Electronic Supplementary Material (ESI) for Chemical Science.

Supporting Information for:

Thorium-ligand multiple bonds via reductive deprotection of a trityl group

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Experimental Details

$[Na(THF)_{4.5}][Th(Cl)_2(NR_2)_3]$ (R = $SiMe_3$)

This procedure was adapted from the previously reported synthesis.[1] To a cold (-25 °C), stirring solution of $ThCl_4(DME)_2$[2] (465.5 mg, 0.84 mmol) in THF (6 mL) was added a cold (-25 °C) solution of $NaNR_2$ (462.0 mg, 2.52 mmol) in THF (6 mL). This mixture was allowed to stir for 72 h, during which time the deposition of a fine white solid was observed. The solvent was then removed in vacuo, and the resulting white solid triturated with diethyl ether (4 mL) and pentane (4 mL). The white powder was then extracted with THF (6 mL) and filtered through a Celite column supported on a glass frit (2 cm × 3 cm). The volume of this filtrate was reduced in vacuo to 5 mL and layered with pentane (8 mL). Storage of this mixture at -25 °C for 24 h resulted in the deposition of colorless needles (595.2 mg, 63%). Melting point = 196-199 °C. ^{1}H NMR (400 MHz, 25 °C, benzene-d_6): δ 0.41 (s, NSiCH_3), 1.41 (m, OCH_2CH_2), 3.59 (m, OCH_2CH_2). $^{13}C\{^1H\}$ NMR (100 MHz, 25 °C, benzene-d_6): δ 4.26 (NSiCH_3), 25.81 (OCH_2CH_2), 68.00 (OCH_2CH_2). IR (KBr pellet, cm^{-1}): 612 (s), 657 (m), 678 (m), 772 (s), 832 (s), 850 (s), 922 (s), 1073 (m), 1183 (w), 1248 (s), 1407 (m).

Synthesis of $[Th(OCPh_3)_2(NR_2)_2]$ (5, R = $SiMe_3$)

To a colorless, stirring solution of $[Th(Cl)(NR_2)_3]$ (**1**) (118.5 mg, 0.16 mmol) in benzene (3 mL) was added a colorless solution of $KOCPh_3$ (134.0 mg, 0.45 mmol) in benzene (3 mL). This was allowed to stir for 12 h, whereupon the solvent was removed in vacuo to afford a white solid. The solid was triturated with pentane (2 × 3 mL). The resulting white powder was extracted with hexanes (9 mL) and filtered through a Celite column supported on glass wool (0.5 cm × 3 cm) to afford a colorless filtrate. The volume of this filtrate was reduced to 3 mL in vacuo. Storage of this solution at -25 °C for 24 h resulted in the deposition of colorless crystals, which were isolated by decanting off the supernatant (56.9 mg, 34%). Anal. Calcd for $C_{49}H_{66}N_2O_2Si_4Th$: C, 55.55; H, 6.28; N, 2.64. Found: C, 55.64; H, 6.58; N, 2.68. ^{1}H NMR (400 MHz, 25 °C, benzene-d_6): δ 0.26 (s, 36H, NSiCH_3), 7.05-7.07 (m, 18H, *m*-C*H* and *p*-C*H*), 7.36-7.40 (m, 12H, *o*-C*H*). $^{13}C\{^1H\}$ NMR (100 MHz, 25 °C, benzene-d_6): δ 4.18 (NSiCH_3), 94.87 ($C(C_6H_5)_3$), 127.25 (*p*-*C*), 129.26 (*m*-*C*), 149.12 (C_{ipso}). The resonance assignable to the *o*-*C* was not observed due to overlap with the benzene-d_6 resonance. IR (KBr Pellet, cm^{-1}): 475 (m), 503 (w), 604 (m), 639 (m), 654 (m), 675 (m), 699 (s), 764 (s), 786 (s), 830 (s), 844 (s), 870 (s), 902 (m), 941 (s), 1012 (s), 1034 (m), 1051 (s), 1088 (m), 1158 (m), 1183 (w), 1208 (w), 1250 (s), 1316 (w), 1398 (w), 1445 (s), 1490 (m), 1598 (m).

Complex 5 Structural Details: Crystals of **5** suitable for X-ray diffraction were grown from a concentrated hexanes solution stored at -25 °C for 24 h. Complex **5** crystallizes in the triclinic spacegroup $P\bar{1}$ as a hexanes solvate, **5**·0.5C_6H_{14}. Complex **5** exhibits Th-O bond lengths (2.131(2) and 2.123(2) Å) comparable to those reported for other complexes with Th-O single bonds (av. 2.20 Å).[3-8] Additionally, in the solid state **5** features a tetrahedral geometry around thorium center with an average L-Th-L angle of 109.3° and a τ_4 value of 0.96.[9] Further crystallographic details can be found in Table S2 and Figure S20.

Raman Spectroscopy: Raman spectra were recorded on a LabRam Aramis microRaman system (Horiba Jobin Yvon) equipped with 1200 grooves/mm holographic gratings, and Peltier-cooled CCD camera. The 633 nm ouput of a Melles Griot He-Ne laser was used to excite the spectra, which were collected in a back scattering geometry using a confocal Raman Microscope (high stability BX40) equipped with Olympus objectives (MPlan 50x). Sample preparation was performed inside the glovebox: Pure crystalline solid samples were placed between a glass microscope slide and coverslip, sealed with a bead of silicone grease, and removed from the glovebox for spectral acquisition.

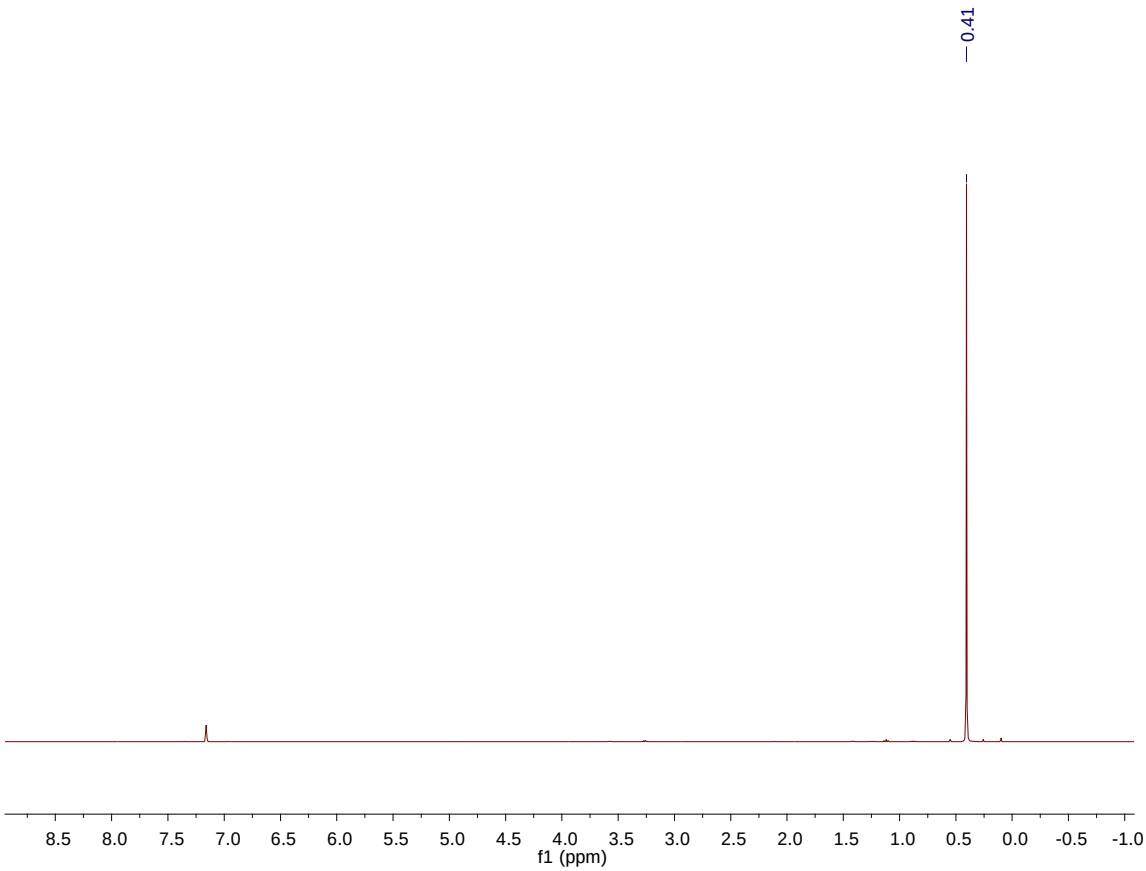


Figure S1. ^{1}H NMR spectrum of [Th(Cl)(NR_2)$_3$] (**1**) in benzene-d_6.

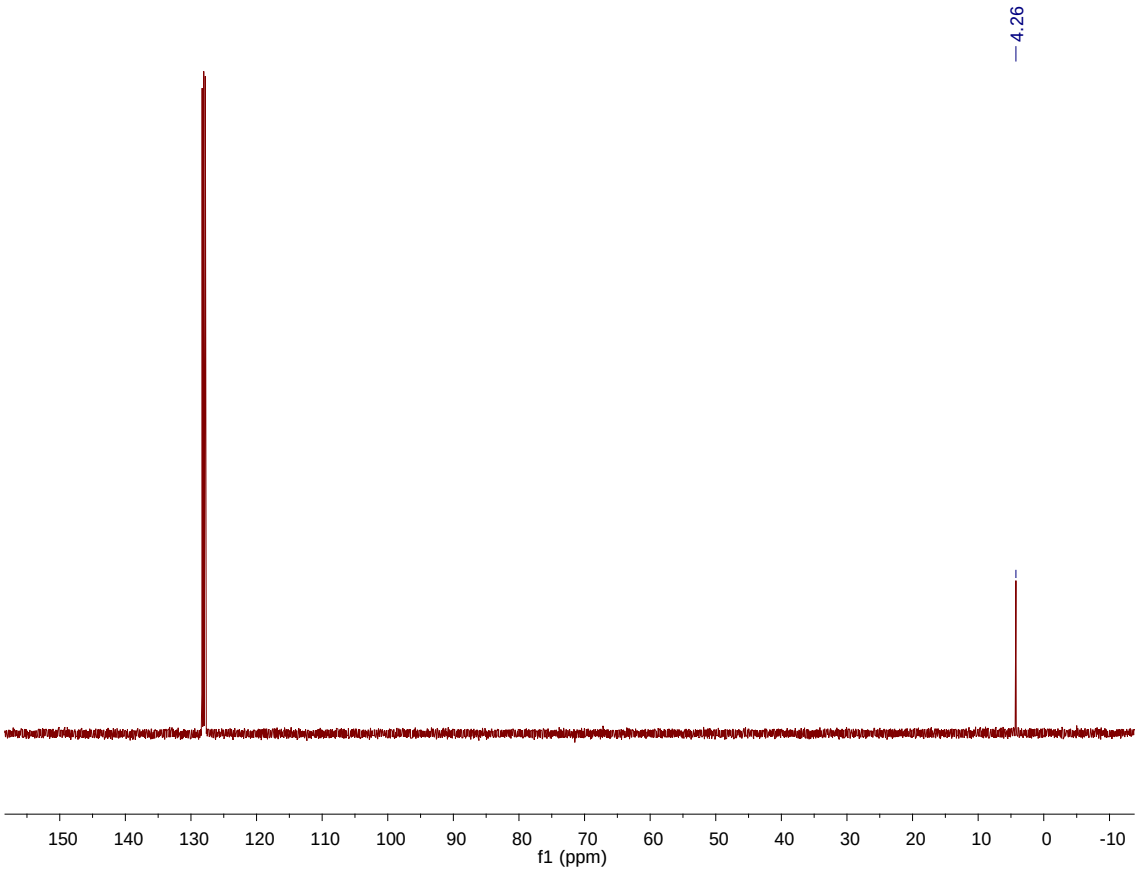


Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of $[Th(Cl)(NR_2)_3]$ (**1**) in benzene-d_6.

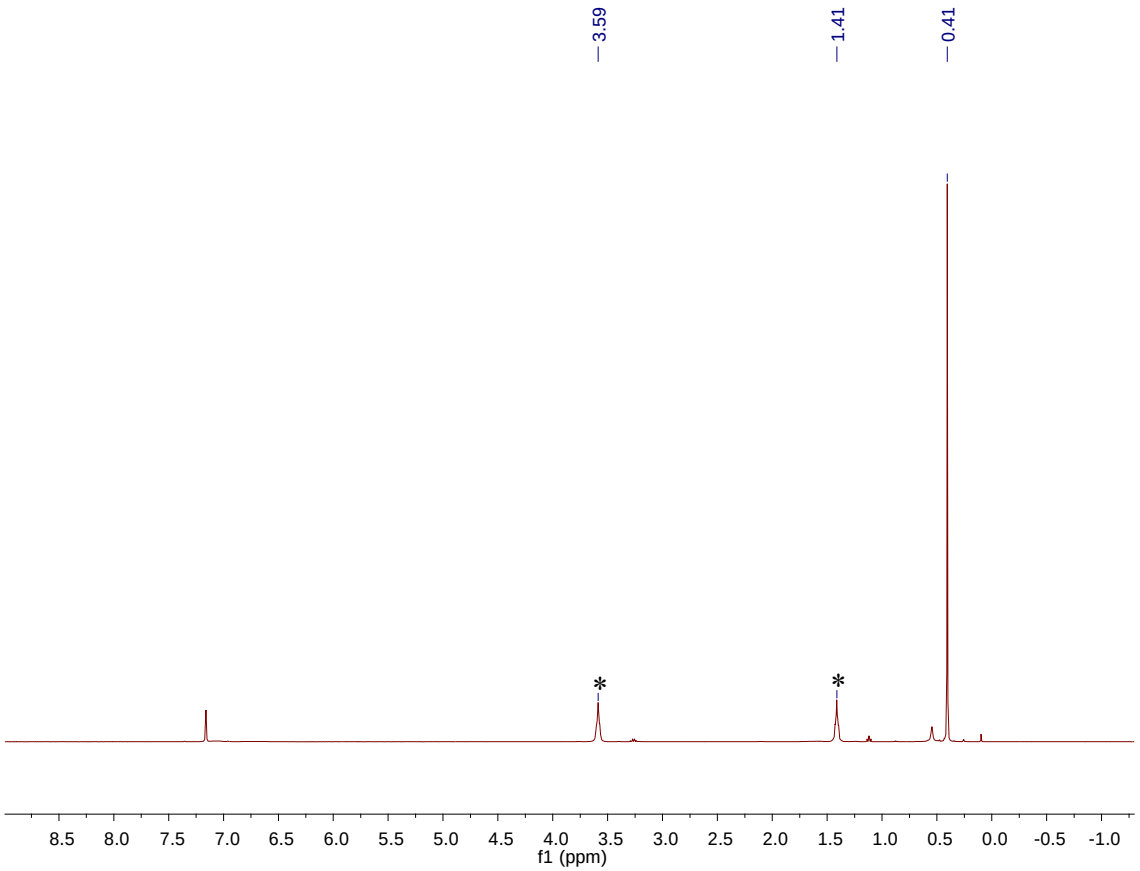


Figure S3. ^{1}H NMR spectrum of $[Na(THF)_{4.5}][Th(Cl)_2(NR_2)_3]$ in benzene-d_6. (*) are assignable to THF that is coordinated to Na^+.

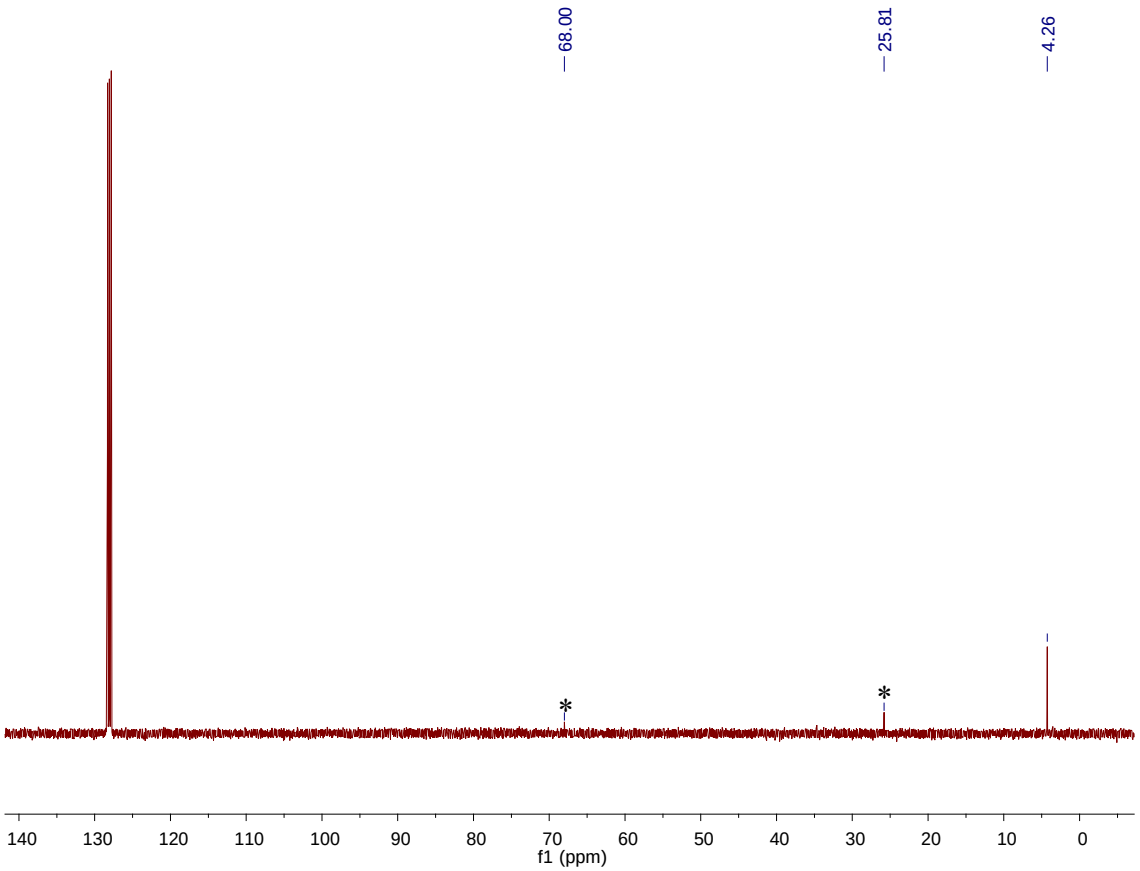


Figure S4. $^{13}C\{^{1}H\}$ NMR spectrum of $[Na(THF)_{4.5}][Th(Cl)_2(NR_2)_3]$ in benzene-d_6. (*) are assignable to THF that is coordinated to Na^+.

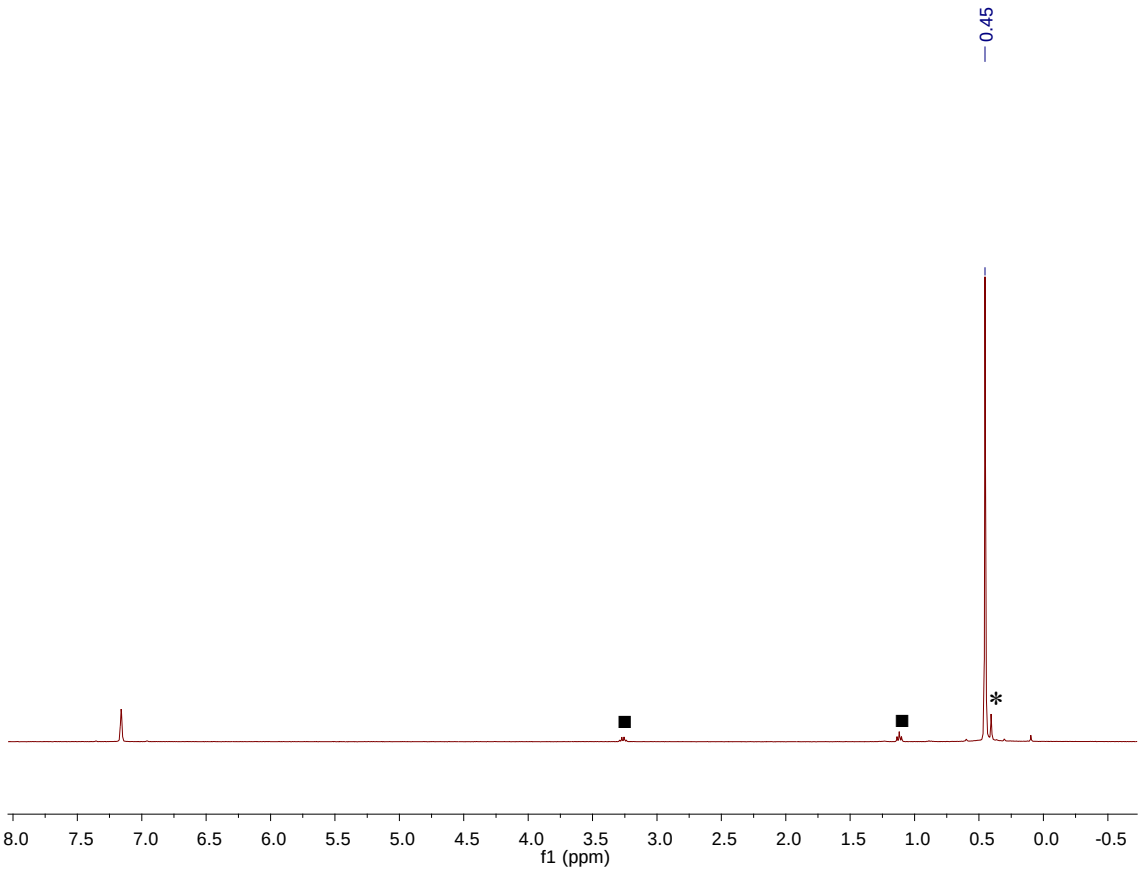


Figure S5. ^{1}H NMR spectrum of [Th(I)(NR_2)$_3$] (**2**) in benzene-d_6. (*) indicates the presence of [Th(Cl)(NR_2)$_3$], and (■) indicates the presence of diethyl ether.

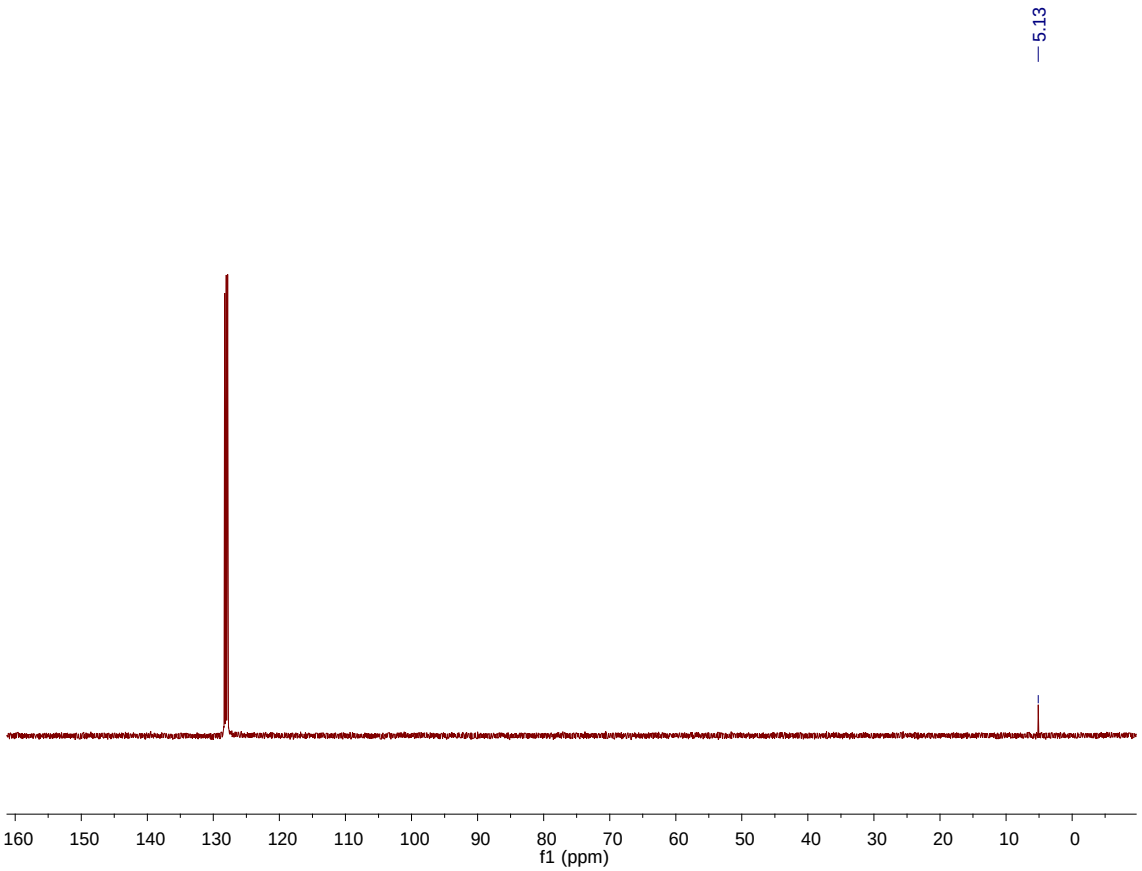


Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum of [Th(I)$(NR_2)_3$] (**2**) in benzene-d_6.

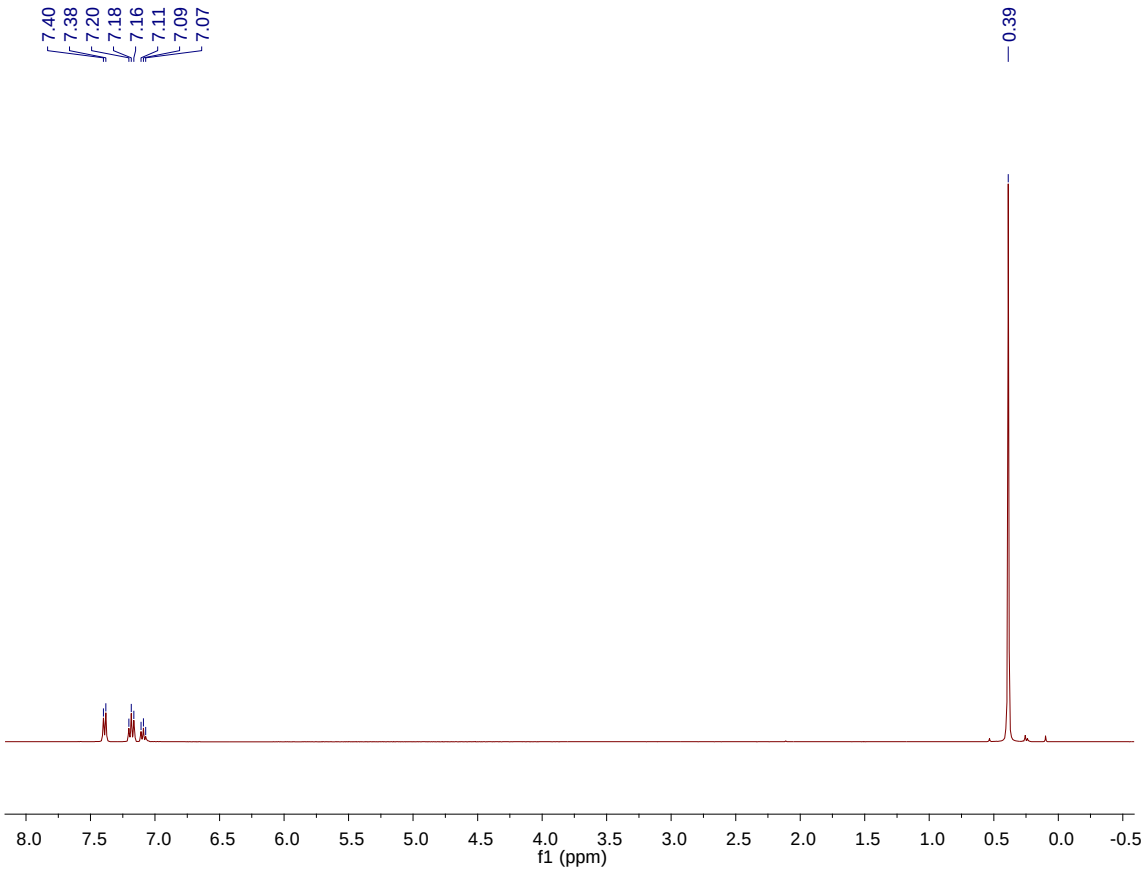


Figure S7. ^{1}H NMR spectrum of [Th(OCPh$_3$)(NR$_2$)$_3$] (**3**) in benzene-d_6.

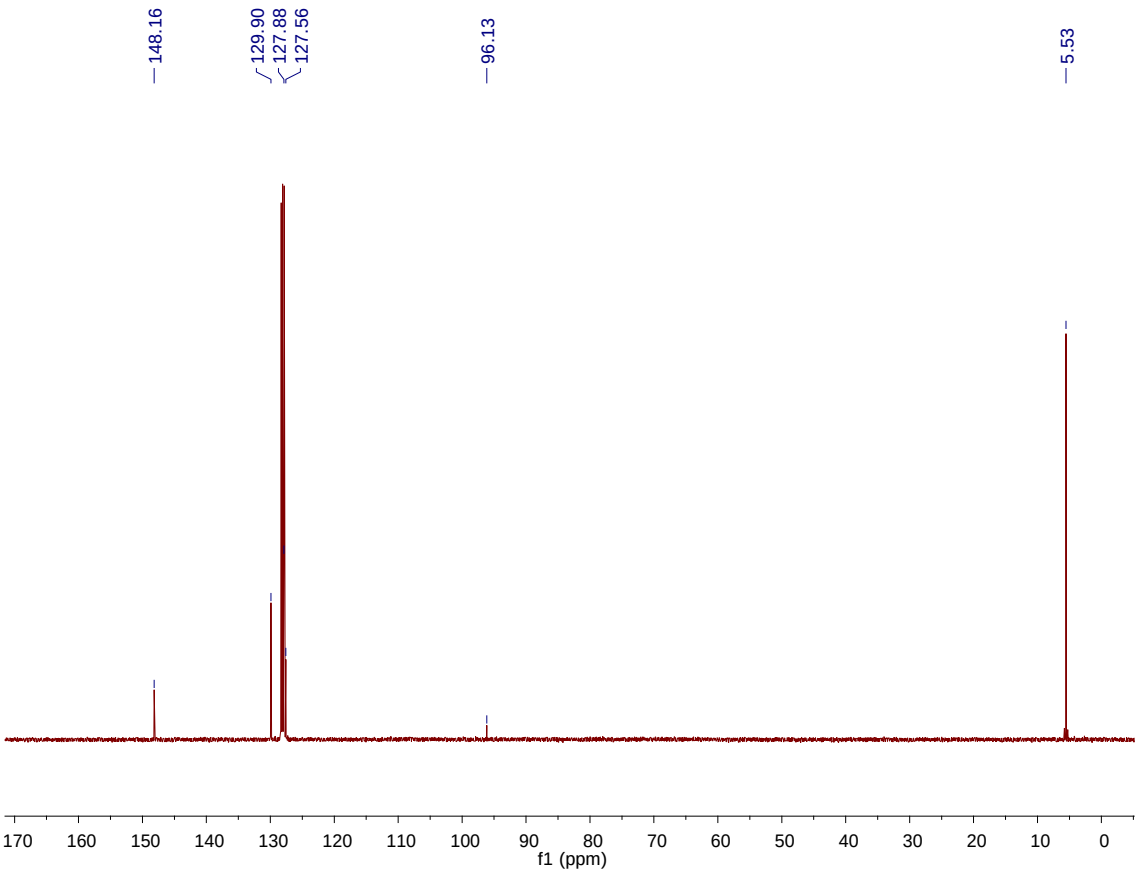


Figure S8. $^{13}C\{^{1}H\}$ NMR spectrum of $[Th(OCPh_3)(NR_2)_3]$ (**3**) in benzene-d_6.

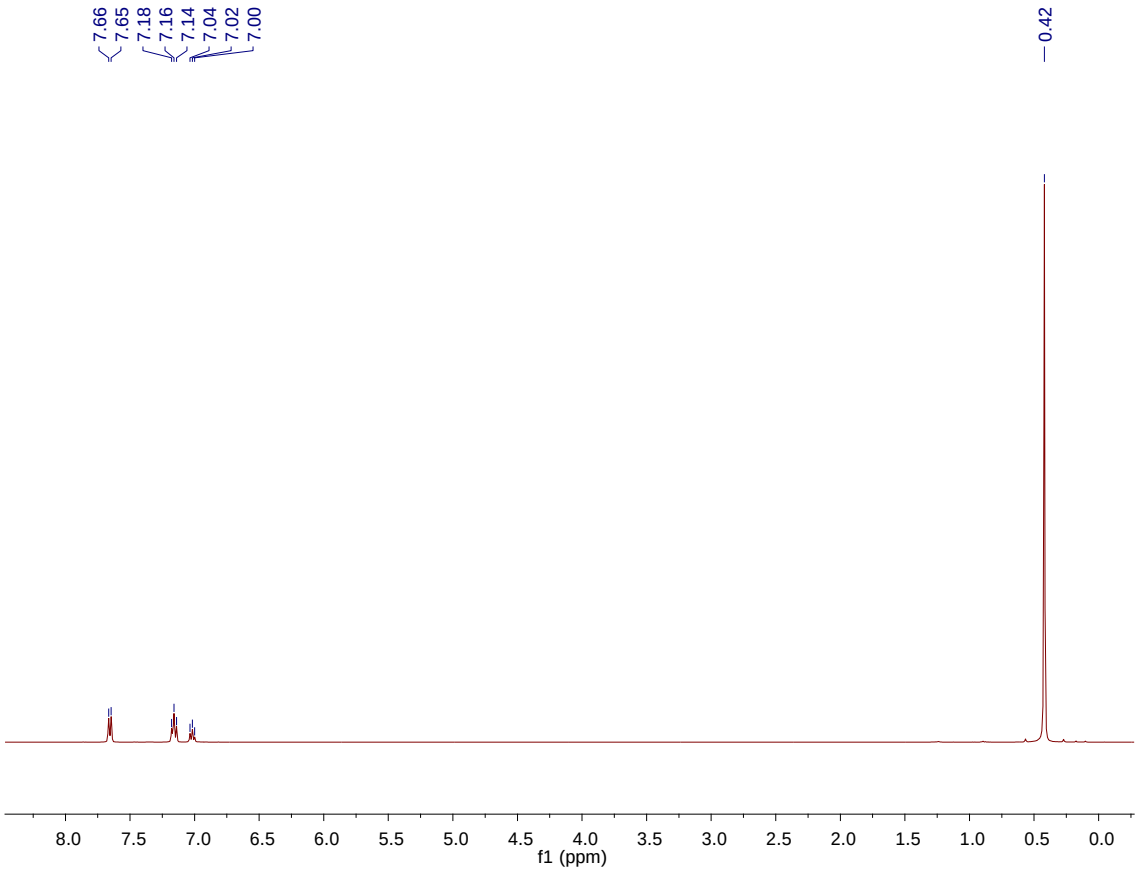


Figure S9. ^{1}H NMR spectrum of [Th(SCPh$_3$)(NR$_2$)$_3$] (**4**) in benzene-d_6.

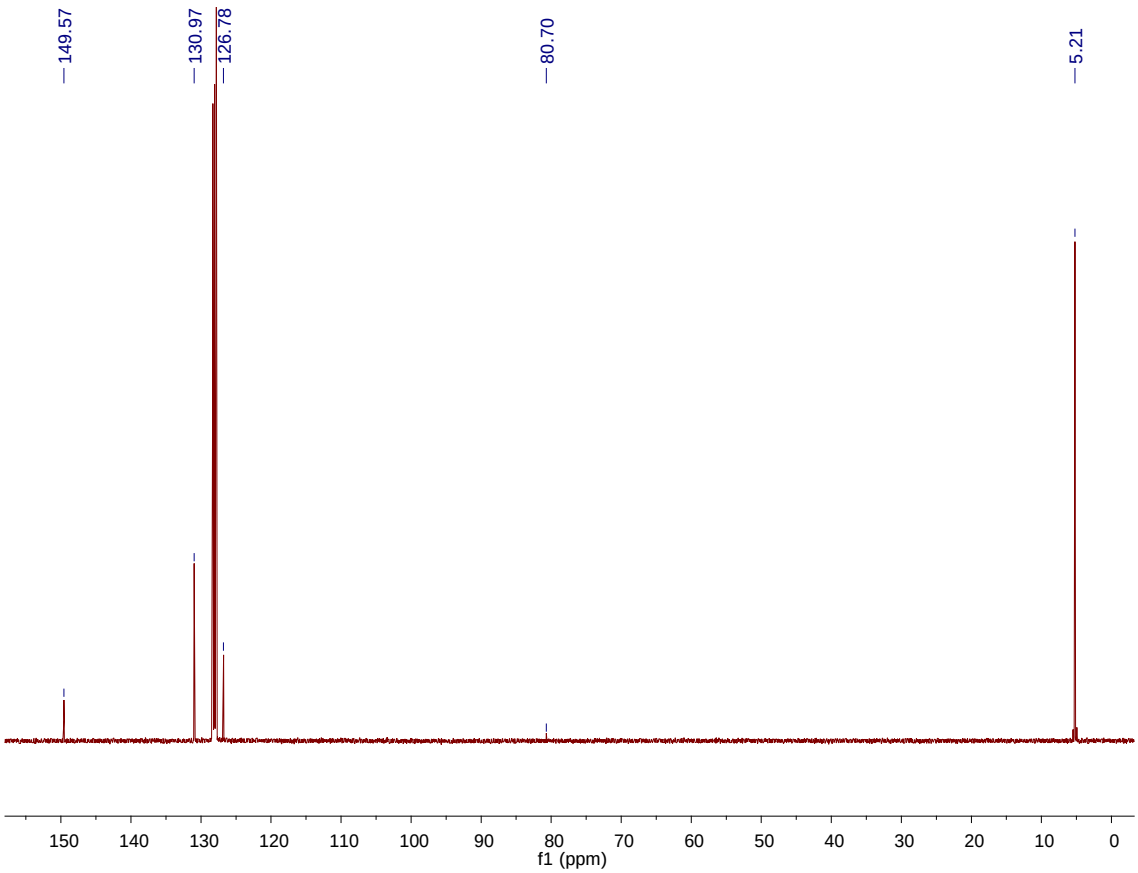


Figure S10. $^{13}C\{^{1}H\}$ NMR spectrum of $[Th(SCPh_3)(NR_2)_3]$ (**4**) in benzene-d_6.

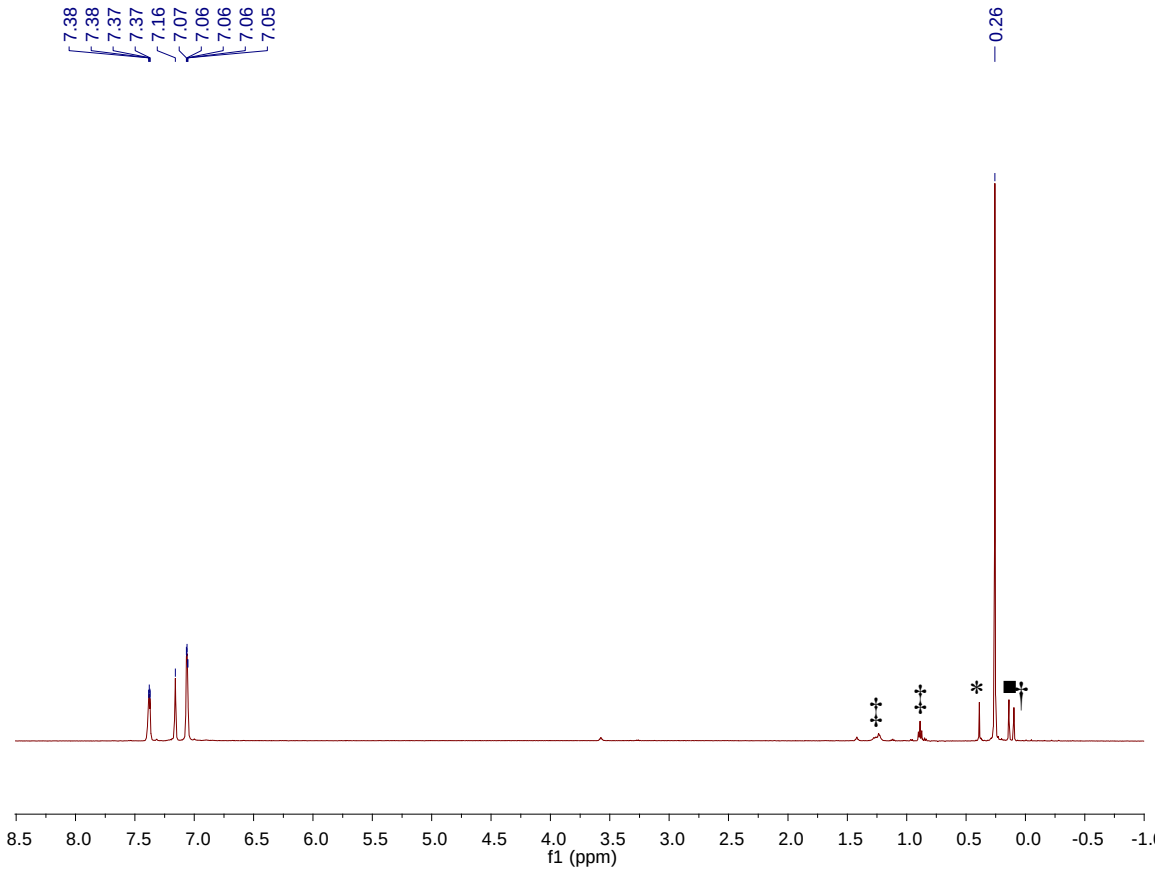


Figure S11. ^{1}H NMR spectrum of [Th(OCPh$_3$)$_2$(NR$_2$)$_2$] (**5**) in benzene-d_6. (*) indicates the presence of **3**, (■) indicates the presence of KN(SiMe$_3$)$_2$, (†) indicates the presence of HN(SiMe$_3$)$_2$, and (‡) indicates the presence of hexanes.

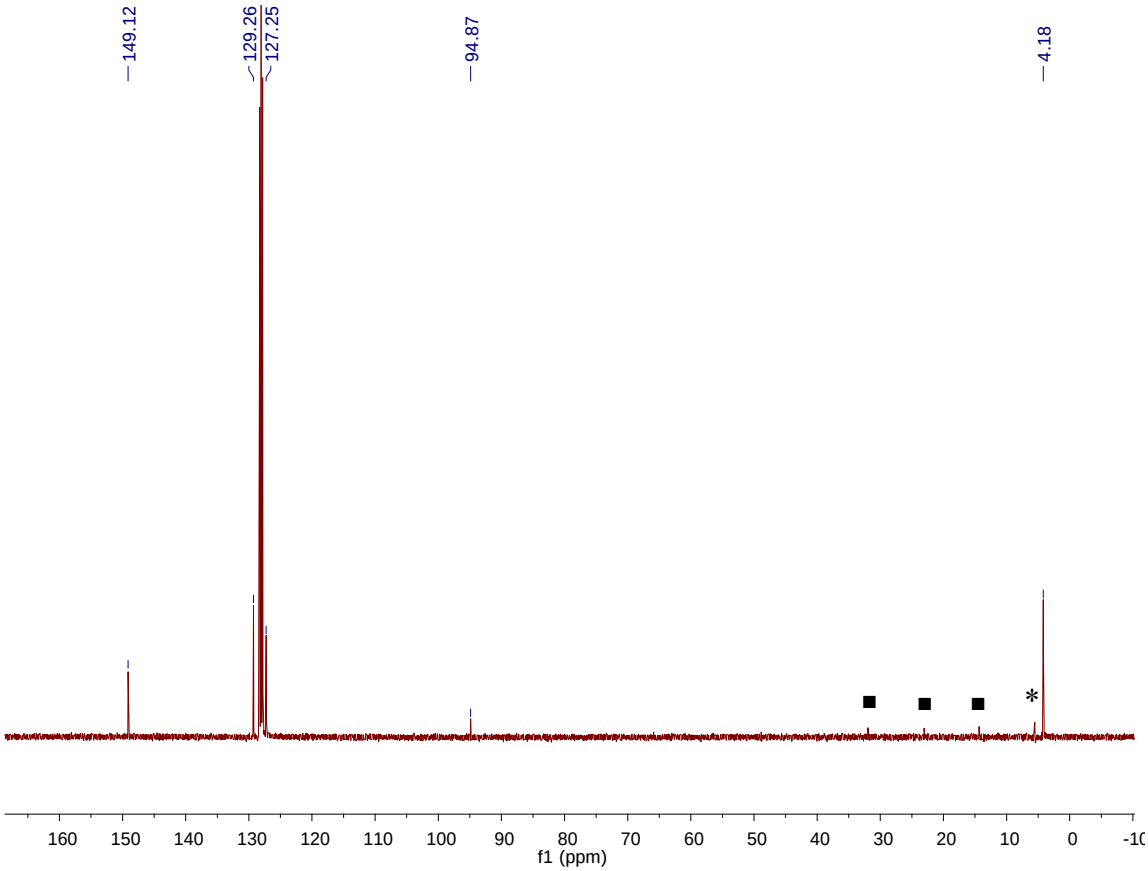


Figure S12. $^{13}C\{^{1}H\}$ NMR spectrum of of $[Th(OCPh_3)_2(NR_2)_2]$ (**5**) in benzene-d_6. (*) indicates the presence of **3**, and (■) indicates the presence of hexanes.

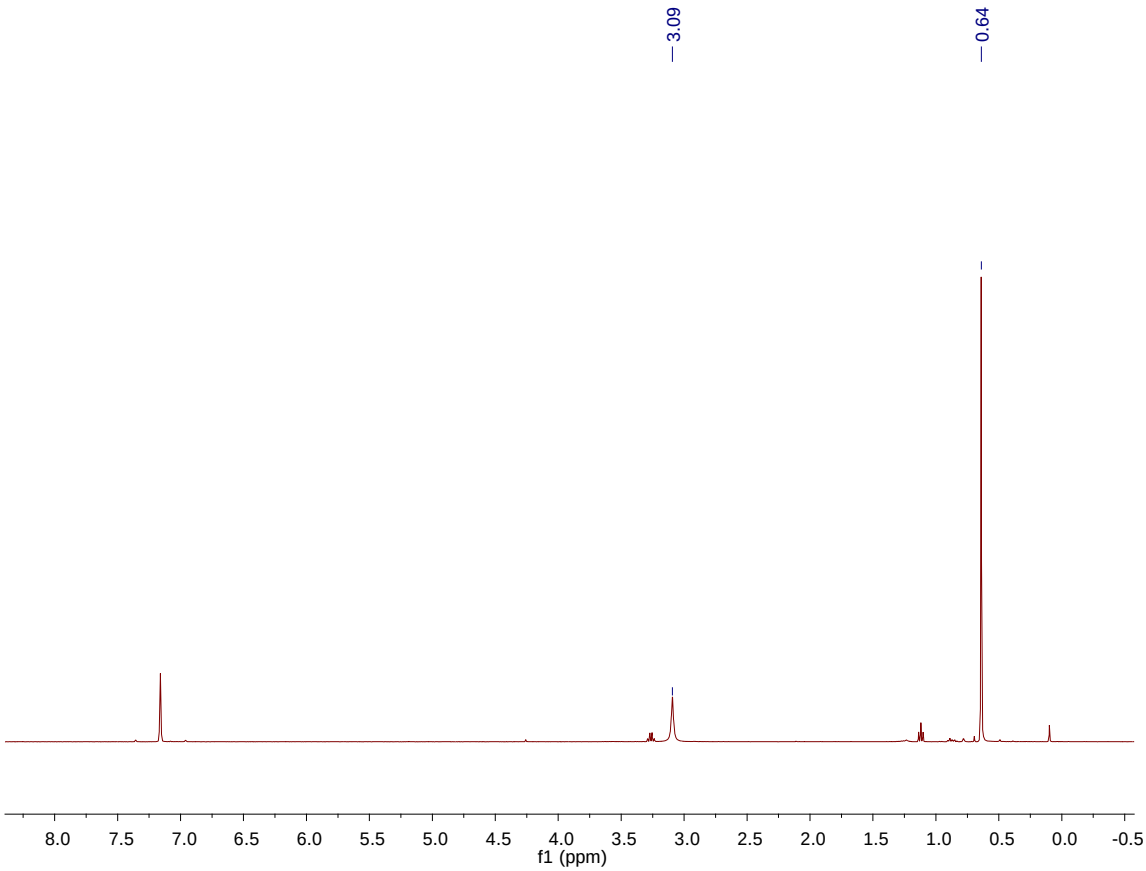


Figure S13. ^{1}H NMR spectrum of [K(18-crown-6)][Th(O)(NR_2)$_3$] (**6**) in benzene-d_6.

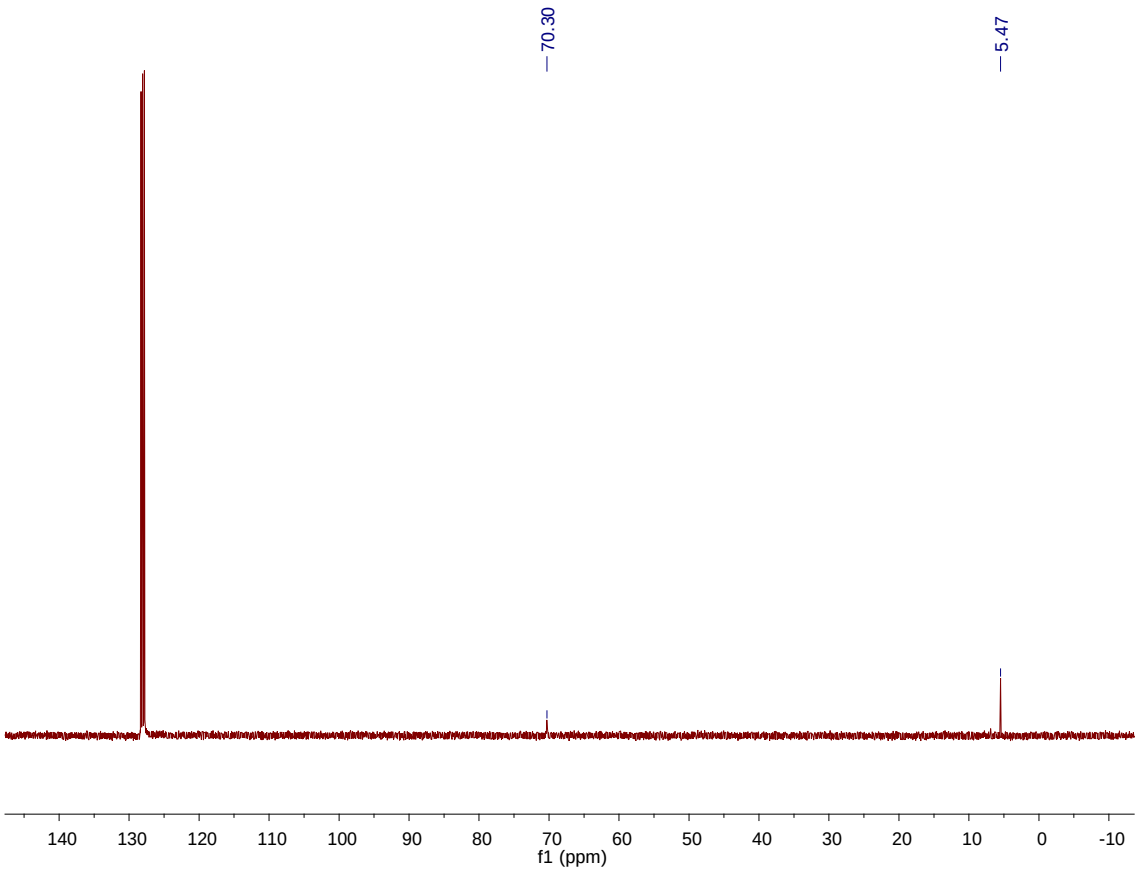


Figure S14. $^{13}C\{^{1}H\}$ NMR spectrum of [K(18-crown-6)][Th(O)(NR_2)$_3$] (**6**) in benzene-d_6.

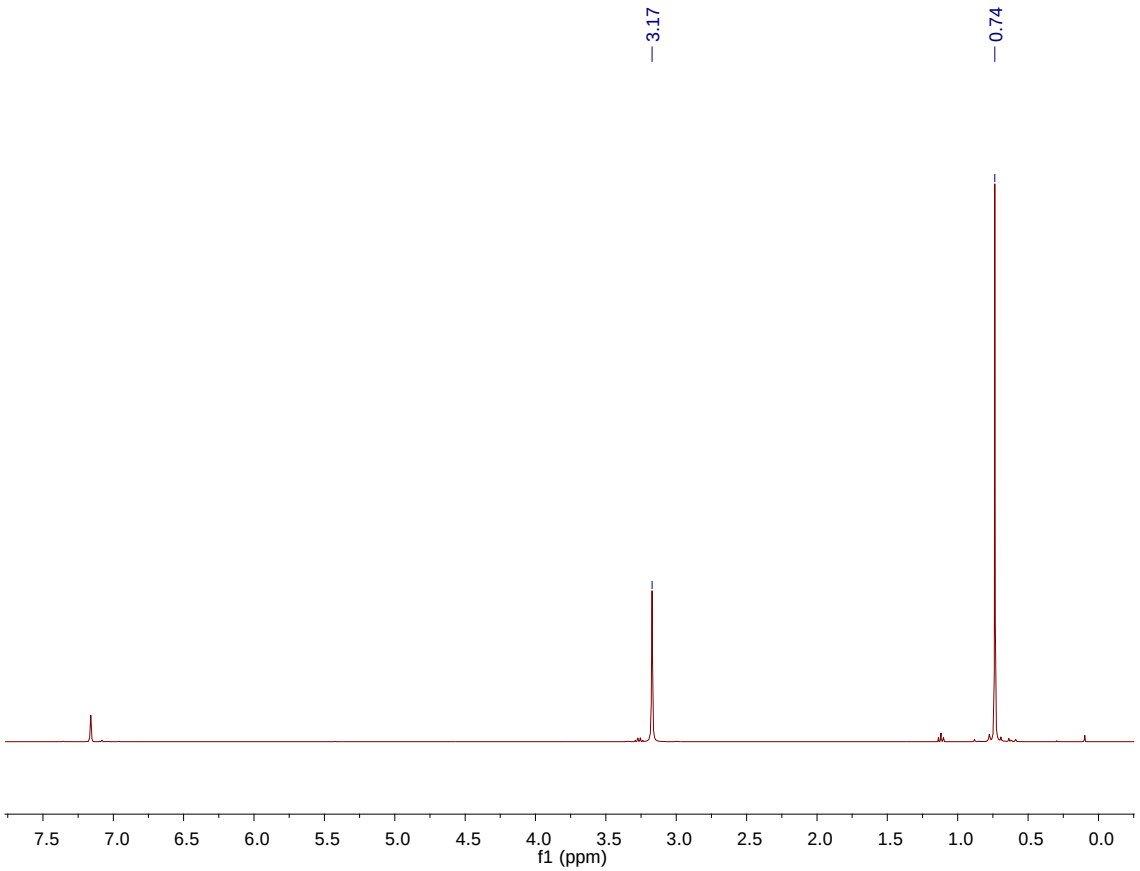


Figure S15. ^{1}H NMR spectrum of [K(18-crown-6)][Th(S)(NR_2)$_3$] (**7**) in benzene-d_6.

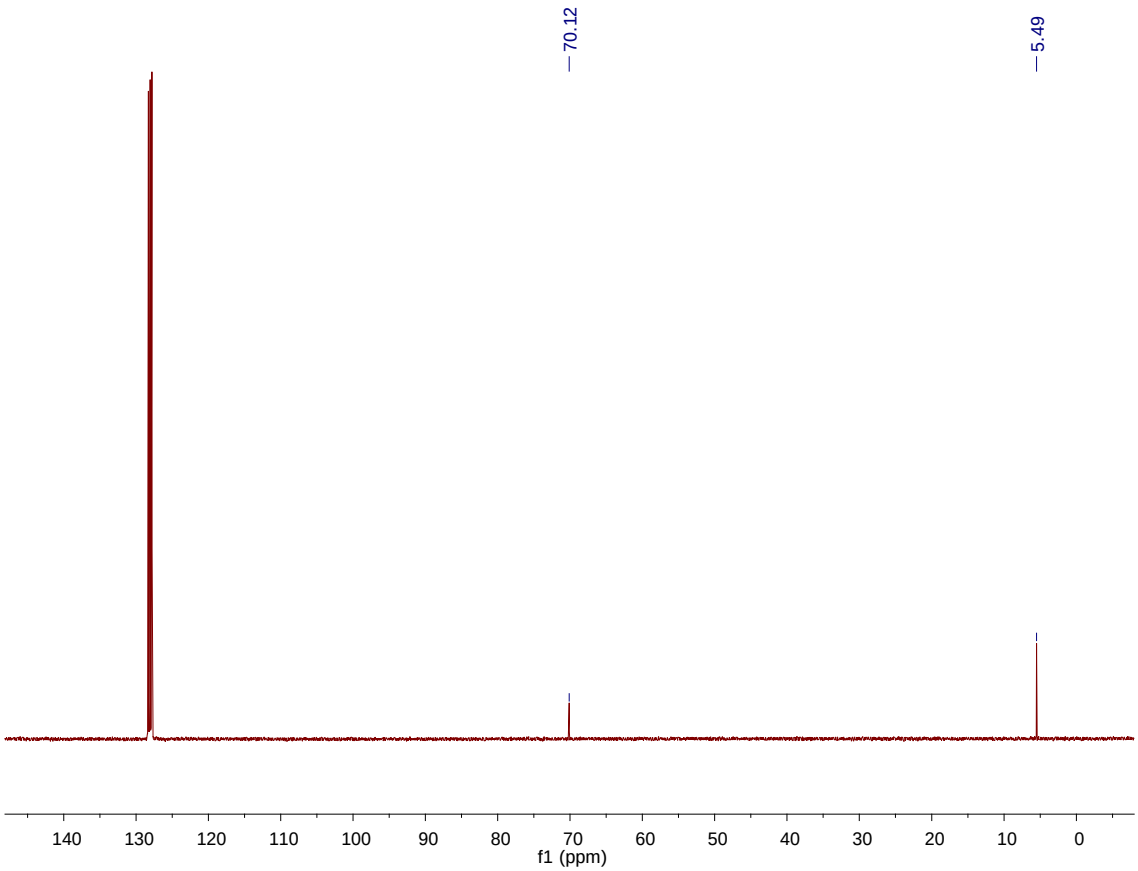


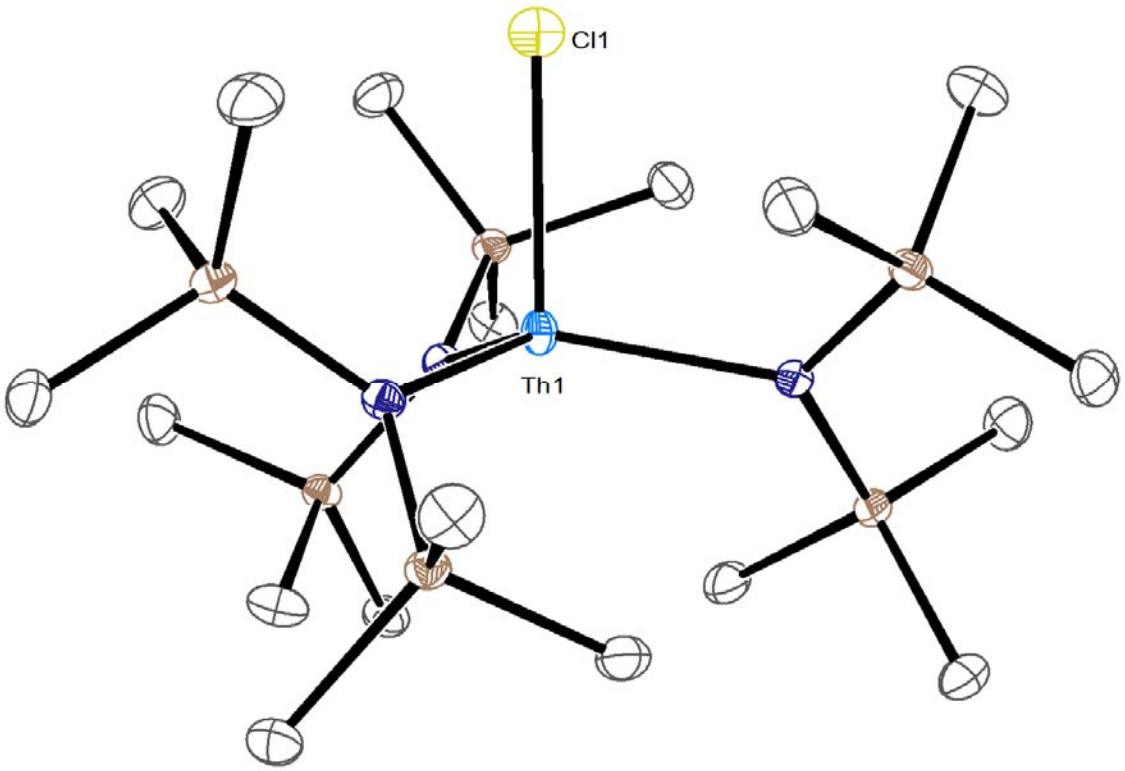
Figure S16. $^{13}C\{^{1}H\}$ NMR spectrum of [K(18-crown-6)][Th(S)$(NR_2)_3$] (**7**) in benzene-d_6.

Table S1. X-ray Crystallographic Data for **1**, $[Na(THF)_{4.5}][Th(Cl)_2(NR_2)_3]$, and **2**.

	1	$[Na(THF)_{4.5}][Th(Cl)_2(NR_2)_3]$	**2**
empirical formula	$C_{18}H_{54}ClN_3Si_6Th$	$C_{36}H_{82}Cl_2N_3NaO_{4.5}Si_6Th$	$C_{18}H_{54}IN_3Si_6Th$
crystal habit, color	block, colorless	needle, colorless	block, colorless
crystal size (mm)	0.1 × 0.1 × 0.1	0.2 × 0.05 × 0.02	0.2 × 0.1 × 0.1
space group	*R*3c	$R\bar{3}$	*R*3c
volume (Å^3)	4953.5(6)	8690(3)	5049(3)
a (Å)	18.430(1)	18.404(4)	18.328(5)
b (Å)	18.430(1)	18.404(4)	18.328(5)
c (Å)	16.840(1)	29.626(7)	17.356(5)
α (deg)	90	90	90
β (deg)	90	90	90
γ (deg)	120	120	120
Z	6	6	6
formula weight (g/mol)	748.67	1131.59	840.10
density (calculated) (Mg/m^3)	1.506	1.288	1.658
absorption coefficient (mm^{-1})	4.825	2.831	5.572
F_{000}	2244	3444	2460
total no. reflections	20265	8328	9620
unique reflections	3383	5914	3344
R_{int}	0.0485	0.0316	0.0324
final R indices (I >2σ(I)]	R_1 = 0.0176 wR_2 = 0.0417	R_1 = 0.0503 wR_2 = 0.1166	R_1 = 0.0295 wR_2 = 0.0681
largest diff. peak and hole (e$^-$ A^{-3})	0.531 and -0.634	1.321 and -1.575	5.273 and -0.996
GOF	1.047	1.000	0.891

Table S2. X-ray Crystallographic Data for **5**, **6**, and **7**.

	5·0.5C_6H_{14}	**4**	**6**·0.5OC_4H_{10}	**7**
empirical formula	$C_{53}H_{73}N_2O_2Si_4Th$	$C_{37}H_{69}N_3SSi_6Th$	$C_{32}H_{83}KN_3O_{7.5}Si_6Th$	$C_{30}H_{78}KN_3O_6SSi_6Th$
crystal habit, color	plate, colorless	needle, colorless	block, colorless	needle, colorless
crystal size (mm)	0.1 × 0.1 × 0.05	0.1 × 0.05 × 0.01	0.1 × 0.1 × 0.1	0.1 × 0.02 × 0.02
space group	$P\bar{1}$	$P\bar{1}$	*P*bca	$P\bar{1}$
volume (Å^3)	2725.4(7)	2372.5(4)	10534(2)	5044.9(11)
a (Å)	12.955(2)	10.594(1)	20.457(3)	12.748 (2)
b (Å)	13.025(2)	11.587(1)	20.307(3)	18.891(2)
c (Å)	16.867(2)	19.595(2)	25.358(3)	21.817(3)
α (deg)	85.654(3)	96.883(2)	90	91.554(2)
β (deg)	77.178(3)	91.006(2)	90	105.863(2)
γ (deg)	79.336(3)	96.270(2)	90	92.564(2)
Z	2	2	8	4
formula weight (g/mol)	1114.53	988.59	1069.69	1048.68
density (calculated) (Mg/m^3)	1.358	1.388	1.349	1.381
absorption coefficient (mm^{-1})	2.862	3.365	3.086	3.258
F_{000}	1134	1010	4392	2144
total no. reflections	56153	19192	51408	63038
unique reflections	11192	10322	13650	24802
R_{int}	0.0655	0.0440	0.1158	0.0408
final R indices (I >2σ(I)]	R_1 = 0.0310 wR_2 = 0.0612	R_1 = 0.0350 wR_2 = 0.0702	R_1 = 0.1001 wR_2 = 0.1885	R_1 = 0.0387 wR_2 = 0.1126
largest diff. peak and hole (e$^-$ A^{-3})	1.598 and -0.757	1.992 and -1.407	6.017 and -3.222	4.482 and -1.860
GOF	1.013	0.957	1.207	0.870



Figures S17. Solid state molecular structure of **1** with 50% probability ellipsoids. Hydrogen atoms have been omitted for clarity. Selected bond lengths (Å) and angles (deg): Th1-Cl1 = 2.647(1), Th1-N = 2.293(2); N-Th1-N = 116.74(3), N-Th1-Cl1 = 100.53(4).

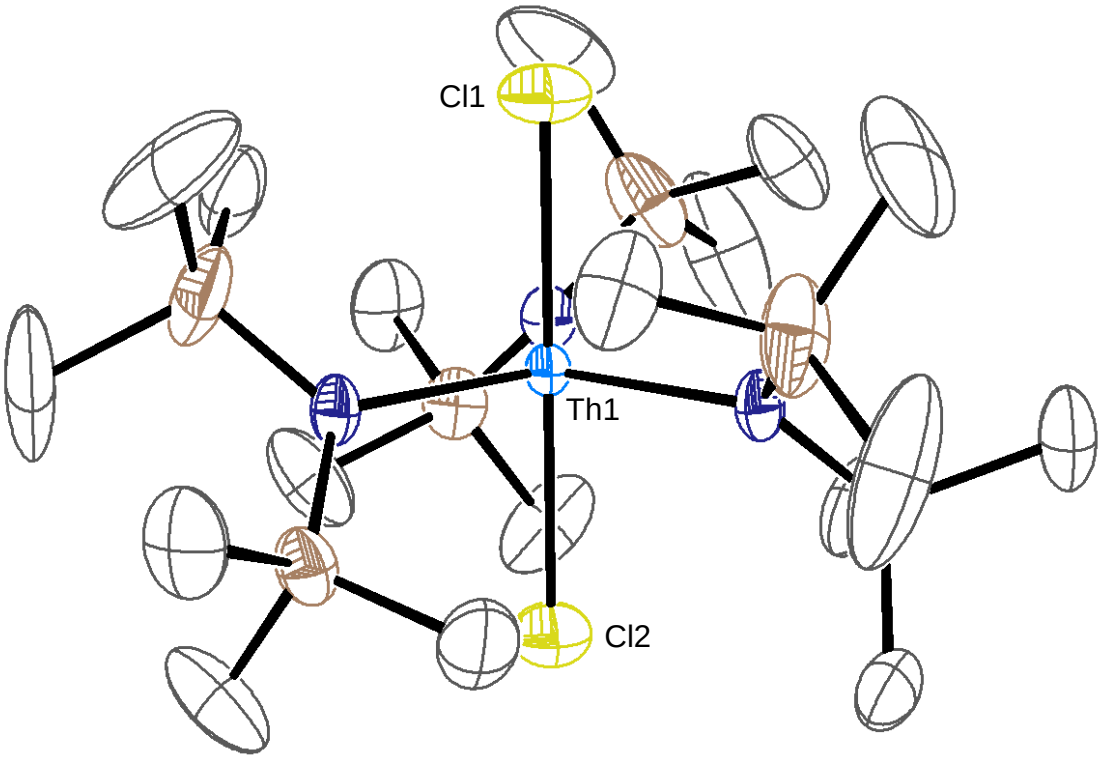
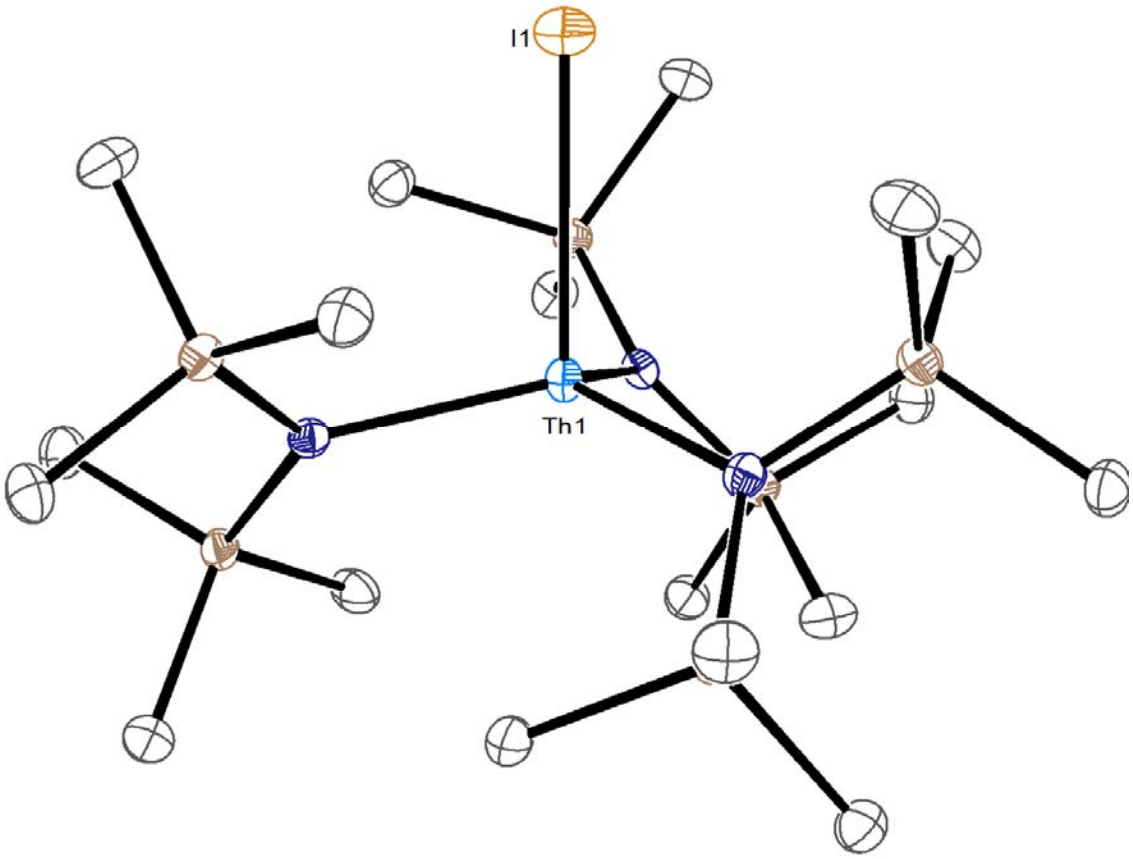


Figure S18. Solid state molecular structure of $[Na(THF)_{4.5}][Th(Cl)_2(NR_2)_3]$ with 50% probability ellipsoids. The Na^+ cation, coordinated molecules of THF, and hydrogen atoms have been omitted for clarity. Selected bond lengths (Å) and angles (deg): Th1-Cl1 = 2.725(3), Th1-Cl2 = 2.743(3), Th1-N = 2.332(4); Cl1-Th1-Cl2 = 180.0, N-Th1-N = 119.93(1).



Figures S19. Solid state molecular structure of **2** with 50% probability ellipsoids. Hydrogen atoms have been omitted for clarity. Selected bond lengths (Å) and angles (deg): Th1-I1 = 3.052(1), Th1-N = 2.299(4); N-Th-N = 116.83(6), N-Th1-I1 = 100.37(9).

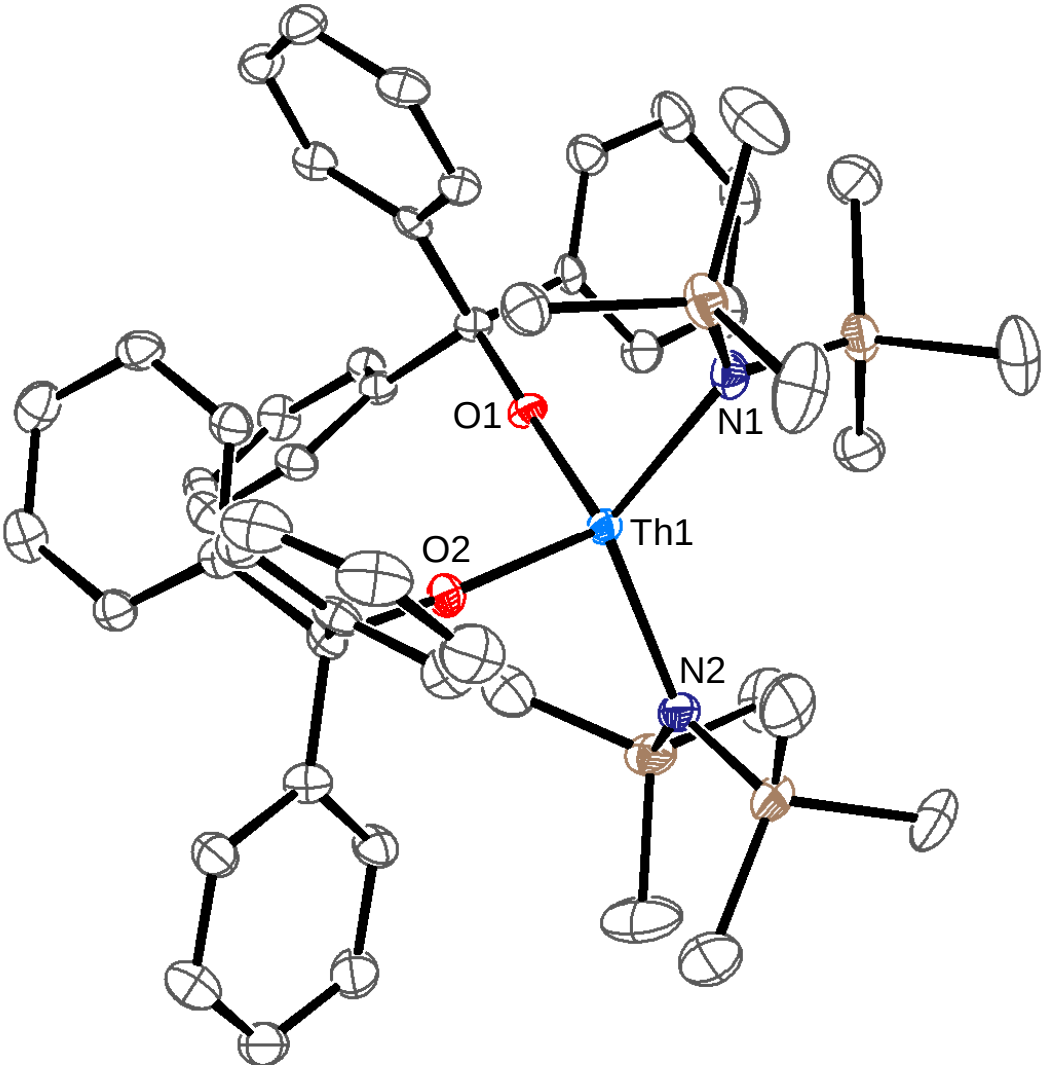


Figure S20. Solid state molecular structure of **5**·0.5C_6H_{14} with 50% probability ellipsoids. A hexanes solvate molecule and hydrogen atoms have been omitted for clarity. Selected bond lengths (Å) and angles (deg): Th1-O1 = 2.123(2), Th1-O2 = 2.131(2), Th1-N1 = 2.358(3), Th1-N2 = 2.367(3); O2-Th1-O1 = 105.05(9), O2-Th1-N1 = 113.70(9), O1-Th1-N1 = 98.95(9), O2-Th1-N2 = 100.35(9), O1-Th1-N2 = 112.7(1), N1-Th1-N2 = 125.1(1).

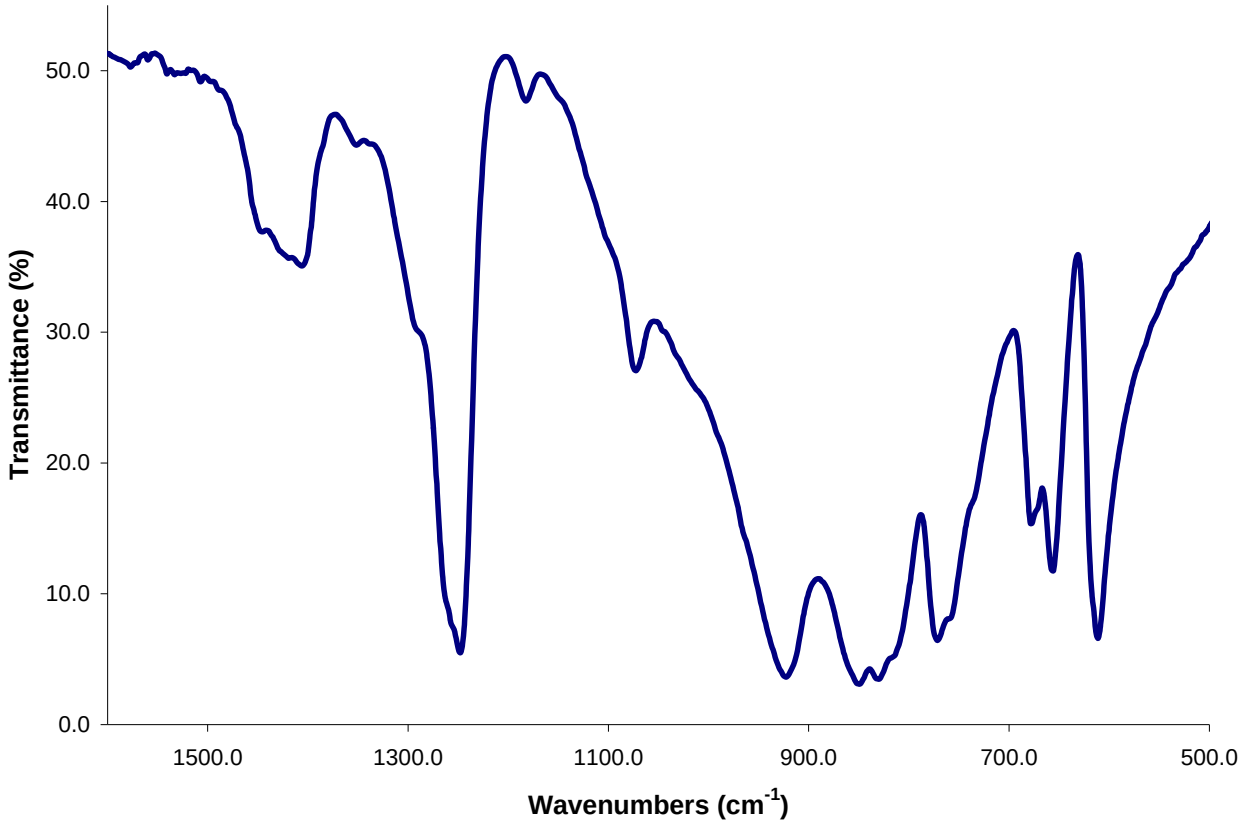


Figure S21. Partial IR spectrum of $[Th(Cl)(NR_2)_3]$ (**1**) (KBr pellet).

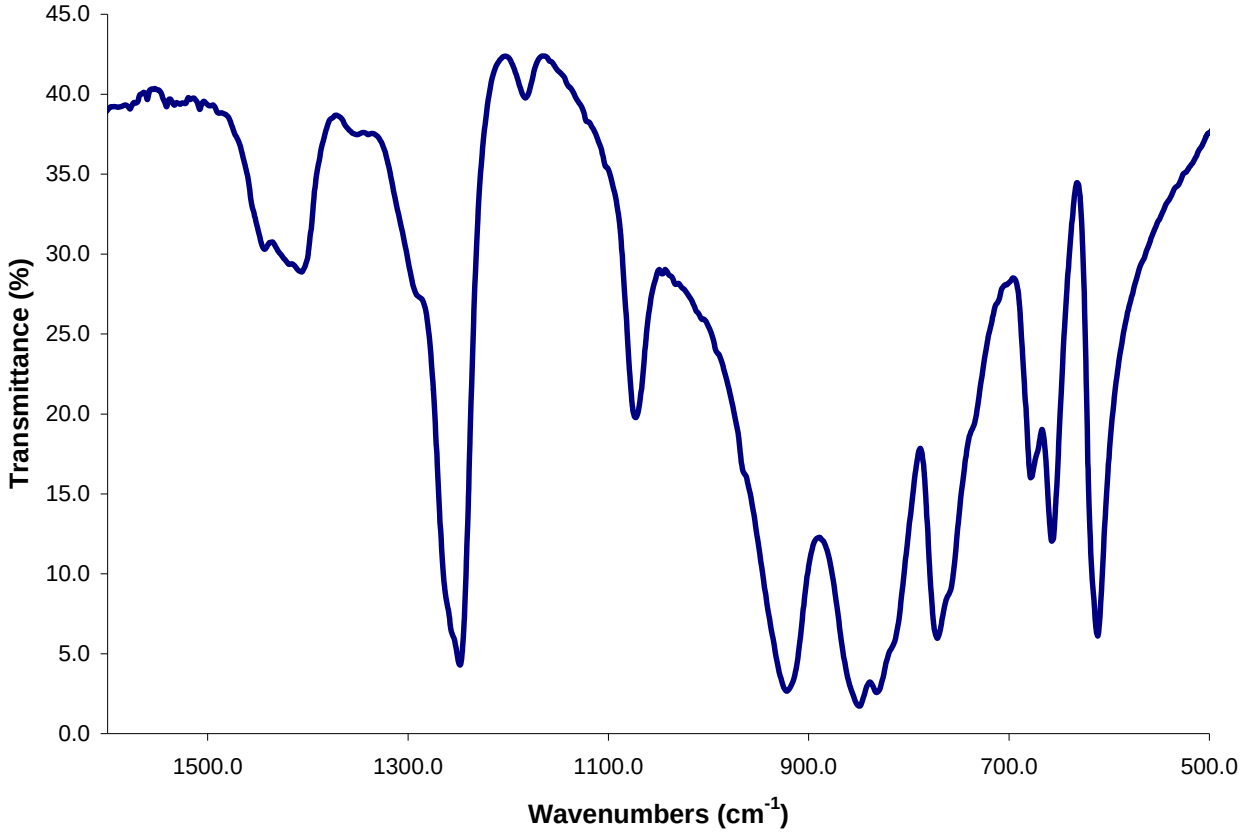


Figure S22. Partial IR spectrum of $[Na(THF)_{4.5}][Th(Cl)_2(NR_2)_3]$ (KBr pellet).

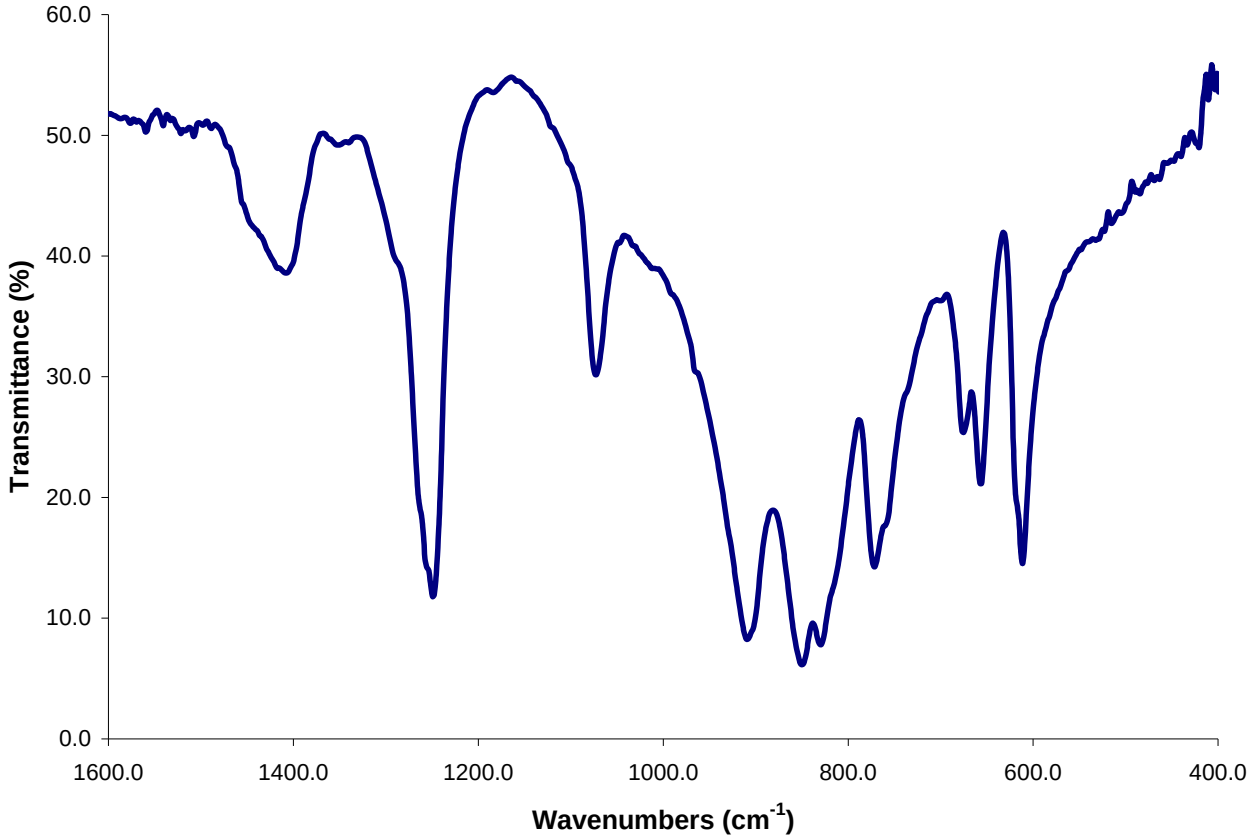


Figure S23. Partial IR spectrum of [Th(I)(NR_2)$_3$] (**2**) (KBr pellet).

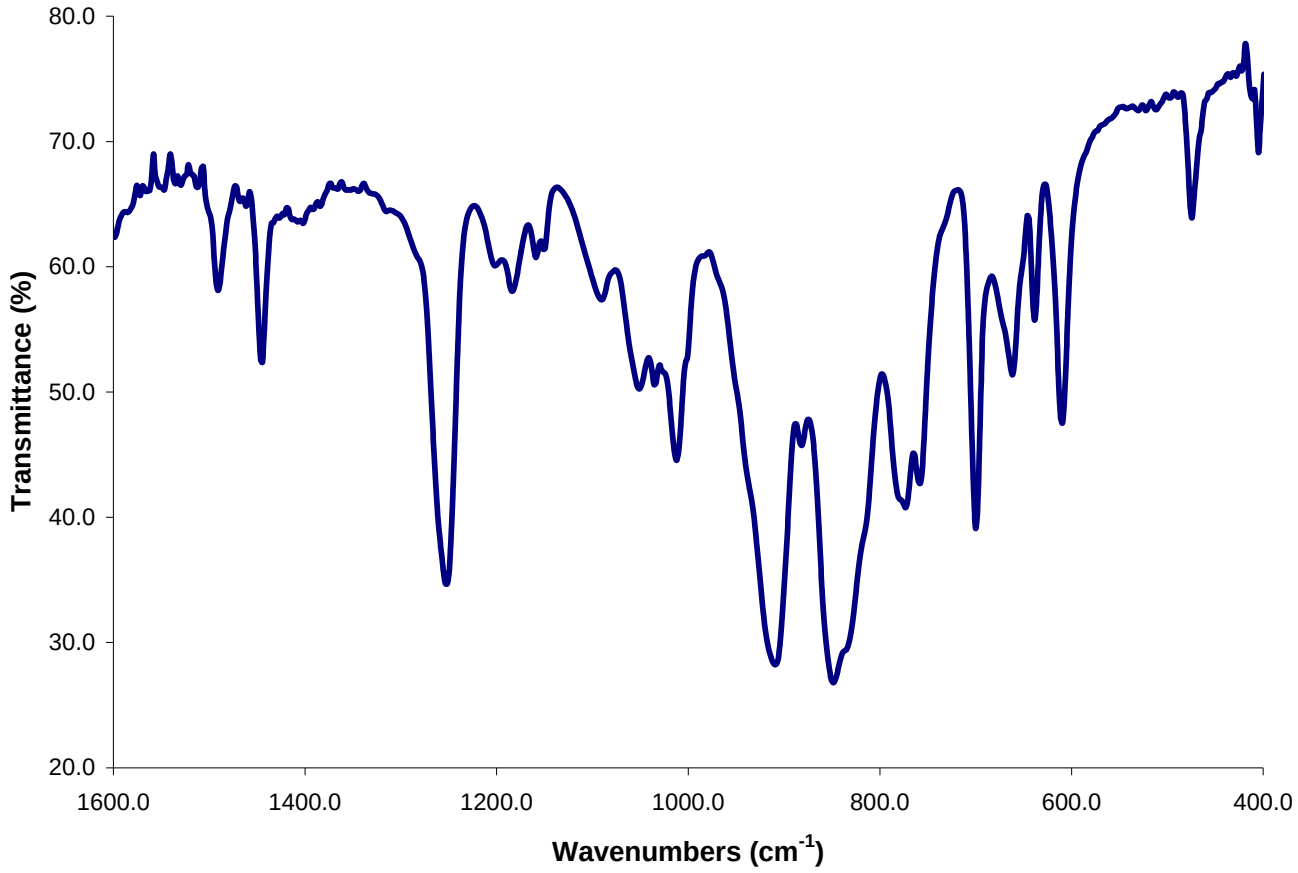


Figure S24. Partial IR spectrum of $[Th(OCPh_3)(NR_2)_3]$ (**3**) (KBr pellet).

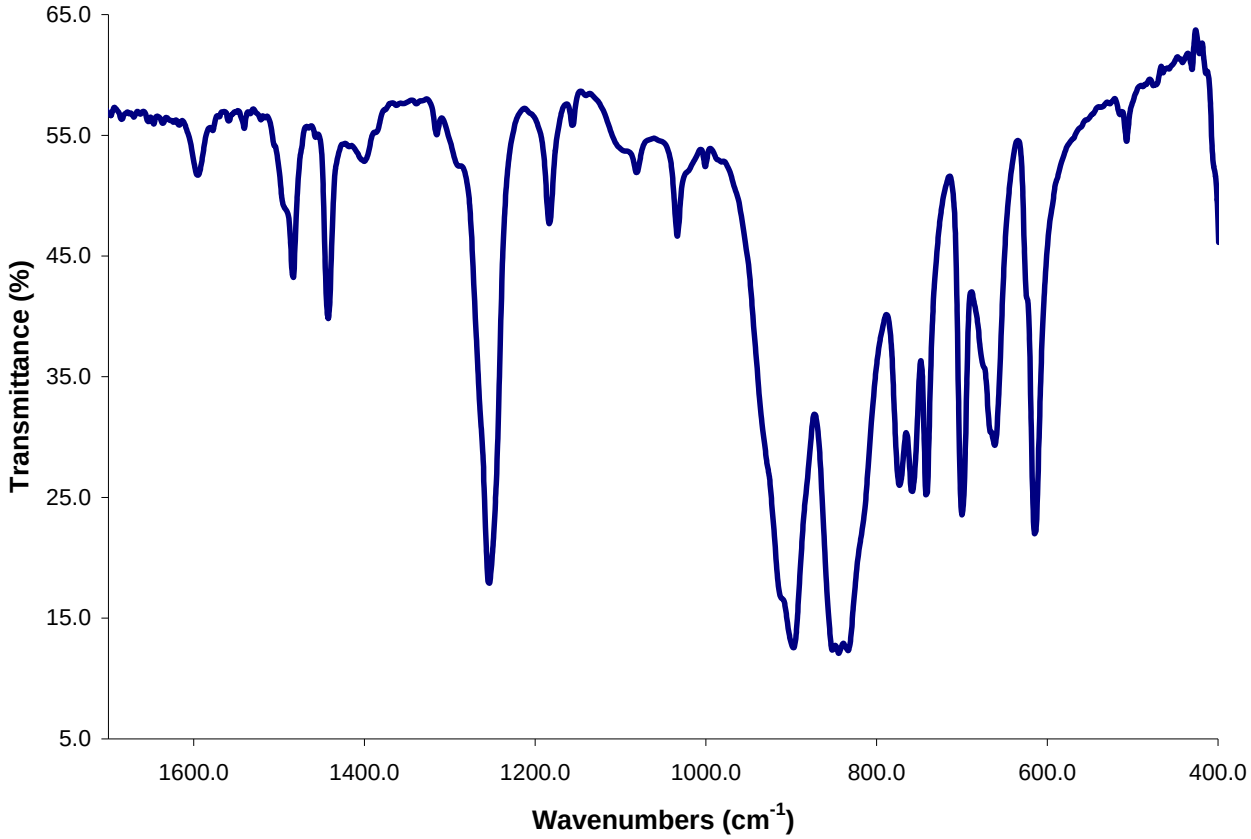


Figure S25. Partial IR spectrum of $[Th(SCPh_3)(NR_2)_3]$ (**4**) (KBr pellet).

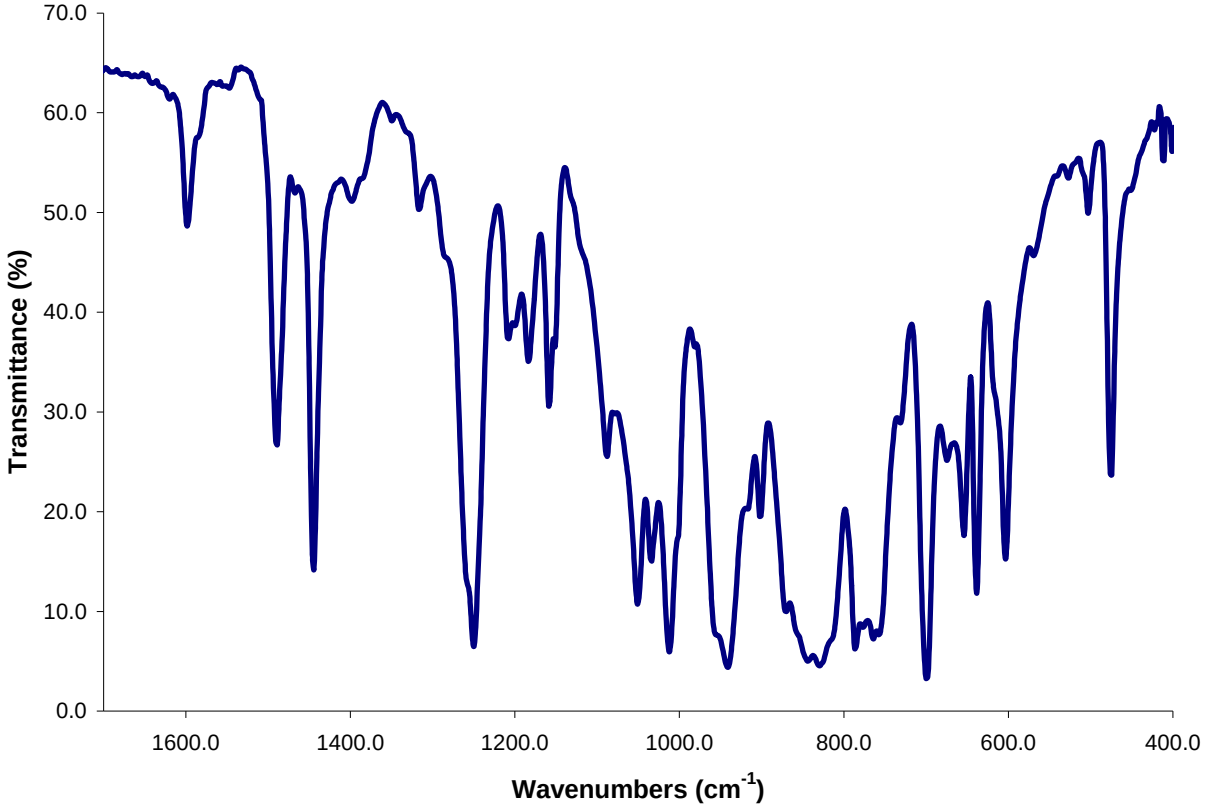


Figure S26. Partial IR spectrum of $[Th(OCPh_3)_2(NR_2)_2]$ (**5**) (KBr pellet).

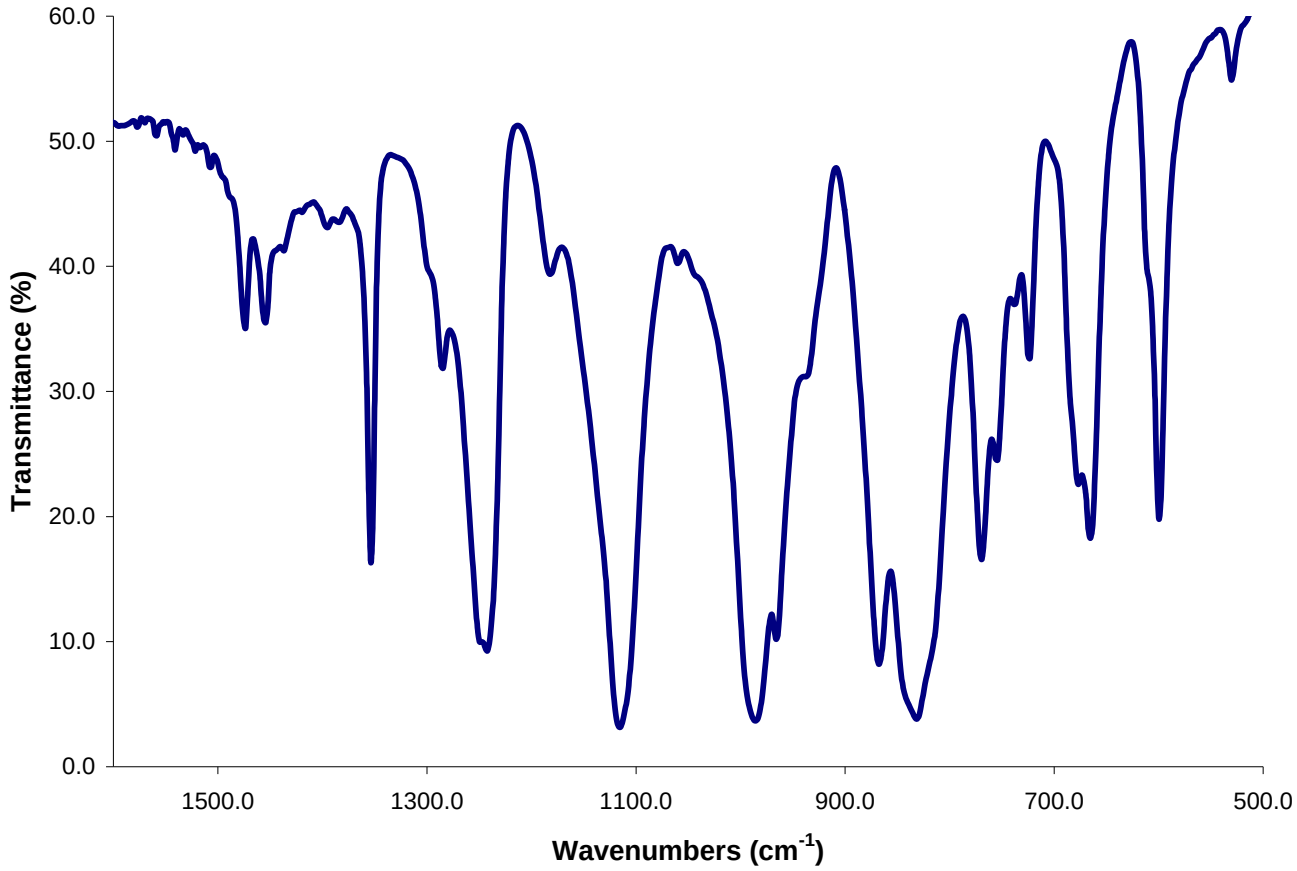


Figure S27. Partial IR spectrum of [K(18-crown-6)][Th(O)(NR_2)$_3$] (**6**) (KBr pellet).

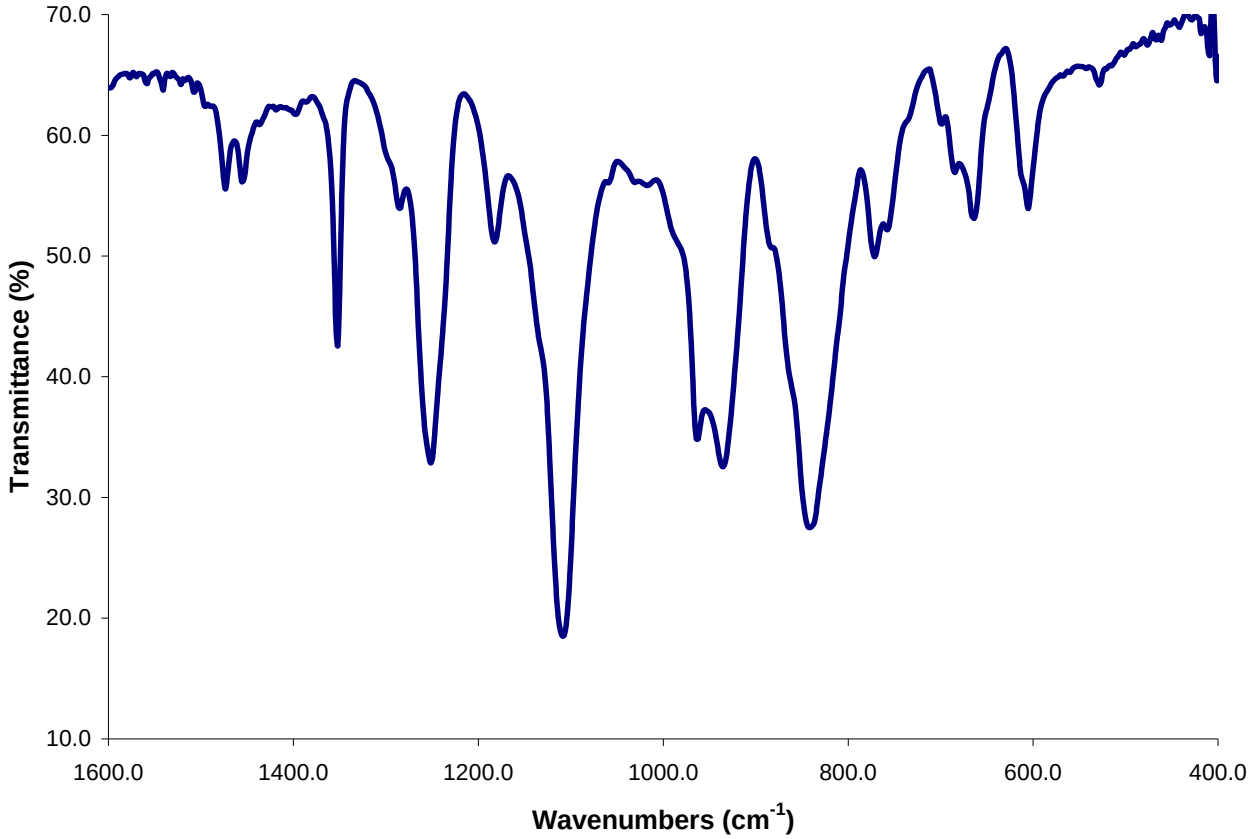


Figure S28. Partial IR spectrum of [K(18-crown-6)][Th(S)(NR_2)$_3$] (**7**) (KBr pellet).

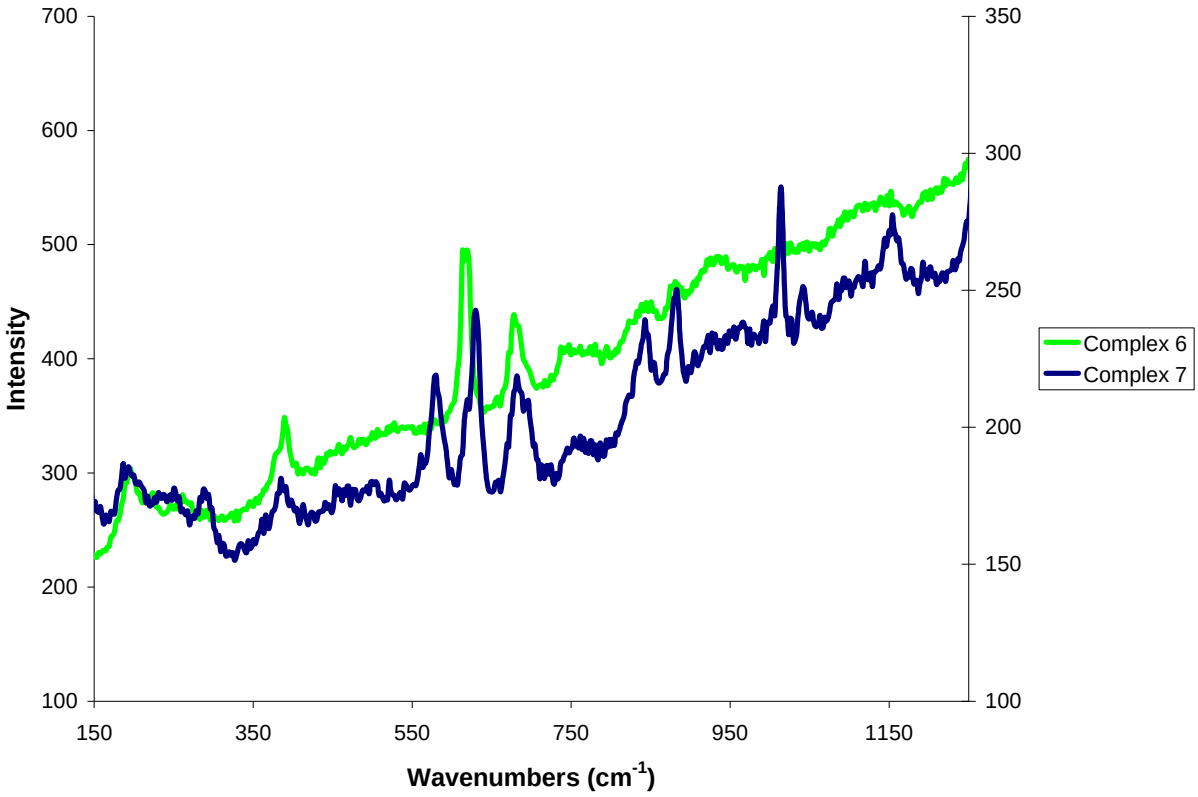


Figure S29. Raman spectra of [K(18-crown-6)][Th(O)(NR_2)$_3$] (**6**) and [K(18-crown-6)][Th(S)(NR_2)$_3$] (**7**).

Converged Cartesian coordinates, total energies, and maximum force at converged geometries

6 – PBE
-4622.3385088 H
4.1×10^{-4}

Th	1.380947	-0.000313	0.000191
O	-0.598611	-0.001070	0.001653
N	1.881537	-1.077986	-2.118594
N	1.883105	2.373319	0.125682
Si	0.805531	-0.781935	-3.464198
Si	3.194863	3.074548	-0.800956
Si	3.192199	-2.232455	-2.263409
Si	0.807424	3.391573	1.054268
K	-3.204329	0.000179	0.000754
N	1.882799	-1.295705	1.992831
Si	3.194675	-0.844605	3.063667
Si	0.806457	-2.608645	2.409951
O	-4.341263	1.760717	2.182644
O	-3.970663	-1.768513	-2.188488
O	-4.340210	1.011379	-2.615536
O	-3.972369	-1.010296	2.626291
O	-3.969133	2.780841	-0.437679
O	-4.342442	-2.769905	0.432440
C	1.631778	4.909961	1.870016
H	2.483971	4.621087	2.509251
H	0.896038	5.434574	2.507773
H	2.000761	5.638464	1.126693
C	0.063503	2.378355	2.493961
H	-0.629849	3.002013	3.089747
H	0.854249	2.022488	3.179043
H	-0.492167	1.494055	2.129415
C	-0.634104	4.086183	0.009161
H	-0.243771	4.634850	-0.866527
H	-1.255132	4.791309	0.594802
H	-1.287446	3.278332	-0.363467
C	2.595283	4.360036	-2.080935
H	1.840130	3.927712	-2.761562
H	3.435516	4.729801	-2.696792
H	2.135281	5.236365	-1.589284
C	4.103142	1.699066	-1.760870
H	4.648153	1.015561	-1.081857
H	4.862619	2.159997	-2.419555
H	3.441794	1.081367	-2.393403
C	4.556281	3.920789	0.236038

H 4.210464 4.841597 0.733876
H 5.404681 4.193384 -0.418926
H 4.940830 3.240400 1.015886
C 2.590581 -3.982941 -2.736639
H 1.835884 -4.355669 -2.021150
H 3.430214 -4.701835 -2.749869
H 2.129562 -3.994720 -3.740917
C 4.100979 -2.377241 -0.592612
H 4.648068 -1.448448 -0.340917
H 4.858691 -3.179804 -0.662500
H 3.439585 -2.614530 0.259018
C 4.554193 -1.758762 -3.514756
H 4.208730 -1.787486 -4.561263
H 5.401901 -2.463104 -3.423202
H 4.939779 -0.743654 -3.315090
C 0.061138 0.971249 -3.305440
H -0.495324 1.097124 -2.357712
H -0.631520 1.175783 -4.143920
H 0.851816 1.742588 -3.338762
C -0.635843 -2.034449 -3.544799
H -0.245492 -3.067115 -3.582268
H -1.256057 -1.879436 -4.448754
H -1.290030 -1.953726 -2.659450
C 1.630151 -0.832466 -5.187020
H 2.482986 -0.135072 -5.254840
H 0.894832 -0.540176 -5.959772
H 1.998271 -1.840250 -5.448256
C 2.595439 -0.381337 4.817643
H 1.840552 0.424560 4.784603
H 3.435868 -0.033888 5.446080
H 2.135201 -1.245753 5.329742
C 4.556982 -2.165349 3.275420
H 4.211381 -3.058463 3.821461
H 5.404989 -1.735457 3.840364
H 4.942077 -2.497820 2.295553
C 4.101369 0.676160 2.354238
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H 3.439307 1.533134 2.139108
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H 2.482301 -4.483929 2.747293
H 0.894276 -4.888909 3.452604

H 1.999392 -3.795285 4.319769
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H -0.245440 -1.567074 4.447124
H -1.256463 -2.910619 3.850889
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C -4.446268 -3.086173 -1.934526
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H -5.586854 -2.331153 2.707851
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C -4.475372 -1.242436 -3.411692
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C -3.852170 -3.583387 -0.631704
H -4.152949 -4.643455 -0.482844
H -2.743758 -3.543958 -0.676897
C -3.883172 3.089225 1.936710
H -2.776396 3.118283 1.884687
H -4.209712 3.770550 2.752767
C -3.849823 2.339717 -2.787770
H -4.150230 2.740796 -3.780381
H -2.741447 2.359247 -2.730694
C -3.882733 0.133439 -3.642721
H -2.776035 0.072548 -3.641270
H -4.208421 0.499689 -4.641008
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H -2.744077 1.185455 3.408907
C -3.885721 -3.220893 1.706489
H -2.778999 -3.190363 1.758887
H -4.212428 -4.268252 1.888383
C -4.447940 -0.131016 3.640011
H -4.147655 -0.497089 4.645270
H -5.557210 -0.071714 3.609316
C -4.474287 3.577411 0.629072
H -5.583219 3.513720 0.664789
H -4.192252 4.642588 0.485905
C -4.444245 3.219540 -1.706051
H -4.142846 4.272831 -1.891725
H -5.553585 3.164546 -1.741991

6 – PBE+D3
-4622.4686717 H
$2.7x10^{-4}$

Th	1.333611	-0.000137	-0.000385
O	-0.646704	0.000366	0.002384
N	1.833855	-1.962291	-1.310741
N	1.836040	2.115872	-1.043861
Si	0.753875	-2.326649	-2.630415
Si	3.135575	2.272535	-2.201877
Si	3.133882	-3.043936	-0.870027
Si	0.759266	3.443115	-0.697986
K	-3.220002	0.000368	0.001308
N	1.839663	-0.155361	2.352527
Si	3.143222	0.765004	3.065040
Si	0.759030	-1.111680	3.331522
O	-4.235695	2.571994	1.184572
O	-3.886059	-2.531950	-1.156799
O	-4.235598	-0.260609	-2.817910
O	-3.886258	0.263357	2.773627
O	-3.886095	2.269603	-1.612966
O	-4.234418	-2.310839	1.637280
C	1.577789	5.165937	-0.731035
H	2.438511	5.218955	-0.042010
H	0.847606	5.935916	-0.420148
H	1.936000	5.437157	-1.739744
C	0.062778	3.232336	1.069453
H	-0.584949	4.086422	1.342102
H	0.881460	3.193227	1.810411
H	-0.527303	2.302115	1.170445
C	-0.699975	3.514575	-1.925052
H	-0.319997	3.554826	-2.961304
H	-1.336016	4.405917	-1.763723
H	-1.333166	2.616417	-1.829907
C	2.514679	2.795309	-3.928927
H	1.743469	2.098204	-4.302316
H	3.339573	2.818575	-4.663999
H	2.064527	3.804278	-3.901460
C	4.022401	0.594720	-2.389652
H	4.534722	0.294345	-1.455287
H	4.806356	0.683733	-3.164215
H	3.354774	-0.234735	-2.679849
C	4.505659	3.498565	-1.697326
H	4.162378	4.546120	-1.691179
H	5.352645	3.426296	-2.404301

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C 2.512516 -4.800226 -0.457072
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H 3.360807 -2.206545 1.540138
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H 4.154586 -3.740785 -3.095938
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H -0.589975 -0.878051 -4.205641
H 0.876411 -0.027152 -3.664047
C -0.705194 -3.423731 -2.075528
H -0.325269 -4.340552 -1.590718
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C -4.350298 -0.848934 3.531467
H -5.459731 -0.904226 3.498869
H -4.036573 -0.752961 4.593031
C -4.351673 -2.632123 -2.498500
H -5.461140 -2.576388 -2.528677
H -4.038363 -3.599419 -2.946477
C -3.685984 -3.479168 1.028714
H -3.925821 -4.383205 1.630217
H -2.581492 -3.400783 0.952258
C -3.745078 3.623064 0.353498
H -2.640702 3.579880 0.279640
H -4.026930 4.614665 0.771030
C -3.687861 0.850400 -3.526257
H -3.929016 0.781386 -4.609628
H -2.583264 0.877298 -3.421456
C -3.745314 -1.506139 -3.312294
H -2.640974 -1.549011 -3.237828
H -4.027005 -1.640422 -4.379835
C -3.688190 2.629838 2.501004
H -3.929405 3.602565 2.982910
H -2.583604 2.525617 2.472023
C -3.742908 -2.115929 2.962612
H -2.638590 -2.028557 2.961166
H -4.022848 -2.973722 3.612858
C -4.291769 1.510773 3.326590
H -3.933317 1.605359 4.374062
H -5.399982 1.593075 3.326765
C -4.351130 3.481757 -1.028690
H -5.460618 3.480542 -0.965381
H -4.037370 4.353306 -1.642253
C -4.291313 2.124981 -2.969878
H -3.932753 2.984894 -3.575366
H -5.399516 2.084073 -3.041417

6-U – PBE
-4691.5761669 H
1.4×10^{-5}

U	-1.397440	-0.001591	-0.040795
O	0.523095	0.025310	-0.084680
N	-1.914142	-0.424586	2.229254
N	-1.853812	2.207013	-0.774321
Si	-0.861040	0.264443	3.447826
Si	-3.196379	3.135316	-0.127633
Si	-3.218073	-1.499544	2.712511
Si	-0.762442	2.950894	-1.924251
K	3.161527	0.008947	0.019643
N	-1.812094	-1.825907	-1.485834
Si	-3.075403	-1.702908	-2.696522
Si	-0.739443	-3.205771	-1.458400
O	4.339875	1.049689	-2.558034
O	3.926948	-1.038864	2.651680
O	4.286989	1.739460	2.243481
O	3.987962	-1.725877	-2.176600
O	3.975958	2.788708	-0.357080
O	4.345903	-2.750037	0.439978
C	-1.564998	4.232114	-3.094760
H	-2.396935	3.796303	-3.674433
H	-0.807259	4.591683	-3.815972
H	-1.953875	5.115654	-2.559002
C	-0.016365	1.627817	-3.082854
H	0.676665	2.092682	-3.810204
H	-0.809116	1.121184	-3.662322
H	0.529625	0.853733	-2.514137
C	0.671152	3.879700	-1.067430
H	0.272016	4.627528	-0.359252
H	1.300833	4.417586	-1.802240
H	1.317951	3.189538	-0.499724
C	-2.637781	4.747819	0.732881
H	-1.918658	4.542774	1.545962
H	-3.501957	5.279537	1.171712
H	-2.148534	5.439946	0.024048
C	-4.138831	2.105635	1.169047
H	-4.625269	1.219684	0.718234
H	-4.946645	2.723903	1.603290
H	-3.499774	1.747653	1.992940
C	-4.529288	3.625596	-1.405078
H	-4.175997	4.364759	-2.142231
H	-5.395927	4.066574	-0.878098
H	-4.890433	2.741946	-1.959796

C -2.601355 -3.010332 3.707247
H -1.830244 -3.574891 3.153650
H -3.435299 -3.701862 3.927140
H -2.160881 -2.706283 4.673954
C -4.123053 -2.162064 1.173068
H -4.650814 -1.355729 0.629050
H -4.894352 -2.888496 1.490398
H -3.452673 -2.662016 0.454323
C -4.592471 -0.686434 3.760468
H -4.258556 -0.395103 4.769641
H -5.428562 -1.400759 3.878694
H -4.991516 0.214933 3.263794
C -0.087959 1.889232 2.806494
H 0.502858 1.729027 1.886485
H 0.571756 2.330484 3.578122
H -0.867726 2.635716 2.573123
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H 0.168544 -1.888205 4.261007
H 1.160464 -0.495444 4.769644
H 1.249222 -1.095637 3.085728
C -1.719295 0.731440 5.089903
H -2.572469 1.412955 4.929412
H -0.996568 1.247793 5.748983
H -2.092044 -0.151334 5.638201
C -2.400317 -1.765257 -4.482697
H -1.624264 -0.996456 -4.646181
H -3.209089 -1.594562 -5.216718
H -1.949054 -2.747752 -4.711032
C -4.444968 -3.028058 -2.582620
H -4.091516 -4.040091 -2.839803
H -5.262049 -2.771308 -3.282376
H -4.874834 -3.068988 -1.566730
C -3.991574 -0.043096 -2.490908
H -4.625618 -0.035669 -1.584242
H -4.668509 0.103693 -3.353285
H -3.324582 0.835936 -2.439309
C 0.007194 -3.402078 0.288283
H 0.545877 -2.490138 0.604404
H 0.710955 -4.255646 0.316359
H -0.780990 -3.599760 1.036037
C -1.573586 -4.880372 -1.848256
H -2.445564 -5.065714 -1.197295
H -0.852609 -5.703469 -1.686618
H -1.916548 -4.945138 -2.895892
C 0.699162 -3.045803 -2.706747
H 0.307934 -2.881655 -3.726341

H 1.315145 -3.965490 -2.730789
H 1.356987 -2.195162 -2.458804
C 4.426041 -2.364586 2.797247
H 4.124173 -2.788796 3.778874
H 5.536088 -2.364779 2.745873
C 4.519819 -3.024235 -1.932275
H 5.627142 -2.976013 -1.851772
H 4.261994 -3.712971 -2.765108
C 4.411083 -0.173406 3.674074
H 5.520342 -0.118523 3.636152
H 4.116345 -0.552656 4.676006
C 3.859504 -3.232020 1.691451
H 4.186019 -4.281656 1.858605
H 2.750112 -3.209856 1.715984
C 3.902863 2.398217 -2.719074
H 2.796564 2.457933 -2.691406
H 4.247404 2.804822 -3.695086
C 3.816450 3.066446 2.014828
H 4.114975 3.735916 2.850856
H 2.709146 3.083170 1.940302
C 3.817223 1.207409 3.480852
H 2.710468 1.149096 3.487833
H 4.134791 1.853808 4.328185
C 3.855107 0.198664 -3.595275
H 4.158447 0.586407 -4.592143
H 2.746782 0.142916 -3.571692
C 3.927800 -3.571645 -0.648968
H 2.822251 -3.592445 -0.721504
H 4.285355 -4.615213 -0.508125
C 4.455892 -1.179818 -3.405778
H 4.155663 -1.826156 -4.258212
H 5.564788 -1.108895 -3.397105
C 4.494185 3.238473 -1.604855
H 5.602489 3.157353 -1.612257
H 4.222748 4.301943 -1.777764
C 4.435768 3.582750 0.731467
H 4.140870 4.644707 0.590641
H 5.543859 3.536055 0.800962

6-U – PBE+D3
-4691.7062677 H
$6.5x10^{-5}$

U	-1.358977	0.000973	-0.033537
O	0.561707	0.039071	-0.103461
N	-1.842432	-0.497286	2.210651
N	-1.824463	2.210316	-0.690851
Si	-0.777615	0.183484	3.416740
Si	-3.157611	3.106842	0.002559
Si	-3.125276	-1.598838	2.670157
Si	-0.737940	2.966013	-1.830177
K	3.160116	0.010522	0.008513
N	-1.782932	-1.758465	-1.524223
Si	-3.045854	-1.600508	-2.723798
Si	-0.700606	-3.125098	-1.516932
O	4.214482	1.030441	-2.619551
O	3.871166	-1.000667	2.616908
O	4.212923	1.779934	2.215287
O	3.888680	-1.729207	-2.156600
O	3.896129	2.759343	-0.403812
O	4.253776	-2.766278	0.450314
C	-1.537970	4.299345	-2.938066
H	-2.381923	3.890454	-3.520108
H	-0.788408	4.681545	-3.655788
H	-1.912493	5.162218	-2.360055
C	-0.054492	1.657881	-3.042480
H	0.603935	2.122748	-3.800516
H	-0.882782	1.166031	-3.583222
H	0.510175	0.870908	-2.511157
C	0.717360	3.820523	-0.941323
H	0.330111	4.533216	-0.191600
H	1.363901	4.383160	-1.641437
H	1.340956	3.079868	-0.414555
C	-2.585079	4.691278	0.900332
H	-1.850624	4.459986	1.692182
H	-3.438221	5.214158	1.369646
H	-2.105470	5.398142	0.199444
C	-4.066942	2.023788	1.278268
H	-4.522614	1.130432	0.809513
H	-4.894871	2.604733	1.725141
H	-3.415312	1.669156	2.093482
C	-4.504696	3.622935	-1.245234
H	-4.159854	4.386003	-1.961695
H	-5.372774	4.039788	-0.701864
H	-4.856752	2.750984	-1.823401

C -2.477834 -3.111960 3.637392
H -1.689509 -3.644434 3.076635
H -3.293453 -3.828870 3.842909
H -2.048322 -2.809561 4.609586
C -4.014185 -2.239562 1.113456
H -4.510106 -1.419109 0.560195
H -4.808607 -2.948551 1.411502
H -3.340414 -2.749185 0.405484
C -4.505231 -0.817941 3.730629
H -4.165595 -0.527934 4.738240
H -5.330937 -1.543533 3.850580
H -4.916635 0.081568 3.241163
C -0.049678 1.830280 2.779722
H 0.570296 1.684263 1.877034
H 0.567424 2.311818 3.561692
H -0.854662 2.537155 2.512415
C 0.665085 -0.994352 3.834873
H 0.274467 -1.982934 4.133697
H 1.282135 -0.609355 4.669198
H 1.322773 -1.141724 2.961799
C -1.620656 0.607491 5.074855
H -2.481787 1.282686 4.930141
H -0.900246 1.116756 5.741466
H -1.982136 -0.292147 5.602908
C -2.365644 -1.639151 -4.506127
H -1.573599 -0.881835 -4.644173
H -3.163759 -1.439712 -5.244100
H -1.929511 -2.625728 -4.746138
C -4.417949 -2.919762 -2.615226
H -4.064382 -3.929773 -2.879962
H -5.240234 -2.659059 -3.306881
H -4.836814 -2.965946 -1.595108
C -3.945097 0.062997 -2.485452
H -4.519794 0.087377 -1.540181
H -4.674622 0.198349 -3.305389
H -3.273567 0.938851 -2.485790
C 0.020424 -3.340784 0.237948
H 0.609335 -2.457658 0.545225
H 0.667023 -4.236400 0.292964
H -0.788440 -3.470418 0.977959
C -1.527202 -4.790450 -1.946348
H -2.397622 -4.988740 -1.296964
H -0.806909 -5.618148 -1.808813
H -1.874130 -4.824083 -2.994145
C 0.738526 -2.903773 -2.749685
H 0.344196 -2.701748 -3.761044

H 1.374427 -3.807570 -2.810832
H 1.374538 -2.051765 -2.457074
C 4.315570 -2.340772 2.801106
H 3.975578 -2.730812 3.784440
H 5.425430 -2.387071 2.771295
C 4.386574 -3.042884 -1.925241
H 5.496099 -3.030116 -1.864783
H 4.089817 -3.721880 -2.753082
C 4.329015 -0.132468 3.648732
H 5.438295 -0.068160 3.634669
H 4.013926 -0.513084 4.643951
C 3.731272 -3.206448 1.703020
H 4.011563 -4.265531 1.893688
H 2.623679 -3.137856 1.712872
C 3.737710 2.368301 -2.756871
H 2.633938 2.401653 -2.671329
H 4.021994 2.784369 -3.748317
C 3.694662 3.083775 1.955415
H 3.954650 3.780413 2.782239
H 2.588993 3.056813 1.864175
C 3.722499 1.240750 3.441731
H 2.617811 1.161837 3.421221
H 4.007658 1.892151 4.296865
C 3.663875 0.158755 -3.605976
H 3.898533 0.526315 -4.628843
H 2.559888 0.100669 -3.507766
C 3.794762 -3.572143 -0.634244
H 2.689200 -3.550938 -0.696285
H 4.114928 -4.628519 -0.498231
C 4.276295 -1.216144 -3.427032
H 3.913565 -1.880427 -4.240462
H 5.383371 -1.149843 -3.495696
C 4.357453 3.222071 -1.668752
H 5.466218 3.168034 -1.719791
H 4.051497 4.277864 -1.830729
C 4.308956 3.598770 0.668879
H 3.964350 4.641597 0.500556
H 5.417112 3.604961 0.751614

7 - PBE
-4945.1865021 H
$1.1x10^{-5}$

Th	1.642819	0.023535	0.142863
S	-0.712137	0.190722	-0.810537
N	2.216596	-2.202208	-0.436507
N	2.735401	1.759724	-1.029608
Si	1.606912	-2.883606	-1.949632
Si	4.370687	1.547161	-1.646285
Si	3.101976	-3.236227	0.678749
Si	1.828695	3.218140	-1.458744
K	-3.769457	0.046246	-0.440211
N	1.213148	0.415509	2.449323
Si	2.277460	1.430459	3.416874
Si	-0.295007	-0.171483	3.143364
O	-5.348973	2.367190	0.611376
O	-3.653188	-2.370252	-1.887415
O	-3.687532	0.063977	-3.385639
O	-5.287358	-0.077651	2.089903
O	-4.026047	2.484215	-1.881965
O	-4.959811	-2.492419	0.603125
C	2.917205	4.768629	-1.711094
H	3.499882	5.019639	-0.807923
H	2.259418	5.629446	-1.933598
H	3.622844	4.669617	-2.554189
C	0.630460	3.673366	-0.049047
H	0.030986	4.556137	-0.342102
H	1.177493	3.931511	0.875455
H	-0.073933	2.850629	0.171176
C	0.831985	2.983674	-3.062010
H	1.495514	2.801054	-3.925747
H	0.213122	3.872251	-3.287092
H	0.168326	2.109685	-2.941760
C	4.454971	1.626466	-3.549362
H	3.781336	0.881423	-4.008117
H	5.481012	1.426996	-3.908869
H	4.157128	2.619890	-3.929227
C	5.028333	-0.165236	-1.120088
H	5.170404	-0.240102	-0.024662
H	6.025129	-0.313596	-1.575920
H	4.389384	-1.008612	-1.433331
C	5.654220	2.779909	-0.958808
H	5.502114	3.809797	-1.319811
H	6.667793	2.462992	-1.267447
H	5.632499	2.801921	0.144765

C 2.103885 -4.775389 1.204821
H 1.131263 -4.490218 1.643059
H 2.657239 -5.366999 1.956932
H 1.898816 -5.439195 0.346042
C 3.514221 -2.258988 2.265029
H 4.229491 -1.435875 2.073798
H 4.007778 -2.942470 2.981038
H 2.633039 -1.824998 2.767393
C 4.794532 -3.847720 0.045019
H 4.711979 -4.572597 -0.780774
H 5.336851 -4.342566 0.872135
H 5.416268 -3.005542 -0.305399
C 1.576999 -1.542263 -3.301190
H 0.960631 -0.671849 -3.011452
H 1.150003 -1.957870 -4.233522
H 2.598279 -1.189486 -3.532631
C -0.144332 -3.613857 -1.760646
H -0.155353 -4.417506 -1.002244
H -0.494275 -4.046580 -2.717553
H -0.850880 -2.825801 -1.446926
C 2.688832 -4.287185 -2.666562
H 3.722329 -3.953450 -2.863244
H 2.254707 -4.611834 -3.630581
H 2.737802 -5.175791 -2.013312
C 1.403124 2.995871 4.068017
H 0.970315 3.583109 3.239151
H 2.110479 3.646003 4.614618
H 0.580754 2.744562 4.761665
C 3.074336 0.554010 4.912529
H 2.350076 0.298231 5.702802
H 3.838454 1.215959 5.360795
H 3.579692 -0.377338 4.602673
C 3.753861 1.999414 2.352659
H 4.412966 1.155456 2.071853
H 4.372400 2.695720 2.949197
H 3.463822 2.520177 1.424077
C -0.741874 -1.869173 2.397083
H -0.856762 -1.821511 1.298346
H -1.698013 -2.224372 2.828224
H 0.028307 -2.624273 2.635695
C -0.247830 -0.463347 5.031957
H 0.515947 -1.207123 5.317566
H -1.230783 -0.852928 5.357627
H -0.054166 0.458811 5.606954
C -1.746081 1.029818 2.835276
H -1.648136 1.939420 3.455341

H -2.717582 0.552928 3.064123
H -1.737532 1.330143 1.771761
C -4.215155 -3.579407 -1.399559
H -3.641283 -4.455855 -1.769894
H -5.269273 -3.686816 -1.736783
C -5.901397 -1.309813 2.458148
H -6.897709 -1.403752 1.975292
H -6.046337 -1.359125 3.558981
C -3.562253 -2.331382 -3.310519
H -4.577097 -2.380445 -3.761733
H -2.973245 -3.197340 -3.679963
C -4.150823 -3.565859 0.116252
H -4.523732 -4.538464 0.503786
H -3.098858 -3.438818 0.446568
C -4.745918 3.563946 0.119063
H -3.686154 3.627607 0.444850
H -5.283252 4.456886 0.505438
C -3.048965 1.299151 -3.719003
H -2.873258 1.359646 -4.815404
H -2.073721 1.378138 -3.196242
C -2.858763 -1.053169 -3.722245
H -1.883456 -0.973387 -3.199352
H -2.679083 -1.082188 -4.819428
C -5.368656 2.320706 2.036379
H -5.922601 3.192959 2.446875
H -4.335995 2.342953 2.443192
C -5.011067 -2.459050 2.025865
H -3.993788 -2.330110 2.452421
H -5.431685 -3.407881 2.424879
C -6.071388 1.049563 2.473567
H -6.206010 1.071900 3.576508
H -7.077412 0.996113 2.004807
C -4.816309 3.558419 -1.396597
H -5.872488 3.451930 -1.727907
H -4.434677 4.531710 -1.775008
C -3.949709 2.446381 -3.305964
H -3.522918 3.396244 -3.693296
H -4.964014 2.317928 -3.742448

7 – PBE+D3
-4945.3178726 H
$1.3x10^{-4}$

Th	1.473094	0.000590	0.000319
S	-1.057203	0.000303	-0.011799
N	1.913564	-2.263877	-0.496493
N	1.910310	1.567752	-1.707679
Si	0.839727	-3.121606	-1.596703
Si	3.195486	1.283713	-2.869105
Si	3.195798	-3.126412	0.336220
Si	0.832299	2.946616	-1.899132
K	-4.044684	-0.003768	-0.005603
N	1.901904	0.700976	2.212141
Si	3.181433	1.854026	2.551466
Si	0.821227	0.175644	3.498842
O	-4.344386	2.892851	0.365078
O	-4.046127	-2.730000	-0.350516
O	-4.326094	-1.132430	-2.702241
O	-4.060999	1.060523	2.528742
O	-4.052169	1.657399	-2.193396
O	-4.339498	-1.775053	2.317459
C	1.652768	4.462446	-2.719675
H	2.531065	4.810537	-2.149082
H	0.923821	5.293315	-2.752732
H	1.976738	4.266834	-3.756705
C	0.265972	3.558601	-0.184591
H	-0.435552	4.407173	-0.293769
H	1.129143	3.916222	0.404516
H	-0.245980	2.765278	0.390749
C	-0.693141	2.515958	-2.953679
H	-0.383323	2.096848	-3.927678
H	-1.315853	3.409606	-3.149670
H	-1.301954	1.762256	-2.425609
C	2.537193	1.124196	-4.649733
H	1.764043	0.338678	-4.714133
H	3.347739	0.868336	-5.355896
H	2.080205	2.069145	-4.994111
C	4.093571	-0.342524	-2.434861
H	4.614792	-0.284413	-1.459467
H	4.874769	-0.524844	-3.195936
H	3.437388	-1.228616	-2.408049
C	4.571192	2.602209	-2.868627
H	4.239294	3.571659	-3.273463
H	5.418377	2.252079	-3.486756
H	4.949497	2.773891	-1.845932

C	2.535123	-4.588596	1.363455
H	1.762819	-4.251428	2.076755
H	3.345199	-5.074008	1.937275
H	2.076622	-5.358024	0.716868
C	4.089074	-1.936442	1.530066
H	4.609516	-1.119373	0.993474
H	4.870296	-2.503096	2.069835
H	3.430122	-1.472184	2.282792
C	4.575425	-3.785727	-0.800968
H	4.245843	-4.622136	-1.437994
H	5.421107	-4.144645	-0.185817
H	4.955049	-2.986466	-1.460985
C	0.284708	-1.946251	-2.991617
H	-0.222612	-1.046022	-2.598093
H	-0.418241	-2.462947	-3.672002
H	1.152280	-1.623424	-3.594294
C	-0.691023	-3.808756	-0.697432
H	-0.385361	-4.441628	0.154885
H	-1.317450	-4.423608	-1.371407
H	-1.294304	-2.969044	-0.311799
C	1.659315	-4.597211	-2.487992
H	2.539325	-4.282329	-3.074958
H	0.930978	-5.044471	-3.189613
H	1.980536	-5.393499	-1.794203
C	2.515030	3.472477	3.304112
H	1.742995	3.920262	2.654237
H	3.323098	4.213933	3.439796
H	2.055015	3.295515	4.292765
C	4.556084	1.199162	3.697073
H	4.220766	1.062381	4.737667
H	5.399806	1.913612	3.706880
H	4.940472	0.229865	3.334907
C	4.081692	2.297612	0.929099
H	4.605985	1.426769	0.489669
H	4.860324	3.049538	1.155162
H	3.425277	2.717654	0.148708
C	0.262618	-1.617309	3.170195
H	-0.244629	-1.721579	2.193293
H	-0.441003	-1.949964	3.956531
H	1.128668	-2.302605	3.189204
C	1.634903	0.132599	5.225011
H	2.514580	-0.533644	5.244890
H	0.904182	-0.254810	5.958985
H	1.955617	1.129597	5.573930
C	-0.707487	1.300889	3.644029
H	-0.399777	2.354178	3.771531

H -1.336772 1.022195 4.510671
H -1.309282 1.220783 2.722561
C -4.293686 -3.600820 0.747772
H -3.823054 -4.590651 0.568896
H -5.384858 -3.752585 0.895440
C -4.360350 0.234114 3.648195
H -5.458896 0.130460 3.782137
H -3.936044 0.671829 4.576432
C -4.334900 -3.289356 -1.627036
H -5.432123 -3.362732 -1.788867
H -3.901631 -4.308487 -1.709569
C -3.665232 -2.992047 1.988258
H -3.742479 -3.717582 2.827439
H -2.591333 -2.795098 1.792142
C -3.709686 3.522749 -0.750241
H -2.630604 3.270933 -0.769100
H -3.813889 4.627941 -0.681981
C -3.654066 -0.234157 -3.588497
H -3.724400 -0.598355 -4.636840
H -2.581824 -0.155635 -3.315065
C -3.690672 -2.412839 -2.685771
H -2.612984 -2.302564 -2.452249
H -3.788820 -2.906859 -3.677410
C -3.680688 3.218382 1.588696
H -3.763239 4.307611 1.797003
H -2.605240 2.953955 1.524583
C -3.713961 -1.120927 3.423868
H -2.634436 -0.973400 3.221356
H -3.820118 -1.733025 4.346399
C -4.315569 2.446271 2.731096
H -3.854490 2.788368 3.681711
H -5.407983 2.645758 2.779325
C -4.348414 3.041021 -2.040333
H -5.446548 3.212323 -2.025552
H -3.916062 3.624363 -2.880553
C -4.292185 1.140200 -3.497618
H -3.823605 1.793373 -4.263798
H -5.382325 1.080802 -3.706233

7-U - PBE
-5014.4187078 H
$2.4x10^{-5}$

U	-1.622346	-0.022566	0.136699
S	0.670375	-0.168308	-0.803673
N	-2.203317	2.137233	-0.395051
N	-2.702749	-1.698176	-0.991120
Si	-1.620137	2.833454	-1.919205
Si	-4.347662	-1.500206	-1.608862
Si	-3.063628	3.193327	0.731492
Si	-1.803388	-3.163467	-1.435686
K	3.750864	-0.042194	-0.437749
N	-1.208299	-0.418315	2.370863
Si	-2.238196	-1.461609	3.358249
Si	0.298250	0.178723	3.072098
O	5.318304	-2.369314	0.600588
O	3.624568	2.376180	-1.882060
O	3.656108	-0.055062	-3.380474
O	5.291403	0.074412	2.078095
O	3.978817	-2.481278	-1.884477
O	4.946414	2.489261	0.600098
C	-2.900922	-4.710461	-1.676414
H	-3.468544	-4.963903	-0.764448
H	-2.244544	-5.569705	-1.909331
H	-3.619279	-4.611846	-2.508310
C	-0.581275	-3.652937	-0.059618
H	0.006636	-4.531973	-0.386705
H	-1.114094	-3.930336	0.867075
H	0.123943	-2.835357	0.170361
C	-0.842546	-2.927716	-3.061425
H	-1.524155	-2.746658	-3.910992
H	-0.230620	-3.818420	-3.297053
H	-0.175793	-2.054421	-2.959002
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