
C -3.145635 0.374869 -0.852720
C -3.247690 1.671677 -0.112920
C -1.889456 2.243468 0.132726
C -0.980063 2.346697 -0.936716
H -1.320739 2.099743 -1.937552
C 0.348182 2.688378 -0.726984
C 0.774177 2.972260 0.583663
H 1.818204 3.211998 0.757827
C -0.127617 2.952258 1.631793
H 0.200138 3.196688 2.636184
C -1.452043 2.567187 1.410796
H -2.140816 2.499697 2.246589
C 1.352583 2.611463 -1.827716
N 2.038430 0.425108 -0.758257
N -2.003924 -0.420866 -0.804061
U -0.001398 0.000238 0.484449
H 1.874403 3.570119 -1.926221
H 0.834794 2.435119 -2.778561
H 3.767218 -1.563263 0.917963
H 3.873691 -2.369615 -0.639549
H -0.755605 -2.418211 -2.811423
H -1.813796 -3.557410 -1.987708
H -3.842512 2.374339 -0.709243
H -3.770140 1.558112 0.845157
P -0.140545 -0.033393 2.751747
H -0.932864 -0.217400 3.159756
H 0.667862 0.153286 3.125552

$LU^{III}SH$. SCF energy = -1910.51130

C -3.145489 0.500939 -0.853828
C -4.134125 -0.053449 -1.619060
H -5.091269 0.395439 -1.844481
C -3.667679 -1.317814 -2.044014
H -4.190571 -2.026869 -2.670239
C -2.409431 -1.472266 -1.531051
C -3.183066 1.817106 -0.139071
C -1.800920 2.304293 0.152384
C -0.872218 2.421812 -0.897900
H -1.207829 2.241504 -1.915000
C 0.468106 2.692369 -0.653768
C 0.885248 2.889657 0.675343
H 1.935701 3.076504 0.874605
C -0.028069 2.837886 1.713277
H 0.298950 2.989402 2.736153
C -1.364946 2.523508 1.454777
H -2.062711 2.424009 2.279922
C 1.486952 2.621888 -1.743119
C 2.428485 1.482410 -1.502334
C 3.691129 1.330634 -2.005195
H 4.219404 2.042966 -2.623128
C 4.153908 0.064037 -1.582887
H 5.112978 -0.383679 -1.802377
C 3.158699 -0.494351 -0.829170
C 3.190120 -1.814266 -0.121058
C 1.805514 -2.302950 0.155855
C 0.885939 -2.414914 -0.903031
H 1.230335 -2.229258 -1.916225
C -0.456442 -2.686723 -0.671937
C -0.885066 -2.890999 0.652457
H -1.937200 -3.078870 0.841633
C 0.019233 -2.844717 1.698515
H -0.316622 -3.001612 2.717709
C 1.358290 -2.529013 1.453253
H 2.048886 -2.433877 2.284919
C -1.465823 -2.610481 -1.769678
N -2.051876 -0.357273 -0.775471
N 2.064430 0.363460 -0.755760
U 0.000977 -0.000132 0.459062
H -2.036304 -3.545184 -1.817047
H -0.947193 -2.509653 -2.730936
H -3.747944 1.754485 0.799146
H -3.706007 2.548459 -0.767212
H 0.976662 2.526137 -2.709347
H 2.057799 3.556815 -1.780625
H 3.718493 -2.542312 -0.748493
H 3.746855 -1.756601 0.822330
S -0.008136 -0.005679 2.565032
H -0.860152 -0.315722 2.880533

$LU^{III}Cl$. SCF energy = -1972.12644

C 3.160747 -0.446279 -0.826263
C 4.142024 0.122424 -1.590282
H 5.109852 -0.307948 -1.806004
C 3.650449 1.371956 -2.030622
H 4.161059 2.086271 -2.660972
C 2.385610 1.502631 -1.527693
C 3.217745 -1.758671 -0.106978
C 1.841866 -2.279240 0.155406
C 0.928051 -2.389677 -0.908712
H 1.272616 -2.180446 -1.917113
C -0.409647 -2.688702 -0.686931
C -0.839490 -2.922992 0.631968
H -1.888855 -3.131656 0.814414
C 0.061856 -2.883923 1.680122
H -0.275424 -3.074091 2.692690
C 1.395438 -2.540169 1.445903
H 2.085173 -2.451428 2.278623
C -1.416667 -2.614088 -1.786527
C -2.385597 -1.502659 -1.527687
C -3.650289 -1.371766 -2.030972
H -4.160784 -2.085901 -2.661620

C -4.141860 -0.122261 -1.590582
H -5.109558 0.308261 -1.806573
C -3.160705 0.446233 -0.826211
C -3.217741 1.758482 -0.106694
C -1.841876 2.279250 0.155429
C -0.928144 2.389557 -0.908783
H -1.272784 2.180153 -1.917124
C 0.409548 2.688615 -0.687147
C 0.839517 2.923101 0.631700
H 1.888910 3.131780 0.813974
C -0.061735 2.884218 1.679924
H 0.275547 3.074563 2.692456
C -1.395358 2.540420 1.445836
H -2.084995 2.451763 2.278644
C 1.416545 2.613896 -1.786778
N 2.047902 0.387888 -0.762486
N -2.048054 -0.388088 -0.762183
U 0.000036 -0.000044 0.476274
H 1.965562 3.560059 -1.854951
H 0.897286 2.481790 -2.743943
H 3.760599 -1.680868 0.843140
H 3.772408 -2.477339 -0.722484
H -0.897404 -2.482315 -2.743744
H -1.965769 -3.560222 -1.854467
H -3.772691 2.477181 -0.721906
H -3.760315 1.680472 0.843571
Cl -0.000253 0.000190 2.566140

$[LTh^{IV}X'']^+$ complexes.

$[LTh^{IV}CH_2Ph]^+$. SCF energy = -1713.44894

C -1.088091 -2.852564 1.043666
C -1.505288 -3.482961 2.184255
H -1.913988 -4.481756 2.246449
C -1.290118 -2.584765 3.254080
H -1.497120 -2.758041 4.300656
C -0.736478 -1.453650 2.719416
C -1.087939 -3.388613 -0.353718
C -0.037514 -2.708788 -1.173842
C 1.266839 -2.589023 -0.660537
H 1.504383 -3.075056 0.280674
C 2.230925 -1.820854 -1.300179
C 1.895144 -1.180042 -2.504572
H 2.635619 -0.556288 -2.994890
C 0.640119 -1.348142 -3.057281
H 0.397580 -0.874644 -4.002136
C -0.333050 -2.090056 -2.382941
H -1.331179 -2.173634 -2.800465
C 3.554814 -1.546447 -0.667679
C 3.676113 -0.088115 -0.362481
C 4.820175 0.648612 -0.233443
H 5.828383 0.288242 -0.381205
C 4.429995 1.951774 0.152402
H 5.079273 2.792351 0.352846
C 3.065124 1.955012 0.225545
C 2.170063 3.094768 0.595584
C 0.878947 2.582355 1.149880
C 0.898198 1.589864 2.145244
H 1.853904 1.283797 2.559734
C -0.266414 0.943905 2.549546
C -1.486986 1.341733 1.982661
H -2.397788 0.826605 2.269137
C -1.530788 2.374600 1.062521
H -2.481707 2.684851 0.648688
C -0.348459 2.969923 0.619546
H -0.383436 3.737626 -0.145897
C -0.233703 -0.247784 3.449485
N -0.608212 -1.582322 1.339634
N 2.557625 0.698606 -0.095997
Th 0.231847 0.085251 -0.199120
H -0.864686 -0.069138 4.327516
H 0.787765 -0.396377 3.820901
H -2.061976 -3.276342 -0.847305
H -0.887413 -4.466544 -0.320249
H 3.661482 -2.160756 0.234893
H 4.362465 -1.841325 -1.347127
H 2.675699 3.715529 1.345133
H 1.960278 3.751591 -0.257920
C -2.521852 1.127916 -1.597673
C -3.382433 2.229530 -1.679537
C -3.041397 -0.046673 -1.042594
C -4.686371 2.157781 -1.222243
H -3.018360 3.151184 -2.125060
C -4.347179 -0.121336 -0.572355
H -2.433303 -0.950873 -0.998040
C -5.174894 0.984257 -0.657089
H -5.334959 3.023319 -1.313417
H -4.715307 -1.049225 -0.147000
H -6.197507 0.932349 -0.300434
C -1.095810 1.199114 -2.003839
H -0.931977 0.620580 -2.919405
H -0.798411 2.227433 -2.241657

$[LTh^{IV}NHPh]^+$. SCF energy = -1729.53641

C -1.071288 -3.053290 -0.031065
C -1.284777 -4.159160 0.744238
H -1.771543 -5.071405 0.429159
C -0.751508 -3.877710 2.021839
H -0.739600 -4.533597 2.880897
C -0.222701 -2.618084 1.965851
C -1.476126 -2.855627 -1.458692
C -0.631581 -1.806241 -2.104368
C 0.770825 -1.912747 -2.051712
H 1.213105 -2.807590 -1.624112
C 1.589024 -0.871071 -2.468798
C 0.992064 0.290891 -2.990698
H 1.627847 1.115866 -3.296219
C -0.383297 0.381616 -3.106598
H -0.839549 1.274177 -3.518684
C -1.195806 -0.657378 -2.645724
H -2.275112 -0.552227 -2.676950
C 3.063374 -0.893361 -2.234334
C 3.451267 0.183068 -1.268804
C 4.684029 0.753804 -1.114358
H 5.560441 0.543901 -1.711122

C	4.594601	1.641014	-0.018048
H	5.386704	2.254226	0.388060
C	3.307433	1.584119	0.439293
C	2.711442	2.355504	1.575661
C	1.505174	1.656618	2.114737
C	1.598361	0.304358	2.497297
H	2.570753	-0.179005	2.478235
C	0.470131	-0.431592	2.829844
C	-0.783838	0.207750	2.811400
H	-1.673441	-0.369645	3.041243
C	-0.883524	1.550290	2.498448
H	-1.853802	2.033671	2.484058
C	0.258204	2.268605	2.132518
H	0.166753	3.307837	1.835107
C	0.535928	-1.907142	3.042658
N	-0.412683	-2.066149	0.699177
N	2.561140	0.686603	-0.321356
Th	0.229369	0.141797	-0.060322
H	0.102624	-2.164772	4.015886
H	1.585914	-2.223204	3.072202
H	-2.531951	-2.572623	-1.550111
H	-1.360704	-3.805287	-1.995022
H	3.357441	-1.885411	-1.870368
H	3.594269	-0.735702	-3.180207
H	3.463639	2.457964	2.367155
H	2.434774	3.374927	1.279224
N	-1.271720	1.757462	-0.555240
H	-0.983966	2.666536	-0.911857
C	-2.656384	1.674319	-0.459736
C	-3.494344	2.731040	-0.829394
C	-3.252337	0.498957	0.018242
C	-4.868995	2.612549	-0.725485
H	-3.056265	3.653604	-1.201156
C	-4.630545	0.388243	0.119017
H	-2.646415	-0.356173	0.327391
C	-5.448872	1.443213	-0.252213
H	-5.496782	3.447619	-1.018883
H	-5.064952	-0.532861	0.493715
H	-6.526175	1.356732	-0.172819

$LTh^{III}X''$ complexes.

$LTh^{III}CH_2Ph$. SCF energy =

C	2.382830	-2.749332	-0.182415
C	3.084463	-3.655218	0.572486
H	3.712517	-4.449801	0.193513
C	2.818983	-3.347082	1.926026
H	3.207084	-3.850682	2.801099
C	1.981807	-2.260208	1.924336
C	2.297873	-2.630882	-1.669081
C	1.907314	-1.240675	-2.053866
C	2.691246	-0.127439	-1.615115
H	3.589162	-0.316620	-1.034307
C	2.267084	1.166703	-1.812068
C	1.040654	1.399178	-2.512449
H	0.695644	2.415316	-2.655804
C	0.435568	0.317064	-3.196483
H	-0.404379	0.501556	-3.856658
C	0.844132	-0.972884	-2.960969
H	0.324260	-1.802510	-3.430404
C	2.945008	2.324710	-1.156864
C	2.003195	2.979262	-0.196442
C	2.038455	4.259647	0.296298
H	2.762529	5.020836	0.040155
C	0.966177	4.372582	1.209130
H	0.691809	5.240594	1.793038
C	0.322913	3.159967	1.213446
C	-0.897235	2.772096	1.986421
C	-0.954925	1.288498	2.160108
C	0.170073	0.609527	2.659741
H	1.033134	1.187544	2.974864
C	0.216571	-0.774009	2.710974
C	-0.891725	-1.505318	2.254042
H	-0.843206	-2.589423	2.257242
C	-2.014494	-0.852316	1.787499
H	-2.870187	-1.410602	1.426344
C	-2.041194	0.544407	1.729786
H	-2.912632	1.038285	1.314448
C	1.463293	-1.495664	3.098995
N	1.687825	-1.872226	0.629269
N	0.945732	2.276673	0.351661
Th	0.272895	-0.029343	-0.272391
H	1.255207	-2.187866	3.923815
H	2.198812	-0.770951	3.471322
H	1.564460	-3.334959	-2.086082
H	3.266044	-2.908163	-2.110179
H	3.854790	1.973513	-0.653503
H	3.259344	3.055545	-1.912507
H	-0.871011	3.260582	2.968738
H	-1.820281	3.109391	1.497189
C	-3.436679	-0.450635	-1.034399
C	-4.225539	0.697400	-0.874034
C	-4.064811	-1.681799	-0.796471
C	-5.552492	0.621301	-0.482727
H	-3.786689	1.670975	-1.081739
C	-5.391498	-1.759583	-0.405384
H	-3.496596	-2.598359	-0.938592
C	-6.148014	-0.608041	-0.238403
H	-6.131390	1.534318	-0.377392
H	-5.842625	-2.733356	-0.237861
H	-7.187943	-0.668476	0.063497
C	-2.024510	-0.370276	-1.436662
H	-1.760591	-1.258859	-2.029884
H	-1.889872	0.496039	-2.104428

$LTh^{III}NHPh$. SCF energy = -1729.69633

C	3.398388	-1.128822	-0.886559
C	4.062480	-2.329880	-0.826826
H	4.817865	-2.674788	-1.519561
C	3.603748	-2.990342	0.335007
H	3.936706	-3.945793	0.717702
C	2.674385	-2.165645	0.922488
C	3.638525	0.015262	-1.828498
C	2.407865	0.851109	-1.979080
C	2.235643	1.999958	-1.230388

H 3.055872 2.343190 -0.603724
C 0.979315 2.648048 -1.128951
C -0.046496 2.241008 -2.050941
H -0.975986 2.799503 -2.089822
C 0.136732 1.143508 -2.861990
H -0.658787 0.833796 -3.530900
C 1.309781 0.356209 -2.760749
H 1.438069 -0.528503 -3.371676
C 0.738433 3.751098 -0.146389
C 0.037466 3.267441 1.092325
C -0.238797 3.958095 2.245706
H 0.048087 4.977648 2.463807
C -0.979560 3.084783 3.074853
H -1.378177 3.300535 4.057252
C -1.126732 1.904307 2.388607
C -1.958319 0.729599 2.783528
C -1.392589 -0.621874 2.444636
C -0.016380 -0.871880 2.519939
H 0.639936 -0.080394 2.884683
C 0.521591 -2.122239 2.205274
C -0.349061 -3.144879 1.832784
H 0.054924 -4.120957 1.581839
C -1.714506 -2.922377 1.793775
H -2.385589 -3.727067 1.511292
C -2.232318 -1.669300 2.082297
H -3.301323 -1.495561 2.013729
C 2.005596 -2.346115 2.248153
N 2.511866 -1.016029 0.174156
N -0.490134 1.987926 1.163312
Th 0.409466 0.185559 -0.196153
H 2.212064 -3.361958 2.597554
H 2.444665 -1.661097 2.986750
H 3.957356 -0.376954 -2.800670
H 4.455911 0.646010 -1.454786
H 1.693774 4.218003 0.121887
H 0.139408 4.540078 -0.622986
H -2.121176 0.780326 3.867998
H -2.957384 0.794803 2.330003
N -1.183807 -1.181462 -1.098653
H -0.832027 -2.077063 -1.434995
C -2.533791 -1.069329 -1.370175
C -3.237256 0.090423 -1.008770
C -3.255879 -2.093114 -1.998428
C -4.590700 0.213134 -1.267306
H -2.714638 0.908872 -0.516052
C -4.610390 -1.962362 -2.251898
H -2.735497 -3.001865 -2.290783
C -5.292900 -0.809894 -1.890432
H -5.104386 1.124353 -0.975700
H -5.139134 -2.774838 -2.741515
H -6.353592 -0.709239 -2.091188

$LU^{III}X''$ complexes.

$LU^{III}CH_2Ph$. SCF energy = -1782.85842

C 0.665108 2.988082 1.204185
C 0.743967 3.763955 2.336593
H 0.974868 4.820323 2.369180
C 0.485199 2.914116 3.436040
H 0.463291 3.187222 4.482114
C 0.247908 1.665970 2.914227
C 0.921291 3.413985 -0.204518
C 0.043178 2.746823 -1.228403
C -1.263617 2.359249 -0.905937
H -1.652447 2.605228 0.079459
C -2.078082 1.684491 -1.814771
C -1.586016 1.438046 -3.096347
H -2.204349 0.905335 -3.812105
C -0.321821 1.876087 -3.452972
H 0.048451 1.696121 -4.457043
C 0.494645 2.506421 -2.522565
H 1.499317 2.808962 -2.802932
C -3.435604 1.212041 -1.388629
C -3.481879 -0.240852 -1.030439
C -4.548749 -1.087797 -1.210539
H -5.473446 -0.843806 -1.715938
C -4.217090 -2.307063 -0.580435
H -4.826731 -3.198139 -0.518280
C -2.958281 -2.145970 -0.057331
C -2.143297 -3.151389 0.701375
C -0.930049 -2.515904 1.303370
C -1.072652 -1.506283 2.274018
H -2.068239 -1.256583 2.627736
C 0.023009 -0.777613 2.737116
C 1.298117 -1.089237 2.233240
H 2.152770 -0.507205 2.560439
C 1.461911 -2.106531 1.301050
H 2.446608 -2.328561 0.907338
C 0.348619 -2.808691 0.829356
H 0.476348 -3.571896 0.069434
C -0.143062 0.409141 3.634366
N 0.354946 1.687458 1.538601
N -2.474832 -0.879439 -0.330036
U -0.197545 -0.165595 0.064315
H 0.478288 0.286467 4.530611
H -1.183791 0.454776 3.979273
H 1.969462 3.243031 -0.490766
H 0.775752 4.500517 -0.263677
H -3.762442 1.826866 -0.537971
H -4.157350 1.386085 -2.193259
H -2.757972 -3.598598 1.493415
H -1.826585 -3.976639 0.051581
C 2.714054 -1.071147 -1.529742
C 3.418869 -2.284354 -1.503960
C 3.453247 0.090164 -1.256206
C 4.770534 -2.333958 -1.206638
H 2.888683 -3.204291 -1.738180
C 4.805510 0.041545 -0.960720
H 2.952482 1.055611 -1.286454
C 5.477505 -1.172001 -0.927685
H 5.281853 -3.292347 -1.203782
H 5.341110 0.963712 -0.755235
H 6.536818 -1.211049 -0.698442
C 1.267869 -1.014995 -1.763353
H 1.008727 -0.201114 -2.458688
H 0.869835 -1.949336 -2.177240

$LU^{III}NHPh$. SCF energy = -1798.94096

C 0.783930 2.909078 -1.284136
C 0.765008 4.276966 -1.148923
H 1.129150 4.992887 -1.873563
C 0.200658 4.557738 0.116584
H 0.030911 5.531888 0.554458
C -0.109493 3.345269 0.681823
C 1.357370 2.117169 -2.415565
C 0.644956 0.821506 -2.690426
C -0.747734 0.728760 -2.558111
H -1.311720 1.625368 -2.311761
C -1.421934 -0.478820 -2.734622
C -0.686581 -1.605274 -3.108579
H -1.199521 -2.552859 -3.242978
C 0.679431 -1.513085 -3.309294
H 1.243704 -2.390513 -3.607518
C 1.344400 -0.316424 -3.077600
H 2.424160 -0.269648 -3.178602
C -2.897163 -0.559197 -2.479664
C -3.238868 -1.174925 -1.157744
C -4.379413 -1.879957 -0.855024
H -5.155321 -2.162504 -1.553708
C -4.354233 -2.123051 0.535545
H -5.096703 -2.648046 1.121103
C -3.192329 -1.564150 1.008483
C -2.681014 -1.566816 2.419094
C -1.523669 -0.631572 2.578012
C -1.701671 0.752516 2.391039
H -2.701807 1.130626 2.201899
C -0.620230 1.630581 2.372754
C 0.672197 1.111866 2.579467
H 1.522278 1.784520 2.542572
C 0.862799 -0.244706 2.799552
H 1.863871 -0.637510 2.934736
C -0.233497 -1.114682 2.785381
H -0.075088 -2.180531 2.908730
C -0.783627 3.069708 1.993814
N 0.242162 2.312858 -0.164870
N -2.479206 -0.978824 -0.020360
U -0.246573 -0.037437 0.173356
H -0.351960 3.711108 2.772732
H -1.853858 3.308357 1.950701
H 2.418925 1.889319 -2.244303
H 1.329852 2.741421 -3.318287
H -3.315491 0.454814 -2.549688
H -3.378446 -1.147872 -3.267855
H -3.488789 -1.272391 3.101468
H -2.367306 -2.572596 2.725986
N 1.402757 -1.606479 -0.002507
H 1.067454 -2.554676 -0.169618
C 2.763413 -1.609938 0.198096
C 3.518740 -2.791618 0.266984
C 3.458225 -0.396006 0.342474
C 4.885877 -2.758265 0.475553
H 3.011243 -3.746940 0.156237
C 4.824787 -0.372897 0.558207
H 2.915252 0.545348 0.269546
C 5.555001 -1.551443 0.627718
H 5.437627 -3.692694 0.522017
H 5.327819 0.583797 0.664214
H 6.626478 -1.529369 0.791562

$[LTh^{IV}X^{**}]^{+}$ complexes.

$[LTh^{IV}SiH_2Ph]^{+}$. SCF energy = -1964.75961

C 2.048447 -3.033021 -0.081525
C 2.572644 -3.998872 0.731003
H 3.080170 -4.896282 0.406533
C 2.319182 -3.600943 2.063746
H 2.597798 -4.130484 2.963853
C 1.664926 -2.402231 2.006272
C 2.040421 -2.997470 -1.577134
C 1.894876 -1.590709 -2.058990
C 2.793302 -0.605559 -1.605870
H 3.631711 -0.907873 -0.985159
C 2.596664 0.741592 -1.888148
C 1.484378 1.112660 -2.663863
H 1.305749 2.164537 -2.862046
C 0.614045 0.151582 -3.149999
H -0.234060 0.442322 -3.759723
C 0.810021 -1.197446 -2.833698
H 0.096150 -1.936644 -3.180601
C 3.433081 1.802285 -1.251911
C 2.587444 2.636559 -0.340898
C 2.833799 3.905776 0.102154
H 3.675332 4.524139 -0.176528
C 1.792003 4.242069 0.997164
H 1.674383 5.171143 1.536752
C 0.947018 3.169314 1.049458
C -0.322496 3.035781 1.829901
C -0.641573 1.593068 2.054193
C 0.325736 0.754579 2.642450
H 1.249831 1.195204 3.005048
C 0.145082 -0.621721 2.712665
C -1.046182 -1.173067 2.207171
H -1.179961 -2.249704 2.235464
C -2.024793 -0.359059 1.664157
H -2.947769 -0.780045 1.280875
C -1.812199 1.021545 1.568926
H -2.569763 1.641881 1.100912
C 1.242983 -1.533351 3.150135
N 1.469577 -2.019327 0.680063
N 1.411069 2.146394 0.224125
Th 0.422381 -0.007323 -0.108700
H 0.895745 -2.165271 3.975841
H 2.078989 -0.938607 3.537576
H 1.233312 -3.609149 -1.998148
H 2.979966 -3.421622 -1.951092
H 4.268331 1.335217 -0.716165
H 3.873054 2.443189 -2.024728
H -0.206351 3.543814 2.794743
H -1.166957 3.518213 1.323009
Si -2.212503 0.034068 -1.737096
C -3.947485 -0.094816 -1.010769
C -4.678463 1.044463 -0.664827
C -4.535351 -1.343663 -0.785511

C -5.945210 0.941693 -0.106841
H -4.268040 2.032419 -0.860906
C -5.801970 -1.450027 -0.231351
H -4.006027 -2.251966 -1.065008
C -6.507912 -0.306139 0.114222
H -6.501098 1.839929 0.142428
H -6.245143 -2.428744 -0.077516
H -7.500758 -0.387836 0.543705
H -2.178676 -0.927665 -2.895237
H -2.134230 1.403362 -2.374511

[LTh^{IV}PHPh]$^{+}$. SCF energy = -2016.03070

C 2.003029 -3.032927 -0.040447
C 2.546416 -3.984732 0.776068
H 3.024929 -4.899614 0.456133
C 2.350955 -3.548621 2.107513
H 2.658570 -4.057958 3.009829
C 1.709243 -2.343916 2.042248
C 1.914562 -3.047444 -1.534462
C 1.780419 -1.654609 -2.059743
C 2.701297 -0.675507 -1.653950
H 3.543167 -0.974894 -1.036508
C 2.520712 0.669964 -1.963685
C 1.408278 1.038059 -2.736411
H 1.241367 2.086596 -2.960037
C 0.521489 0.077421 -3.194195
H -0.322691 0.374803 -3.804401
C 0.689927 -1.264853 -2.834804
H -0.028486 -2.008270 -3.161605
C 3.386934 1.730364 -1.368103
C 2.575784 2.598104 -0.456991
C 2.852979 3.873758 -0.051239
H 3.697166 4.471477 -0.364752
C 1.840492 4.246238 0.862846
H 1.750158 5.189450 1.382911
C 0.982442 3.186757 0.962004
C -0.270554 3.089221 1.773958
C -0.588687 1.656170 2.055252
C 0.396328 0.830226 2.626312
H 1.336093 1.276029 2.938595
C 0.213498 -0.544115 2.744714
C -0.992489 -1.106153 2.295214
H -1.126269 -2.181469 2.353630
C -1.988942 -0.303437 1.763783
H -2.924339 -0.734899 1.426890
C -1.779344 1.075235 1.632632
H -2.550079 1.689341 1.180176
C 1.326672 -1.442042 3.173757
N 1.471016 -1.990962 0.715339
N 1.409205 2.138676 0.151414
Th 0.371737 -0.013710 -0.112509
H 1.007439 -2.049007 4.028843
H 2.173658 -0.835102 3.515842
H 1.068645 -3.649813 -1.887771
H 2.819702 -3.512096 -1.943674
H 4.226578 1.260866 -0.841196
H 3.820189 2.347743 -2.163393
H -0.131204 3.630422 2.717497
H -1.123917 3.556254 1.267481
P -2.102439 0.111286 -1.528001
H -2.138464 -0.769662 -2.637196
C -3.809385 -0.083427 -0.914009
C -4.542049 1.049377 -0.558964
C -4.419813 -1.336386 -0.814923
C -5.844398 0.932104 -0.093603
H -4.102222 2.035090 -0.681841
C -5.726188 -1.448234 -0.367586
H -3.870102 -2.229356 -1.096384
C -6.439061 -0.315754 0.003081
H -6.402624 1.823512 0.173112
H -6.190978 -2.426937 -0.306543
H -7.460811 -0.406960 0.355358

[LTh^{IV}SPh]$^{+}$. SCF energy = -2072.30397

C 2.161468 -2.910108 -0.115355
C 2.779337 -3.837746 0.675202
H 3.313707 -4.711725 0.330274
C 2.578127 -3.439150 2.017406
H 2.935349 -3.941285 2.905343
C 1.858480 -2.278504 1.984463
C 2.064393 -2.900980 -1.608507
C 1.861308 -1.506850 -2.107596
C 2.715356 -0.483787 -1.660040
H 3.563027 -0.746762 -1.034210
C 2.458887 0.852857 -1.943867
C 1.339930 1.173200 -2.730087
H 1.117869 2.215742 -2.933599
C 0.523241 0.173093 -3.227640
H -0.337304 0.424922 -3.835106
C 0.768504 -1.164411 -2.896877
H 0.088009 -1.935109 -3.241065
C 3.248255 1.948912 -1.308018
C 2.369482 2.742917 -0.393797
C 2.549399 4.030322 0.026771
H 3.348284 4.692057 -0.276694
C 1.509113 4.316451 0.941356
H 1.346919 5.244452 1.471272
C 0.732887 3.195461 1.027128
C -0.507216 2.997148 1.840238
C -0.715868 1.542031 2.108104
C 0.337701 0.785037 2.653465
H 1.246819 1.296263 2.955901
C 0.262916 -0.599235 2.750030
C -0.909650 -1.243620 2.318032
H -0.962528 -2.326586 2.364039
C -1.972155 -0.509415 1.823096
H -2.877397 -1.005097 1.492628
C -1.867280 0.880796 1.697458
H -2.687558 1.436195 1.255918
C 1.446129 -1.420918 3.139080
N 1.572971 -1.918966 0.667351
N 1.237641 2.189662 0.205155
Th 0.324373 -0.011053 -0.110938
H 1.193005 -2.060134 3.992768
H 2.257970 -0.760922 3.467897
H 1.247027 -3.536459 -1.970648

H 2.989283 -3.314401 -2.028463
H 4.104957 1.518751 -0.775002
H 3.657319 2.611376 -2.079278
H -0.405353 3.538641 2.788395
H -1.395399 3.404108 1.341811
S -1.982965 -0.296159 -1.529083
C -3.645713 -0.292484 -0.909851
C -4.348878 0.904438 -0.799101
C -4.284472 -1.497324 -0.624486
C -5.671986 0.893579 -0.382599
H -3.866021 1.839532 -1.063759
C -5.607513 -1.496909 -0.208997
H -3.748650 -2.432924 -0.745604
C -6.303518 -0.303785 -0.081761
H -6.214890 1.829899 -0.304941
H -6.099245 -2.439795 0.006816
H -7.339623 -0.308415 0.238040

$LTh^{III}X^{**}$ complexes.

$LTh^{III}SiH_2Ph$. SCF energy = -1964.92645

C 2.690318 -2.653233 -0.272166
C 3.397669 -3.588244 0.441651
H 4.081756 -4.318954 0.032364
C 3.048987 -3.411854 1.799580
H 3.417793 -3.972054 2.648227
C 2.157393 -2.369818 1.844158
C 2.656925 -2.430411 -1.749979
C 2.142850 -1.063609 -2.070652
C 2.846072 0.092706 -1.625877
H 3.775733 -0.039534 -1.079117
C 2.319894 1.358227 -1.772932
C 1.060657 1.515202 -2.438560
H 0.629208 2.502361 -2.543607
C 0.482093 0.400372 -3.079503
H -0.402183 0.533454 -3.692172
C 0.994318 -0.866158 -2.887144
H 0.495468 -1.721897 -3.330323
C 2.937069 2.540110 -1.100009
C 2.008588 3.071157 -0.053333
C 1.992620 4.317824 0.519276
H 2.660400 5.135039 0.283737
C 0.951184 4.313908 1.473335
H 0.649159 5.129759 2.115809
C 0.373790 3.070011 1.423196
C -0.822628 2.590481 2.183695
C -0.865793 1.097927 2.215384
C 0.242898 0.387654 2.711339
H 1.077814 0.944398 3.126069
C 0.305901 -0.994516 2.644823
C -0.765681 -1.692293 2.059598
H -0.703781 -2.772229 1.973521
C -1.871574 -1.010729 1.588529
H -2.704961 -1.542379 1.143056
C -1.917309 0.386221 1.659660
H -2.779892 0.906553 1.258115
C 1.536284 -1.736351 3.047574
N 1.912780 -1.883769 0.572784
N 1.014158 2.276205 0.487968
Th 0.480471 -0.018118 -0.229032
H 1.281363 -2.510882 3.781244
H 2.226732 -1.043727 3.545814
H 2.018362 -3.173334 -2.246600
H 3.664660 -2.574797 -2.163200
H 3.902860 2.245914 -0.669775
H 3.142953 3.328518 -1.834900
H -0.781466 2.982299 3.207936
H -1.756172 2.964284 1.744171
Si -2.261968 -0.176123 -1.750491
C -4.000188 -0.369771 -0.998728
C -4.746690 0.741996 -0.596186
C -4.569978 -1.630312 -0.793874
C -5.998250 0.604540 -0.013110
H -4.350252 1.741970 -0.760913
C -5.820951 -1.776183 -0.211272
H -4.032321 -2.520036 -1.115137
C -6.539410 -0.657459 0.184628
H -6.558722 1.487462 0.279894
H -6.241667 -2.768005 -0.073949
H -7.519705 -0.768090 0.636977
H -2.205453 -1.305794 -2.756143
H -2.413424 1.054629 -2.615168

$LTh^{III}PHPh$. SCF energy = -2016.19604

C 1.697842 -3.194814 -0.045605
C 2.142631 -4.217921 0.753933
H 2.509505 -5.177080 0.414436
C 2.011626 -3.776373 2.089570
H 2.266525 -4.322788 2.987185
C 1.509235 -2.500818 2.034584
C 1.564322 -3.196774 -1.535737
C 1.565232 -1.801731 -2.071680
C 2.587722 -0.919970 -1.693305
H 3.395299 -1.293940 -1.071424
C 2.562774 0.421454 -2.052063
C 1.487090 0.893140 -2.816549
H 1.438127 1.947766 -3.066475
C 0.487255 0.029851 -3.228280
H -0.339087 0.403309 -3.820891
C 0.518876 -1.314988 -2.844843
H -0.282188 -1.981502 -3.142714
C 3.577732 1.381760 -1.524427
C 2.922986 2.351627 -0.593138
C 3.364781 3.594235 -0.214700
H 4.259151 4.088292 -0.569721
C 2.438295 4.082023 0.735505
H 2.469161 5.033289 1.248898
C 1.472808 3.117087 0.876340
C 0.233551 3.136590 1.713104
C -0.255563 1.744581 1.962877
C 0.580611 0.800828 2.620862

H 1.558912 1.123461 2.966744
C 0.235814 -0.529987 2.708379
C -1.034179 -0.954475 2.190157
H -1.305324 -2.001304 2.240184
C -1.956109 0.009870 1.752904
H -2.955298 -0.291023 1.461280
C -1.576048 1.332843 1.612722
H -2.279794 2.059038 1.222270
C 1.208841 -1.566249 3.163994
N 1.304438 -2.114463 0.722145
N 1.749414 2.032953 0.065136
Th 0.296367 0.030879 -0.011042
H 0.791986 -2.135725 4.004482
H 2.116808 -1.072334 3.532777
H 0.644279 -3.700575 -1.859815
H 2.397995 -3.762382 -1.970922
H 4.379392 0.819189 -1.028532
H 4.042230 1.928324 -2.353890
H 0.439355 3.656203 2.658986
H -0.564817 3.708315 1.220827
P -2.153523 0.160276 -1.581674
H -2.292213 -0.821398 -2.601307
C -3.856313 0.103807 -0.931545
C -4.463124 1.272492 -0.465720
C -4.600982 -1.079309 -0.895992
C -5.753594 1.256046 0.042968
H -3.923792 2.213075 -0.529316
C -5.897505 -1.091057 -0.408466
H -4.153640 -2.002425 -1.251785
C -6.478210 0.074661 0.072819
H -6.201652 2.178275 0.400149
H -6.457105 -2.021539 -0.396434
H -7.491306 0.062251 0.460927

LTh^{III}SPh. SCF energy = -2072.46921

C 2.817451 -2.450609 -0.265726
C 3.635190 -3.286881 0.451204
H 4.346902 -3.989379 0.039704
C 3.352696 -3.057659 1.817388
H 3.810402 -3.539719 2.670681
C 2.388531 -2.083066 1.861016
C 2.676763 -2.313557 -1.747058
C 2.100830 -0.977372 -2.090477
C 2.756043 0.212464 -1.653946
H 3.691036 0.123491 -1.108520
C 2.165890 1.447830 -1.797063
C 0.898524 1.540296 -2.457423
H 0.416816 2.505291 -2.550449
C 0.376231 0.404081 -3.105884
H -0.527994 0.490078 -3.695013
C 0.946608 -0.837716 -2.910766
H 0.488570 -1.718155 -3.348816
C 2.711646 2.664282 -1.124943
C 1.724234 3.162489 -0.117015
C 1.609610 4.420982 0.417470
H 2.226009 5.275233 0.173414
C 0.551230 4.369731 1.351981
H 0.181476 5.178584 1.967421
C 0.064502 3.086623 1.327071
C -1.092929 2.533119 2.096802
C -0.971121 1.049271 2.228524
C 0.231715 0.499518 2.700603
H 1.020128 1.170056 3.027954
C 0.450143 -0.869059 2.706686
C -0.561784 -1.717171 2.230437
H -0.378794 -2.786064 2.194034
C -1.760992 -1.193363 1.788340
H -2.543286 -1.843798 1.416302
C -1.962908 0.190664 1.780008
H -2.892925 0.590109 1.391324
C 1.782797 -1.437445 3.065074
N 2.034090 -1.690126 0.582525
N 0.776013 2.314875 0.427170
Th 0.379502 -0.036960 -0.258696
H 1.671597 -2.182348 3.862171
H 2.419322 -0.637675 3.465107
H 2.026299 -3.097134 -2.158650
H 3.658188 -2.453284 -2.221280
H 3.675424 2.419610 -0.660716
H 2.903596 3.452085 -1.864237
H -1.116322 2.994507 3.092166
H -2.053269 2.770639 1.621041
S -1.999250 -0.764205 -1.548664
C -3.642414 -0.682279 -0.898004
C -4.313550 0.538195 -0.798703
C -4.325615 -1.849082 -0.551729
C -5.623217 0.588620 -0.347129
H -3.801338 1.448536 -1.094053
C -5.635730 -1.792582 -0.100607
H -3.823446 -2.805931 -0.655189
C -6.290591 -0.574758 0.008615
H -6.128312 1.547466 -0.280003
H -6.150323 -2.712038 0.161542
H -7.316365 -0.533169 0.358977

LU^{III}X** complexes.

LU^{III}SiH$_2$Ph. SCF energy = -2033.89215

C -1.583204 -3.191850 -0.114272
C -2.234953 -4.086943 -0.918798
H -2.530892 -5.091453 -0.649100
C -2.439888 -3.444054 -2.156864
H -2.945603 -3.849982 -3.022096
C -1.920178 -2.179021 -2.046391
C -1.101921 -3.400885 1.284467
C -0.946321 -2.088260 1.975992
C -2.020672 -1.190677 1.978163
H -2.966992 -1.509403 1.551564
C -1.885575 0.105212 2.451003
C -0.645775 0.510282 2.970874
H -0.525163 1.531010 3.318503
C 0.410832 -0.382226 3.027240
H 1.359515 -0.067605 3.447678
C 0.270024 -1.673612 2.509521
H 1.113783 -2.355103 2.510845

C -2.984952 1.093668 2.274072
C -2.559136 2.181133 1.344149
C -3.097995 3.434124 1.263720
H -3.884396 3.833175 1.889472
C -2.457373 4.079012 0.194377
H -2.653026 5.078028 -0.170251
C -1.550590 3.194444 -0.329558
C -0.691640 3.480092 -1.516535
C -0.340948 2.202337 -2.199232
C -1.350338 1.263883 -2.497515
H -2.386283 1.526571 -2.304694
C -1.034057 -0.017297 -2.943992
C 0.300671 -0.344479 -3.153075
H 0.557837 -1.344855 -3.486576
C 1.274076 0.597760 -2.951023
H 2.297511 0.345264 -3.155115
C 0.962701 1.853888 -2.442319
H 1.748218 2.564691 -2.231259
C -2.056331 -1.083518 -3.071658
N -1.351641 -1.997370 -0.777727
N -1.560073 1.990664 0.392718
U -0.213733 -0.053914 0.172587
H -1.996150 -1.502205 -4.083245
H -3.050662 -0.630346 -2.972414
H -0.145706 -3.938450 1.313003
H -1.823807 -4.024811 1.826007
H -3.877425 0.569312 1.910205
H -3.253198 1.538246 3.239801
H -1.275458 4.099969 -2.208289
H 0.214598 4.051486 -1.279273
Si 2.104180 -0.218430 0.995936
C 3.698001 -0.053944 0.513365
C 4.395959 1.160245 0.637778
C 4.409545 -1.155678 -0.004669
C 5.729121 1.271046 0.253396
H 3.880732 2.034248 1.046676
C 5.742440 -1.045873 -0.384969
H 3.902069 -2.119569 -0.104863
C 6.404848 0.169492 -0.259485
H 6.250251 2.226868 0.358219
H 6.271196 -1.916294 -0.783337
H 7.452190 0.258103 -0.558289
H 2.402380 -1.406353 1.384810
H 2.273211 0.614724 1.959413

LU^{III}PHPh. SCF energy = -2085.45256

C 1.918937 -3.115940 0.000691
C 2.454048 -4.077541 0.823034
H 2.920152 -5.001243 0.507782
C 2.258947 -3.627963 2.147804
H 2.558220 -4.127568 3.059117
C 1.626329 -2.411776 2.058555
C 1.831462 -3.120753 -1.491903
C 1.716650 -1.721982 -2.009371
C 2.657178 -0.757629 -1.614969
H 3.491078 -1.065990 -0.991837
C 2.512640 0.582742 -1.956931
C 1.404909 0.965799 -2.726238
H 1.262080 2.014431 -2.963953
C 0.492268 0.019817 -3.162753
H -0.356923 0.325767 -3.761685
C 0.638389 -1.319016 -2.790255
H -0.099606 -2.049971 -3.101183
C 3.430734 1.629963 -1.415135
C 2.683071 2.547836 -0.499185
C 3.039073 3.811373 -0.093933
H 3.910820 4.364174 -0.416693
C 2.058523 4.228372 0.833589
H 2.016381 5.172107 1.360211
C 1.151386 3.201624 0.931941
C -0.095254 3.137275 1.754976
C -0.471197 1.711293 2.008702
C 0.473284 0.834706 2.573804
H 1.436923 1.229184 2.880539
C 0.209549 -0.523556 2.707975
C -1.026159 -1.020357 2.267449
H -1.217987 -2.086071 2.332727
C -1.975246 -0.169953 1.726124
H -2.932063 -0.551770 1.392066
C -1.691612 1.194120 1.592704
H -2.429019 1.848370 1.141546
C 1.260143 -1.479587 3.170784
N 1.399504 -2.073168 0.739458
N 1.513559 2.149368 0.116704
U 0.346792 -0.003664 -0.115211
H 0.889214 -2.056369 4.026980
H 2.130492 -0.913110 3.526023
H 0.972939 -3.703872 -1.850052
H 2.727417 -3.599589 -1.906767
H 4.268297 1.141312 -0.900824
H 3.863894 2.208605 -2.240169
H 0.070333 3.654663 2.708352
H -0.936030 3.645787 1.265624
P -2.154190 0.113595 -1.605473
H -2.201031 -1.007623 -2.479537
C -3.841216 -0.032688 -0.929427
C -4.512391 1.113144 -0.491332
C -4.520658 -1.253656 -0.845308
C -5.793455 1.040381 0.035595
H -4.032809 2.082632 -0.597211
C -5.808288 -1.323161 -0.339422
H -4.028544 -2.161344 -1.181883
C -6.450010 -0.178186 0.113994
H -6.289474 1.947586 0.367401
H -6.314010 -2.283103 -0.292799
H -7.456368 -0.235388 0.515200

LU^{III}SPh at PBE. SCF energy = -2141.72523

C 2.403039 -2.797541 -0.157392
C 3.122431 -3.681005 0.610349
H 3.731636 -4.496500 0.244686
C 2.894614 -3.322573 1.957532
H 3.305258 -3.795681 2.839121
C 2.059106 -2.232327 1.935613
C 2.274009 -2.761119 -1.646874
C 1.926324 -1.380352 -2.107318

C 2.696106 -0.289949 -1.670728
H 3.573522 -0.481207 -1.060587
C 2.326788 1.020307 -1.952884
C 1.168395 1.246534 -2.709463
H 0.855388 2.266965 -2.903453
C 0.421925 0.182177 -3.183139
H -0.477256 0.359712 -3.758910
C 0.790301 -1.128965 -2.867975
H 0.165650 -1.952962 -3.194021
C 3.056677 2.181568 -1.359042
C 2.168156 2.918932 -0.406673
C 2.295982 4.212950 0.036602
H 3.047720 4.924394 -0.277191
C 1.273238 4.415294 0.989927
H 1.069591 5.318713 1.548646
C 0.570273 3.237630 1.065203
C -0.627115 2.924285 1.905087
C -0.737421 1.447132 2.116410
C 0.363397 0.735596 2.624992
H 1.251486 1.285983 2.919681
C 0.355145 -0.651620 2.706976
C -0.787827 -1.346653 2.283652
H -0.784732 -2.431116 2.310569
C -1.890374 -0.660279 1.807989
H -2.772081 -1.196151 1.478995
C -1.859445 0.734221 1.711433
H -2.713634 1.255590 1.293472
C 1.576251 -1.419277 3.096038
N 1.734918 -1.889962 0.637679
N 1.101684 2.294812 0.209465
U 0.308003 -0.016963 -0.114411
H 1.347468 -2.082762 3.939101
H 2.345037 -0.718668 3.446464
H 1.507948 -3.458995 -2.008978
H 3.222381 -3.077263 -2.099476
H 3.965341 1.817552 -0.862267
H 3.384939 2.862623 -2.153591
H -0.535583 3.433636 2.872677
H -1.556547 3.288333 1.448295
S -2.017316 -0.606999 -1.534464
C -3.657545 -0.482341 -0.893361
C -4.308410 0.750497 -0.812665
C -4.364300 -1.631189 -0.530046
C -5.618400 0.831252 -0.365436
H -3.780466 1.646981 -1.122246
C -5.674235 -1.544820 -0.084523
H -3.876349 -2.597225 -0.612154
C -6.308229 -0.313980 0.004676
H -6.106039 1.800128 -0.313618
H -6.205204 -2.451084 0.190838
H -7.334028 -0.248717 0.351427

$[LTh^{IV}X^{\dagger}]^{+}$ complexes.

$[LTh^{IV}CPh_3]^{+}$. SCF energy = -2175.11529

C -1.116729 -3.297949 1.241939
C -1.699145 -4.498776 0.937185
H -1.557694 -5.426937 1.473275
C -2.523989 -4.279274 -0.186224
H -3.153967 -5.001000 -0.686669
C -2.415469 -2.952343 -0.502782
C -0.167836 -3.024722 2.366003
C -0.129326 -1.563907 2.657719
C -1.339573 -0.875207 2.847415
H -2.268949 -1.434448 2.857728
C -1.365736 0.501684 2.988066
C -0.155593 1.213766 2.947307
H -0.182130 2.295269 3.037866
C 1.044189 0.545448 2.807983
H 1.982888 1.086199 2.790242
C 1.054946 -0.842151 2.643830
H 2.003430 -1.346222 2.497668
C -2.647270 1.250989 3.041161
C -2.753213 2.115848 1.832270
C -3.466361 3.276586 1.719346
H -4.006924 3.768968 2.515347
C -3.399460 3.662257 0.364181
H -3.873053 4.518197 -0.096130
C -2.636285 2.726485 -0.279615
C -2.337084 2.694255 -1.742946
C -1.956095 1.318980 -2.164913
C -2.765504 0.236686 -1.796166
H -3.696469 0.429220 -1.273165
C -2.384338 -1.072607 -2.059133
C -1.175177 -1.304392 -2.726637
H -0.858945 -2.323766 -2.917643
C -0.398439 -0.239611 -3.151626
H 0.517415 -0.426830 -3.695761
C -0.775073 1.067014 -2.851560
H -0.145276 1.896674 -3.149330
C -3.186337 -2.218100 -1.545733
N -1.532464 -2.307193 0.357334
N -2.196124 1.746879 0.607572
Th -0.553586 -0.055943 0.131071
H -3.427466 -2.905975 -2.363235
H -4.140563 -1.845465 -1.152666
H 0.848606 -3.383608 2.158152
H -0.504219 -3.568460 3.257506
H -3.484058 0.545153 3.111843
H -2.681859 1.877694 3.939377
H -3.234855 3.008608 -2.290076
H -1.539601 3.390833 -2.021893
C 2.053089 0.276148 -0.379942
C 2.086396 -0.965337 -1.228828
C 2.693610 -1.131575 -2.482044
C 1.489935 -2.107520 -0.683709
C 2.653288 -2.345489 -3.145519
H 3.247070 -0.323615 -2.937887
C 1.429704 -3.330246 -1.344438
H 1.144109 -2.083537 0.349669
C 2.005068 -3.447032 -2.594326
H 3.152420 -2.441401 -4.104714
H 0.939253 -4.173898 -0.869721
H 1.978911 -4.390965 -3.127586
C 3.231287 0.328190 0.565626
C 3.726504 1.541022 1.065549
C 3.928738 -0.828216 0.941572
C 4.816471 1.588398 1.921315

H 3.270402 2.478664 0.770936
C 5.017875 -0.779658 1.798067
H 3.638869 -1.792634 0.540559
C 5.467982 0.428036 2.306074
H 5.166125 2.552354 2.277363
H 5.528753 -1.702192 2.055428
H 6.324253 0.466167 2.969887
C 1.808735 1.615544 -1.016663
C 2.350395 2.092530 -2.218730
C 1.018159 2.520246 -0.295087
C 2.100308 3.379386 -2.662141
H 3.018994 1.477596 -2.802342
C 0.757903 3.814878 -0.733465
H 0.676855 2.258812 0.709315
C 1.296453 4.247326 -1.929969
H 2.558254 3.720751 -3.585137
H 0.145156 4.474717 -0.128446
H 1.115147 5.256566 -2.282980

$[LTh^{IV}SiPh_3]^+$. SCF energy = -2426.46177

C -1.574027 -3.426795 0.720551
C -2.144698 -4.569795 0.236146
H -2.138400 -5.536879 0.718808
C -2.734856 -4.243377 -1.007073
H -3.275885 -4.909085 -1.664629
C -2.510298 -2.912417 -1.219698
C -0.816048 -3.247147 1.996904
C -0.851245 -1.813595 2.416234
C -2.091669 -1.152814 2.523919
H -3.005023 -1.724079 2.387939
C -2.162367 0.215738 2.743892
C -0.964681 0.942075 2.884965
H -1.018559 2.016177 3.030660
C 0.258035 0.300012 2.827165
H 1.184565 0.849759 2.950333
C 0.314484 -1.075345 2.571744
H 1.283408 -1.555230 2.490207
C -3.453976 0.956577 2.673601
C -3.417214 1.913852 1.525246
C -4.180538 3.034176 1.348946
H -4.902993 3.427478 2.050138
C -3.861831 3.553108 0.073846
H -4.288423 4.426866 -0.398244
C -2.907259 2.734783 -0.463536
C -2.248694 2.856121 -1.799983
C -1.739451 1.523855 -2.242845
C -2.601455 0.412640 -2.255345
H -3.653212 0.560731 -2.028904
C -2.124084 -0.869663 -2.505716
C -0.753402 -1.043925 -2.751525
H -0.366029 -2.044645 -2.910236
C 0.102292 0.045759 -2.774837
H 1.157497 -0.097215 -2.975834
C -0.391661 1.327562 -2.518428
H 0.287564 2.171887 -2.509268
C -2.999636 -2.069342 -2.353912
N -1.777224 -2.369329 -0.165393
N -2.598081 1.701520 0.417583
Th -1.021614 -0.107570 0.087792
H -2.987167 -2.660359 -3.276794
H -4.036566 -1.746761 -2.199666
H 0.227957 -3.570350 1.904460
H -1.268797 -3.873844 2.774605
H -4.281432 0.242604 2.581364
H -3.617387 1.511518 3.604793
H -2.978979 3.235899 -2.524628
H -1.416311 3.569940 -1.787048
Si 2.126747 0.255693 -0.054292
C 2.898233 -1.131052 -1.100569
C 4.203741 -1.028427 -1.593962
C 2.222150 -2.333885 -1.319922
C 4.789803 -2.066651 -2.301604
H 4.784894 -0.129987 -1.405758
C 2.805597 -3.383454 -2.017184
H 1.216283 -2.475790 -0.924084
C 4.090343 -3.245778 -2.518220
H 5.802865 -1.960595 -2.676206
H 2.259487 -4.310156 -2.162970
H 4.551946 -4.060210 -3.066677
C 3.237615 0.314636 1.492716
C 3.591374 1.507346 2.130824
C 3.740710 -0.876364 2.028210
C 4.396993 1.509513 3.261022
H 3.258477 2.459069 1.727372
C 4.544883 -0.879506 3.158507
H 3.529851 -1.822204 1.533825
C 4.870996 0.315374 3.782735
H 4.666406 2.451245 3.728793
H 4.930723 -1.817638 3.544874
H 5.504741 0.316799 4.663282
C 2.293721 1.959074 -0.884685
C 2.946574 2.188687 -2.098116
C 1.643566 3.048908 -0.290735
C 2.947706 3.444770 -2.690871
H 3.463323 1.375577 -2.598959
C 1.647506 4.308969 -0.871653
H 1.116337 2.918695 0.654367
C 2.298534 4.508521 -2.080904
H 3.464867 3.595194 -3.633305
H 1.142970 5.135564 -0.381140
H 2.304350 5.489977 -2.543069

$[LTh^{IV}NPh_2]^+$. SCF energy = -1960.38059

C -3.200849 1.671837 0.128055
C -4.123625 2.425557 -0.543485
H -5.133314 2.632055 -0.217323
C -3.505289 2.873881 -1.731956
H -3.940801 3.502341 -2.495942
C -2.227831 2.386279 -1.724796
C -3.392083 0.957892 1.429848
C -2.075612 0.712005 2.090143
C -1.179913 1.780740 2.267236
H -1.503666 2.784323 2.008486
C 0.120894 1.569073 2.704987

C 0.530425 0.256507 2.992965
H 1.553850 0.083466 3.310246
C -0.357704 -0.799079 2.874899
H -0.037271 -1.809351 3.103620
C -1.657902 -0.572675 2.418601
H -2.335460 -1.408222 2.282794
C 1.123692 2.674072 2.723095
C 2.205590 2.405837 1.725885
C 3.478226 2.905867 1.732797
H 3.907845 3.538293 2.496847
C 4.100567 2.463846 0.544050
H 5.108132 2.680183 0.217689
C 3.185009 1.701324 -0.127413
C 3.382867 0.989399 -1.429282
C 2.068777 0.732129 -2.090019
C 1.163368 1.792797 -2.266305
H 1.477903 2.799072 -2.006638
C -0.135412 1.569619 -2.704345
C -0.532895 0.253619 -2.993503
H -1.554683 0.071543 -3.311013
C 0.364847 -0.793895 -2.876284
H 0.053696 -1.806865 -3.105894
C 1.662866 -0.556021 -2.419656
H 2.347965 -1.385487 -2.284413
C -1.148272 2.665423 -2.721530
N -2.003677 1.620827 -0.581186
N 1.988542 1.638539 0.582149
Th -0.001852 0.378155 -0.000018
H -1.593730 2.747782 -3.719505
H -0.649842 3.621547 -2.519573
H -3.909639 0.000219 1.297739
H -4.025579 1.571780 2.081692
H 0.616523 3.625803 2.522167
H 1.568523 2.759504 3.721097
H 4.011200 1.608946 -2.080761
H 3.908713 0.036236 -1.297243
N 0.009677 -1.911682 -0.000906
C -1.204820 -2.604573 0.034656
C -1.379246 -3.774373 0.784422
C -2.321176 -2.053120 -0.601601
C -2.630467 -4.351595 0.898003
H -0.524664 -4.223651 1.279444
C -3.579547 -2.624709 -0.461445
H -2.215745 -1.179171 -1.242892
C -3.740897 -3.777198 0.287401
H -2.744770 -5.260888 1.479332
H -4.429333 -2.174242 -0.963739
H -4.717962 -4.236396 0.384852
C 1.229977 -2.594331 -0.036070
C 1.413948 -3.763515 -0.784481
C 2.341785 -2.032946 0.599456
C 2.669837 -4.330710 -0.897292
H 0.563096 -4.220257 -1.279103
C 3.604714 -2.594523 0.460143
H 2.229271 -1.158744 1.239235
C 3.775474 -3.746648 -0.287228
H 2.791567 -5.239712 -1.477571
H 4.450811 -2.136538 0.961876
H 4.756245 -4.198025 -0.384008

$[LTh^{IV}PPh_2]^+$. SCF energy = -2246.87572

C -1.849216 -3.094559 -0.976586
C -2.508702 -3.775374 -1.961222
H -2.702084 -4.838740 -1.978202
C -2.877231 -2.828215 -2.944024
H -3.419560 -3.017719 -3.859578
C -2.437104 -1.610512 -2.507633
C -1.234986 -3.660768 0.264516
C -1.091944 -2.598063 1.303406
C -2.207027 -1.823561 1.659170
H -3.176518 -2.072434 1.238143
C -2.081557 -0.716603 2.495011
C -0.814426 -0.388702 2.997579
H -0.705174 0.493695 3.619441
C 0.287646 -1.173356 2.694848
H 1.259286 -0.928699 3.104228
C 0.150287 -2.271066 1.838468
H 1.020293 -2.862196 1.577855
C -3.230899 0.202605 2.741897
C -2.955266 1.545780 2.143837
C -3.544161 2.735228 2.470869
H -4.270195 2.889717 3.256543
C -3.040974 3.705462 1.574707
H -3.296485 4.755231 1.542179
C -2.156841 3.067129 0.750806
C -1.342993 3.661858 -0.353849
C -0.951928 2.599626 -1.327706
C -1.945520 1.781938 -1.898211
H -2.989126 2.001036 -1.693972
C -1.610166 0.682320 -2.680467
C -0.253733 0.387969 -2.893996
H 0.007388 -0.493773 -3.470040
C 0.736825 1.200553 -2.364004
H 1.783256 0.994552 -2.550839
C 0.381185 2.306102 -1.579554
H 1.160486 2.920908 -1.143603
C -2.649640 -0.278263 -3.152481
N -1.781751 -1.736539 -1.283273
N -2.072944 1.715371 1.077627
Th -0.725076 0.017400 0.009568
H -2.588105 -0.388110 -4.241383
H -3.645235 0.125255 -2.931421
H -0.252063 -4.106320 0.068686
H -1.873697 -4.467591 0.643876
H -4.145677 -0.241433 2.330566
H -3.392953 0.313480 3.820235
H -1.935770 4.432047 -0.861852
H -0.439518 4.157770 0.021214
P 2.075480 0.165223 0.420619
C 3.084413 -1.350178 0.514132
C 4.099829 -1.453576 1.469037
C 2.856742 -2.432254 -0.339377
C 4.858766 -2.607904 1.568364
H 4.298016 -0.619016 2.134591
C 3.609792 -3.593258 -0.229690
H 2.095157 -2.357983 -1.110694
C 4.611011 -3.682956 0.724739
H 5.646478 -2.671266 2.311895
H 3.424263 -4.422853 -0.904296

H	5.205603	-4.586539	0.806660
C	3.240323	1.465756	-0.086773
C	4.250645	1.227417	-1.022370
C	3.134906	2.739919	0.477354
C	5.121218	2.240865	-1.388896
H	4.364061	0.238163	-1.455167
C	3.999274	3.755401	0.096208
H	2.387288	2.926782	1.243076
C	4.993961	3.508918	-0.838073
H	5.905364	2.039099	-2.111412
H	3.909365	4.737431	0.549192
H	5.678298	4.299245	-1.127027

$LTh^{III}X^{+}$ complexes.

$LTh^{III}CPh_3$. SCF energy = -2175.28305

C	0.625729	-1.075952	3.163441
C	0.502840	-1.886690	4.265862
H	1.135948	-1.861342	5.142474
C	-0.592173	-2.749563	4.028625
H	-0.978022	-3.513292	4.689570
C	-1.094796	-2.414760	2.797314
C	1.650156	-0.015756	2.937562
C	1.128898	1.319189	2.471255
C	-0.238455	1.564215	2.363578
H	-0.937530	0.808763	2.715301
C	-0.742789	2.796539	1.949499
C	0.148621	3.819860	1.667830
H	-0.222999	4.791723	1.357148
C	1.515237	3.598943	1.793291
H	2.212777	4.402257	1.578652
C	2.005349	2.361565	2.173302
H	3.076534	2.203407	2.242768
C	-2.224662	2.945367	1.835697
C	-2.815482	2.436998	0.557770
C	-3.827719	3.075162	-0.117964
H	-4.235726	4.045159	0.133197
C	-4.261309	2.201746	-1.135305
H	-5.060393	2.362774	-1.846101
C	-3.482420	1.076690	-1.038343
C	-3.580202	-0.154584	-1.883828
C	-2.779566	-1.273198	-1.306249
C	-3.056515	-1.751561	0.015475
H	-3.896089	-1.332490	0.560110
C	-2.204163	-2.638073	0.632647
C	-1.066468	-3.112082	-0.083073
H	-0.372181	-3.775128	0.415499
C	-0.938658	-2.845816	-1.464409
H	-0.144818	-3.315085	-2.034701
C	-1.782569	-1.936519	-2.063830
H	-1.658943	-1.684086	-3.110262
C	-2.300315	-2.956037	2.089825
N	-0.353118	-1.389165	2.238534
N	-2.562554	1.195604	-0.006611
Th	-0.627984	-0.385324	0.026012
H	-2.357862	-4.041462	2.238794
H	-3.225794	-2.527220	2.494104
H	2.423363	-0.333380	2.222393
H	2.188864	0.132356	3.880624
H	-2.685974	2.427795	2.689970
H	-2.502640	3.999495	1.923884
H	-4.637823	-0.443209	-1.971399
H	-3.229878	0.040577	-2.905347
C	1.783109	0.130430	-1.103967
C	2.103945	-1.303171	-1.412260
C	2.564310	-1.736829	-2.664098
C	2.053538	-2.259595	-0.392834
C	2.903884	-3.058141	-2.891008
H	2.694887	-1.012012	-3.460240
C	2.408320	-3.586321	-0.610290
H	1.761329	-1.968221	0.616476
C	2.820682	-3.994337	-1.865207
H	3.261744	-3.359883	-3.870643
H	2.363967	-4.295054	0.210592
H	3.097971	-5.028013	-2.043416
C	2.988765	0.868685	-0.616473
C	3.296936	2.174242	-1.027746
C	3.946546	0.243804	0.197582
C	4.444281	2.825888	-0.607515
H	2.637390	2.693058	-1.712292
C	5.095386	0.893305	0.617192
H	3.808086	-0.789109	0.493957
C	5.352645	2.200058	0.232440
H	4.636185	3.835082	-0.960396
H	5.801938	0.361899	1.247914
H	6.253267	2.709440	0.557894
C	0.858979	0.857514	-1.988950
C	0.295525	0.356398	-3.179045
C	0.306646	2.077425	-1.524836
C	-0.651963	1.074242	-3.897436
H	0.631486	-0.593911	-3.571997
C	-0.644446	2.785092	-2.241270
H	0.659844	2.485986	-0.580906
C	-1.120667	2.298170	-3.448204
H	-1.028123	0.660229	-4.828780
H	-1.041811	3.705981	-1.828809
H	-1.870668	2.845770	-4.006810

$LTh^{III}SiPh_3$. SCF energy = -2426.623483

C	-1.653958	-3.448712	0.823590
C	-2.184742	-4.633710	0.379799
H	-2.174398	-5.574230	0.913587
C	-2.727468	-4.382273	-0.900054
H	-3.227439	-5.088131	-1.548934
C	-2.513898	-3.053312	-1.164847
C	-0.911789	-3.201652	2.098295
C	-0.955636	-1.752376	2.457581
C	-2.197454	-1.093906	2.512029
H	-3.103657	-1.672237	2.360706
C	-2.282460	0.273620	2.709022
C	-1.094388	1.010795	2.857865
H	-1.157785	2.087234	2.980338
C	0.130568	0.374427	2.836213
H	1.051125	0.933243	2.962186
C	0.199956	-1.006815	2.623373

H 1.171520 -1.484554 2.577207
C -3.586745 0.991657 2.626223
C -3.579320 1.900804 1.440415
C -4.369568 2.999012 1.212252
H -5.106660 3.405477 1.891643
C -4.045736 3.468405 -0.080598
H -4.476923 4.315707 -0.595970
C -3.064756 2.640324 -0.566196
C -2.349484 2.700340 -1.876050
C -1.763977 1.366451 -2.210534
C -2.604157 0.217920 -2.320507
H -3.676518 0.338651 -2.197132
C -2.073366 -1.043334 -2.479734
C -0.655180 -1.196256 -2.563261
H -0.234623 -2.187292 -2.672061
C 0.156355 -0.045175 -2.683899
H 1.216730 -0.153174 -2.880063
C -0.385897 1.210180 -2.508941
H 0.254464 2.084230 -2.546508
C -2.923890 -2.265713 -2.368649
N -1.847007 -2.449438 -0.113851
N -2.754284 1.659434 0.356594
Th -1.051444 -0.111956 -0.072344
H -2.811686 -2.887620 -3.265505
H -3.978840 -1.968144 -2.315852
H 0.136510 -3.519235 2.027631
H -1.364296 -3.798537 2.900298
H -4.400057 0.256521 2.572254
H -3.750119 1.578363 3.538424
H -3.048586 3.029813 -2.657248
H -1.541388 3.443600 -1.854970
Si 2.150392 0.212200 -0.022710
C 3.185784 -0.988566 -1.092706
C 4.524008 -0.714117 -1.396222
C 2.673295 -2.215114 -1.518577
C 5.301915 -1.608981 -2.114498
H 4.974355 0.212242 -1.049512
C 3.447545 -3.122684 -2.230281
H 1.644919 -2.476220 -1.279194
C 4.763676 -2.817029 -2.536531
H 6.336836 -1.367902 -2.338259
H 3.021024 -4.071187 -2.542502
H 5.372911 -3.520899 -3.094889
C 3.217633 0.269293 1.572908
C 3.570656 1.449811 2.233056
C 3.668540 -0.930734 2.135619
C 4.320560 1.433779 3.402021
H 3.274623 2.408755 1.817407
C 4.417289 -0.955304 3.302497
H 3.450565 -1.872006 1.634643
C 4.742610 0.230488 3.945592
H 4.584780 2.370072 3.884959
H 4.757225 -1.904204 3.706855
H 5.330827 0.216306 4.857590
C 2.289424 1.974872 -0.750492
C 2.949685 2.294953 -1.939396
C 1.579108 3.007043 -0.123565
C 2.904496 3.576612 -2.472798
H 3.505566 1.527340 -2.469691
C 1.533820 4.292052 -0.644056
H 1.035852 2.805422 0.799651
C 2.197768 4.580809 -1.827893
H 3.426238 3.792162 -3.400596
H 0.973404 5.066735 -0.129450
H 2.162027 5.581702 -2.245760

$LTh^{III}NPh_2$. SCF = -1960.53762

C -1.822886 3.020416 0.405241
C -2.217818 4.249439 -0.063597
H -2.966740 4.887889 0.385394
C -1.478528 4.498673 -1.241771
H -1.532673 5.373053 -1.875632
C -0.655212 3.416864 -1.424161
C -2.402431 2.280303 1.568013
C -1.438093 1.355194 2.249411
C -0.093961 1.721867 2.395781
H 0.222199 2.702916 2.051057
C 0.838877 0.868663 2.977358
C 0.405994 -0.372257 3.450460
H 1.126144 -1.052414 3.895272
C -0.927134 -0.729773 3.352234
H -1.257146 -1.694364 3.723583
C -1.842374 0.120183 2.743034
H -2.876265 -0.188765 2.629226
C 2.280875 1.264987 3.025173
C 3.085416 0.587734 1.963381
C 4.407654 0.224835 2.039396
H 5.042065 0.320208 2.910478
C 4.774544 -0.252026 0.761889
H 5.745611 -0.614223 0.452744
C 3.653333 -0.170099 -0.026450
C 3.502687 -0.586417 -1.459134
C 2.207741 -0.117434 -2.040425
C 1.953959 1.274795 -2.224427
H 2.734610 1.986526 -1.970076
C 0.705758 1.737204 -2.577025
C -0.340058 0.789668 -2.845581
H -1.322726 1.148241 -3.124407
C -0.016778 -0.584832 -2.916981
H -0.774046 -1.299368 -3.221587
C 1.220138 -1.035953 -2.513022
H 1.431200 -2.100197 -2.495483
C 0.359345 3.188636 -2.503331
N -0.847756 2.486529 -0.416956
N 2.589372 0.343202 0.694710
Th 0.294227 0.317090 -0.228795
H -0.049566 3.530008 -3.462951
H 1.273951 3.767562 -2.323021
H -3.282251 1.695131 1.268505
H -2.765207 3.017641 2.296242
H 2.345807 2.357776 2.928706
H 2.708058 1.010056 4.000693
H 4.349833 -0.195498 -2.040507
H 3.551233 -1.679238 -1.548899
N -1.159583 -1.529383 -0.013377
C -2.548524 -1.610428 -0.040731
C -3.248269 -2.679726 0.534248
C -3.295823 -0.558147 -0.583024
C -4.631867 -2.686973 0.563320

H -2.691992 -3.504054 0.968278
C -4.680422 -0.565692 -0.536334
H -2.783171 0.277421 -1.056520
C -5.361415 -1.630812 0.033695
H -5.148147 -3.528235 1.016100
H -5.230028 0.267076 -0.964163
H -6.445406 -1.641125 0.060820
C -0.377741 -2.669713 -0.151580
C -0.690879 -3.721101 -1.031863
C 0.858709 -2.722316 0.508477
C 0.209563 -4.741667 -1.256111
H -1.645837 -3.711769 -1.546357
C 1.774295 -3.736969 0.248544
H 1.097061 -1.994778 1.283088
C 1.457268 -4.752162 -0.633488
H -0.055379 -5.540463 -1.942525
H 2.728491 -3.732261 0.765481
H 2.159985 -5.555090 -0.826389

LTh^{III}PPh$_2$. SCF energy = -2247.03916

C -2.066105 3.090992 0.446165
C -2.648401 3.951005 1.342814
H -2.962259 4.965858 1.140243
C -2.745932 3.255162 2.569798
H -3.159953 3.621947 3.499338
C -2.229520 2.003317 2.353112
C -1.693315 3.335899 -0.980624
C -1.535383 2.042280 -1.714426
C -2.619107 1.135657 -1.803420
H -3.568805 1.410671 -1.352307
C -2.454852 -0.135535 -2.314449
C -1.181336 -0.501547 -2.868106
H -1.045412 -1.495259 -3.275863
C -0.186812 0.474799 -3.000396
H 0.739782 0.229611 -3.503568
C -0.325605 1.712418 -2.397015
H 0.480011 2.436012 -2.446292
C -3.512297 -1.180770 -2.188865
C -3.018470 -2.298390 -1.326056
C -3.475901 -3.590176 -1.259134
H -4.271603 -4.015230 -1.855354
C -2.722249 -4.236184 -0.254339
H -2.815427 -5.261554 0.076798
C -1.831634 -3.310424 0.228390
C -0.782158 -3.512246 1.274811
C -0.388301 -2.203357 1.877630
C -1.381519 -1.359828 2.410382
H -2.407966 -1.711907 2.441602
C -1.078586 -0.085289 2.858192
C 0.247565 0.372292 2.757700
H 0.478218 1.386183 3.067895
C 1.236611 -0.451630 2.253543
H 2.261348 -0.106913 2.180803
C 0.915561 -1.742434 1.818136
H 1.693004 -2.369825 1.397352
C -2.149113 0.854218 3.304409
N -1.795817 1.874243 1.045911
N -1.993923 -2.097894 -0.417955
Th -0.707047 -0.001489 -0.164563
H -1.925507 1.225617 4.311813
H -3.100336 0.310632 3.370692
H -0.753172 3.899005 -1.052675
H -2.459835 3.963270 -1.455650
H -4.422127 -0.726113 -1.776233
H -3.775605 -1.575516 -3.178525
H -1.174318 -4.178397 2.053731
H 0.113064 -3.999576 0.868032
P 2.144536 -0.154670 -0.990474
C 2.875506 1.491973 -0.665865
C 4.117115 1.834879 -1.215383
C 2.189569 2.484965 0.039052
C 4.644182 3.105138 -1.061132
H 4.668103 1.088406 -1.779597
C 2.701541 3.769287 0.172218
H 1.236271 2.266544 0.519214
C 3.934482 4.083289 -0.374574
H 5.610908 3.341061 -1.495541
H 2.137259 4.517989 0.719688
H 4.343501 5.082366 -0.265892
C 3.351088 -1.326805 -0.294175
C 4.377679 -0.994137 0.595921
C 3.232820 -2.670550 -0.676490
C 5.240434 -1.963929 1.085200
H 4.510564 0.039066 0.901894
C 4.085518 -3.638853 -0.174598
H 2.462919 -2.951417 -1.391248
C 5.098032 -3.291804 0.710643
H 6.031680 -1.676213 1.771341
H 3.969147 -4.671369 -0.490222
H 5.774211 -4.047436 1.096175