SUPPLEMENTARY INFORMATION

Advancing understanding of comparison of M-O covalency in isostructural M-OSiMe$_3$ (M = Ce, Th, U) complexes

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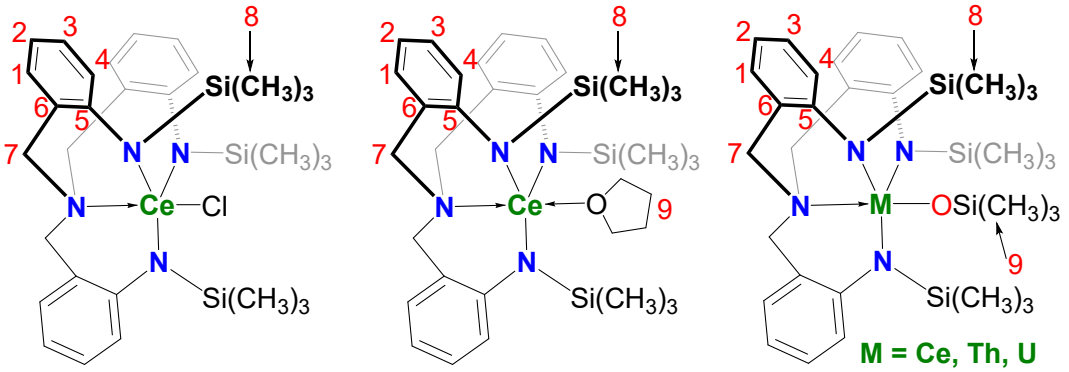

Figure S1. The structure of the synthetic complexes and the labeled C-atomic numbers.

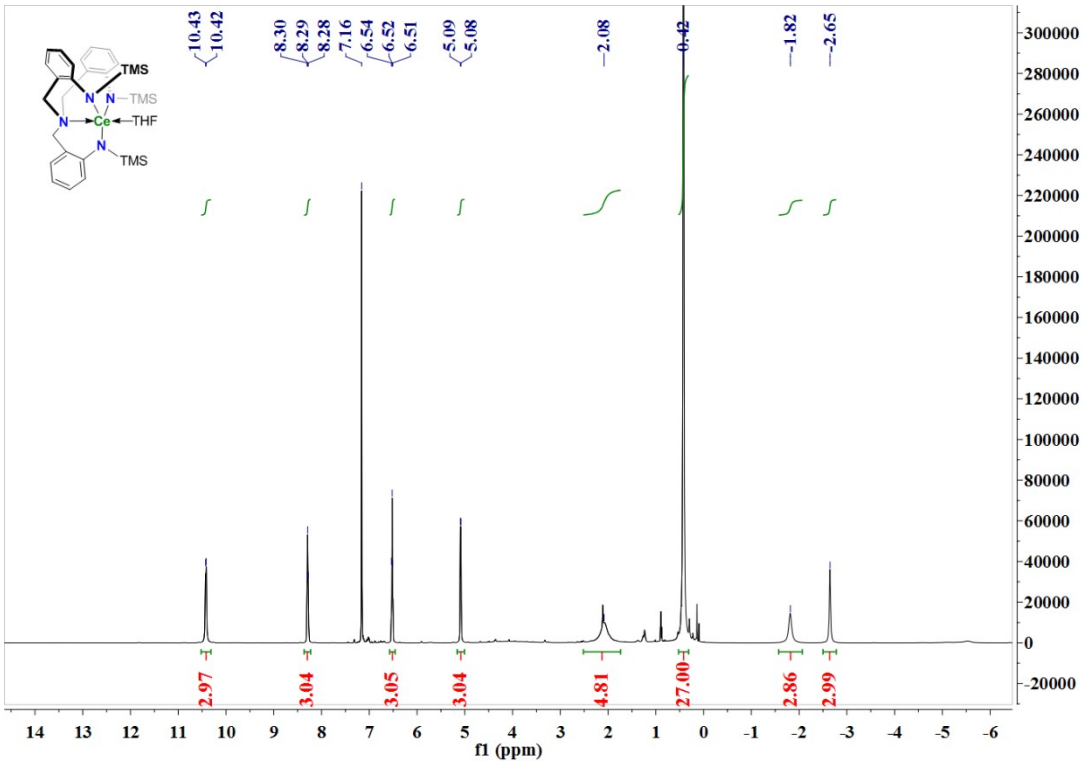

Figure S2. ^{1}H NMR (500 MHz, 298 K) spectrum of B in benzene-d_6.

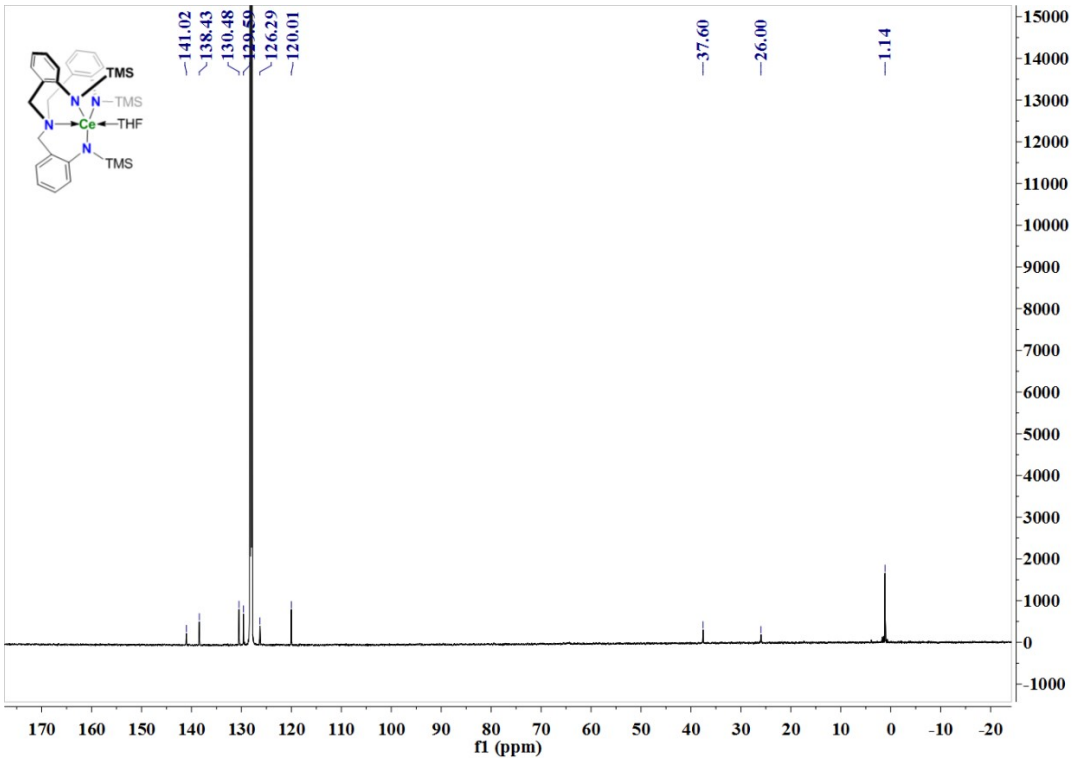

Figure S3. ^{13}C {^{1}H} NMR (125 MHz, 298 K) spectrum of B in benzene-d_6.

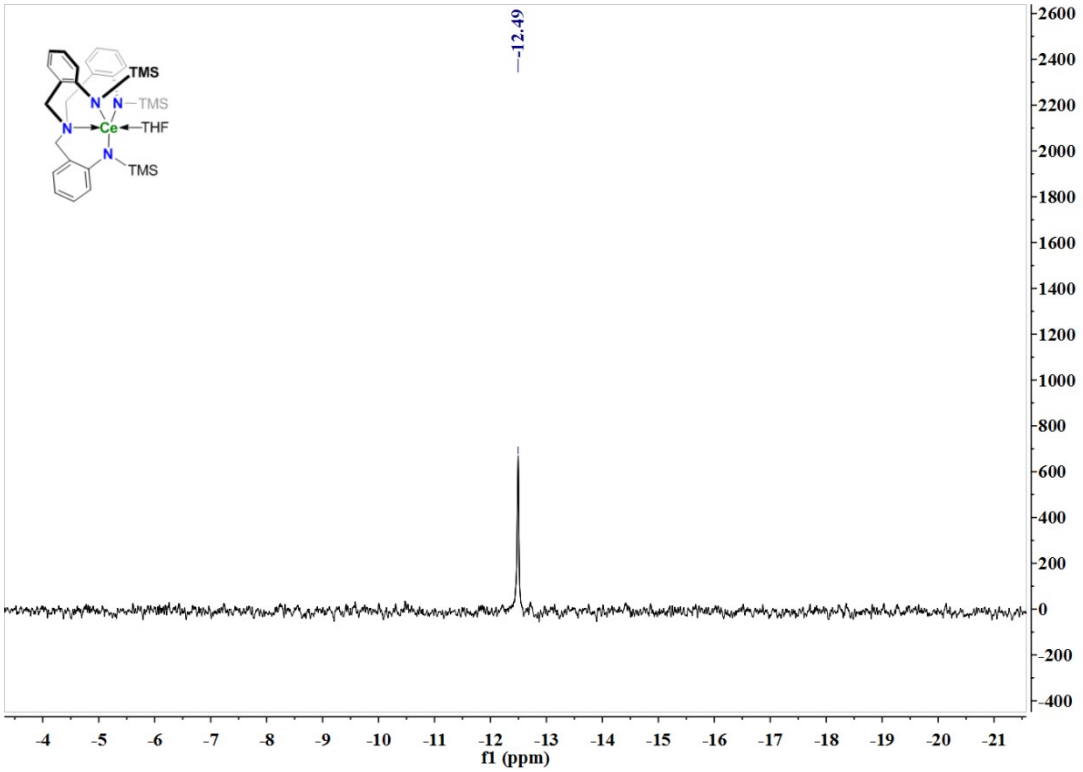

Figure S4. ^{29}Si {^{1}H} NMR (99 MHz, 298 K) spectrum of B in benzene-d_6.

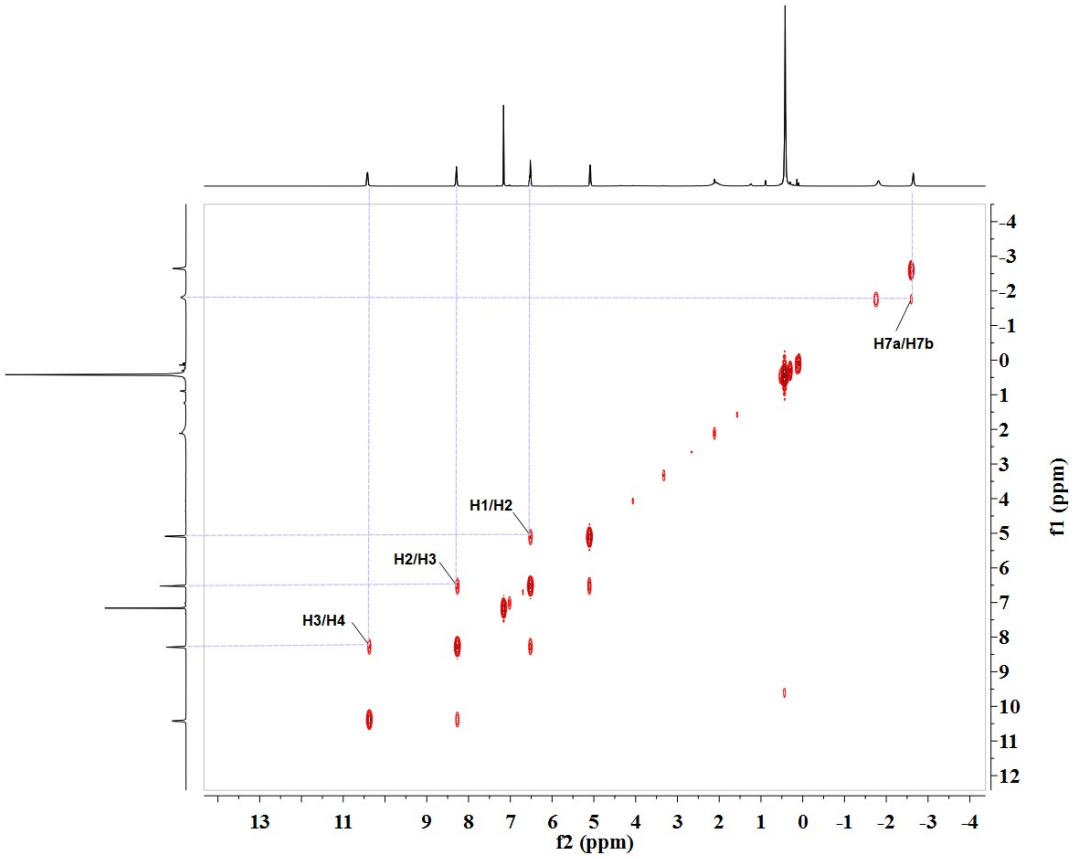

Figure S5. ^{1}H-^{1}H COSY (C_6D_6, 298 K) spectrum of B.

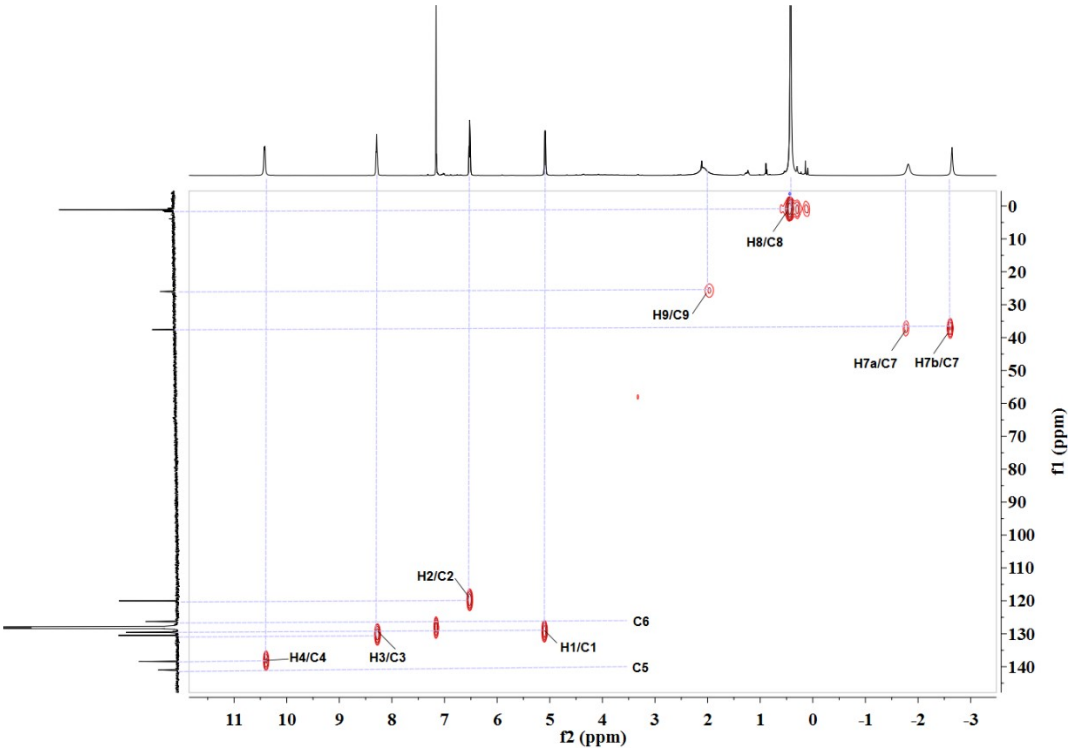

Figure S6. ^{1}H-^{13}C HSQC (C_6D_6, 298 K) spectrum of B.

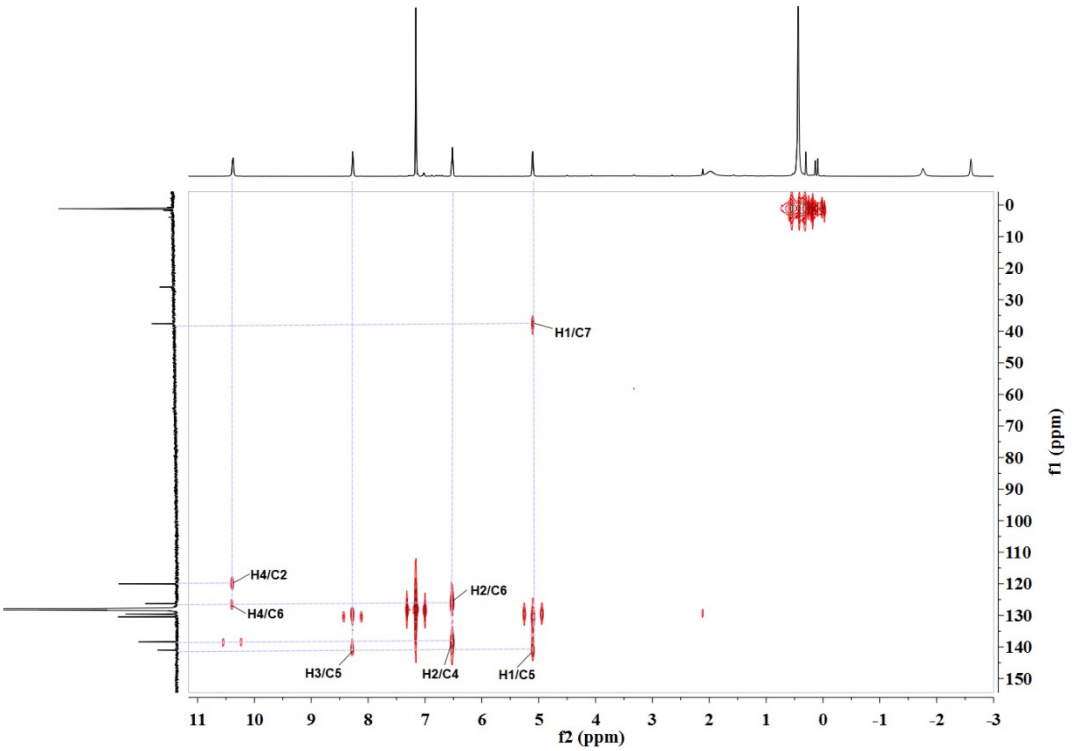

Figure S7. ^{1}H-^{13}C HMBC (C_6D_6, 298 K) spectrum of B.

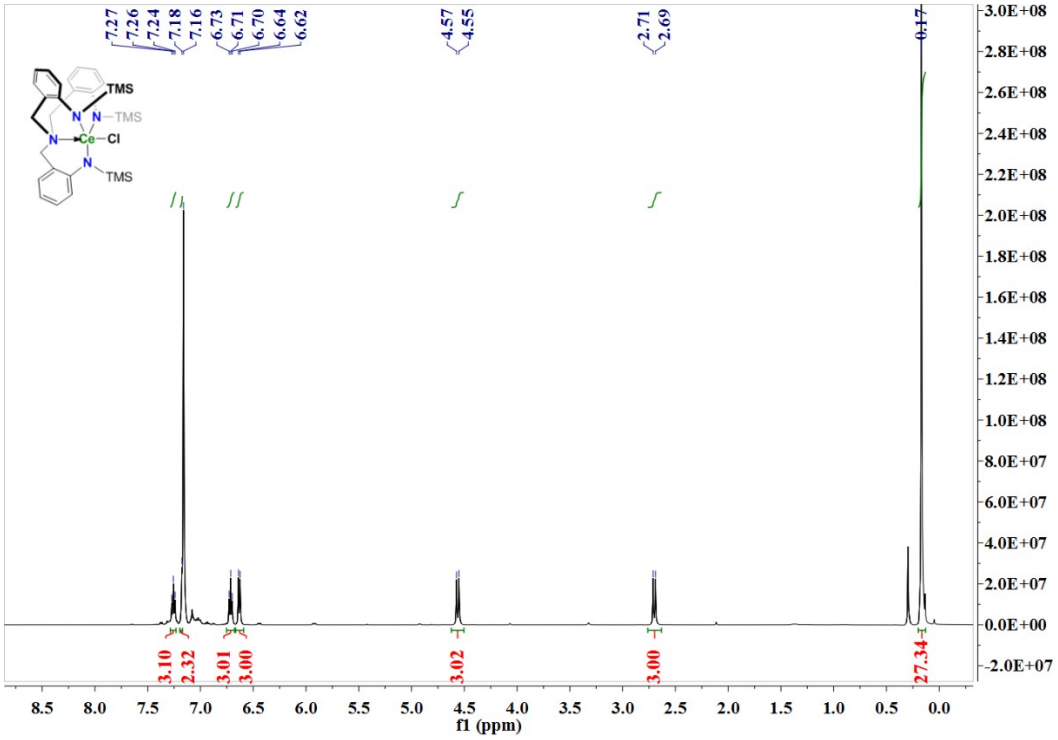

Figure S8. ^{1}H NMR (500 MHz, 298 K) spectrum of 1Ce in benzene-d_6.

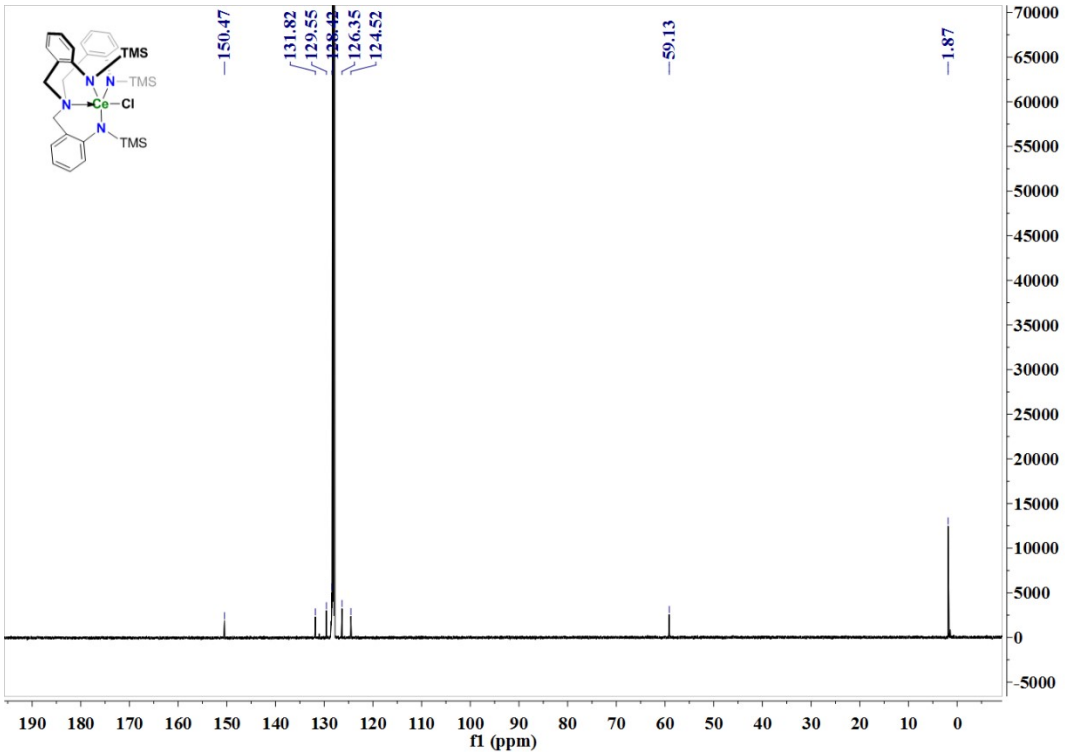

Figure S9. ^{13}C {^{1}H} NMR (125 MHz, 298 K) spectrum of 1Ce in benzene-d_6.

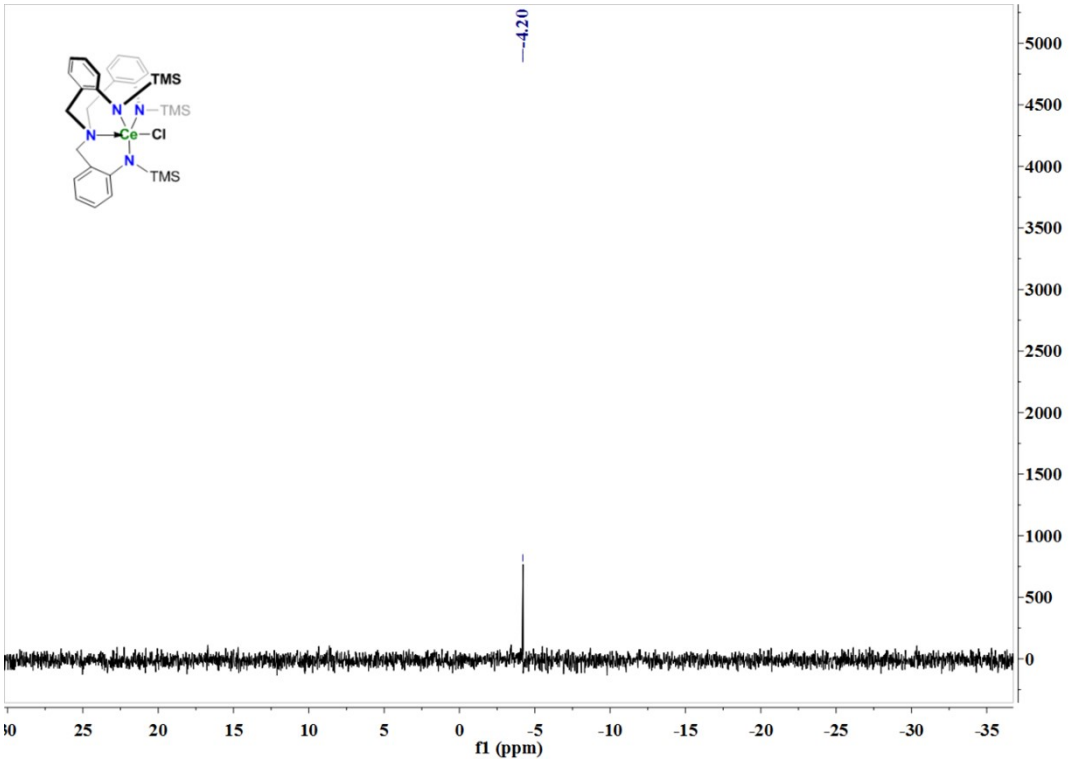

Figure S10. ^{29}Si {^{1}H} NMR (99 MHz, 298 K) spectrum of 1Ce in benzene-d_6.

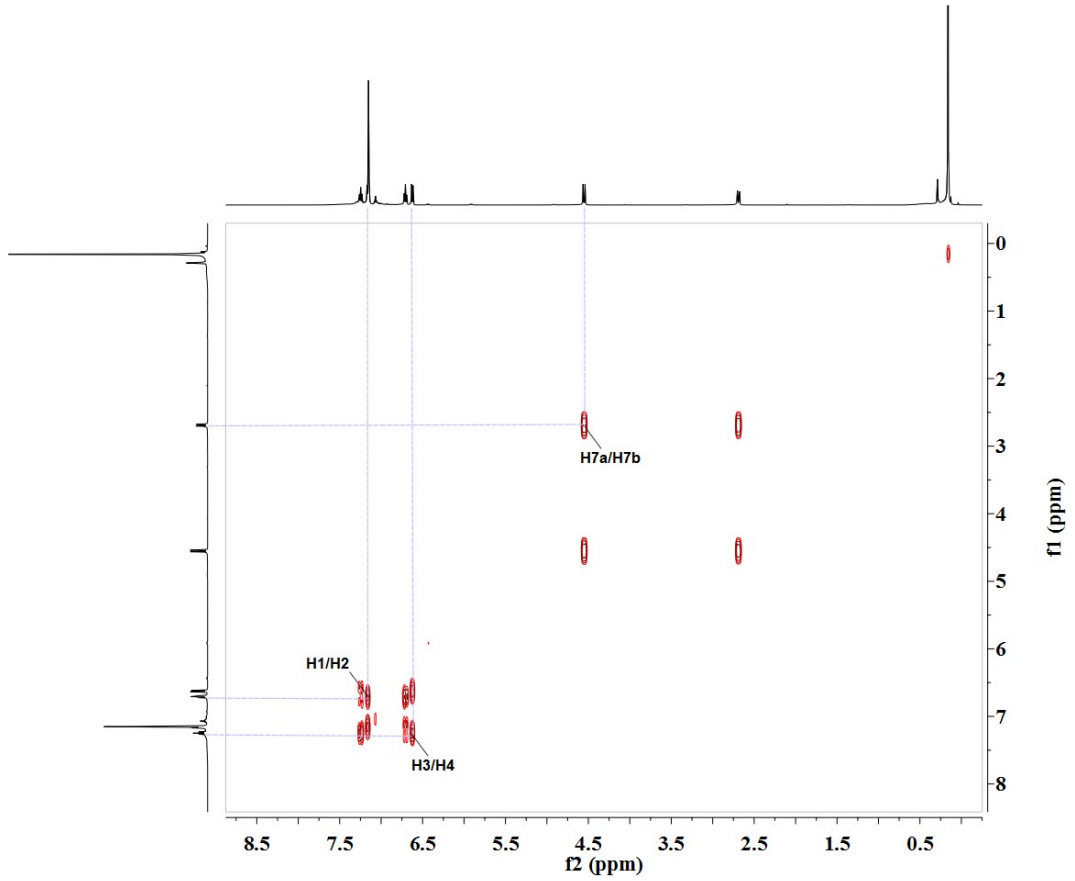

Figure S11. ^{1}H-^{1}H COSY (C_6D_6, 298 K) spectrum of 1Ce.

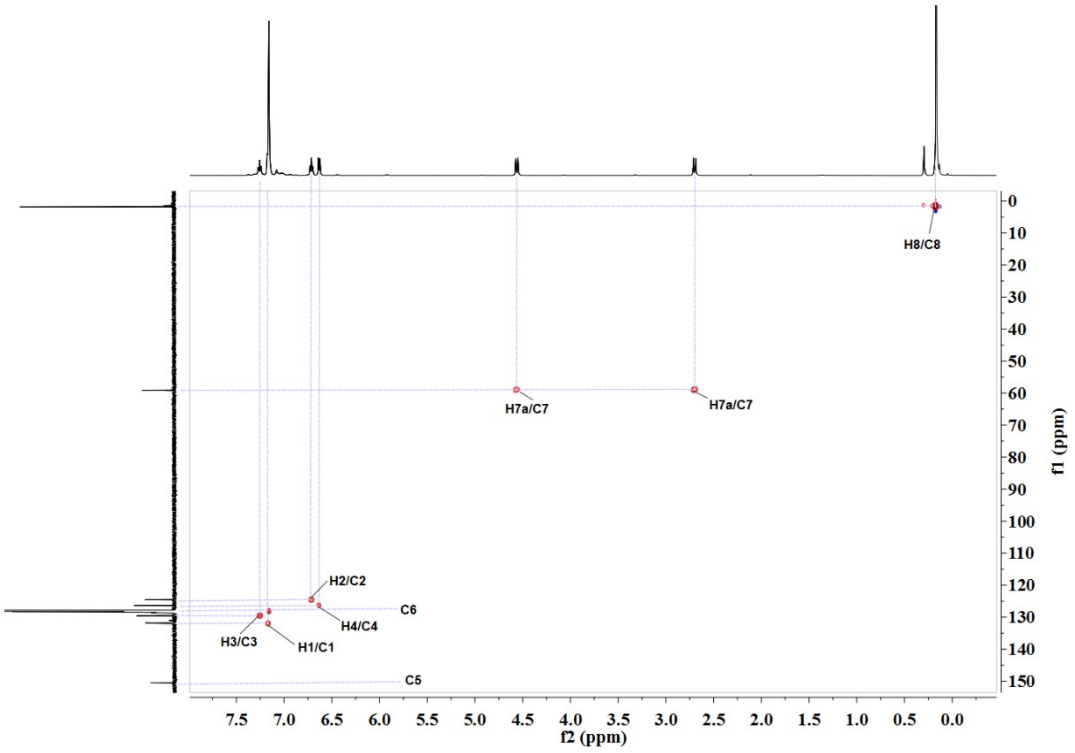

Figure S12. ^{1}H-^{13}C HSQC (C_6D_6, 298 K) spectrum of 1Ce.

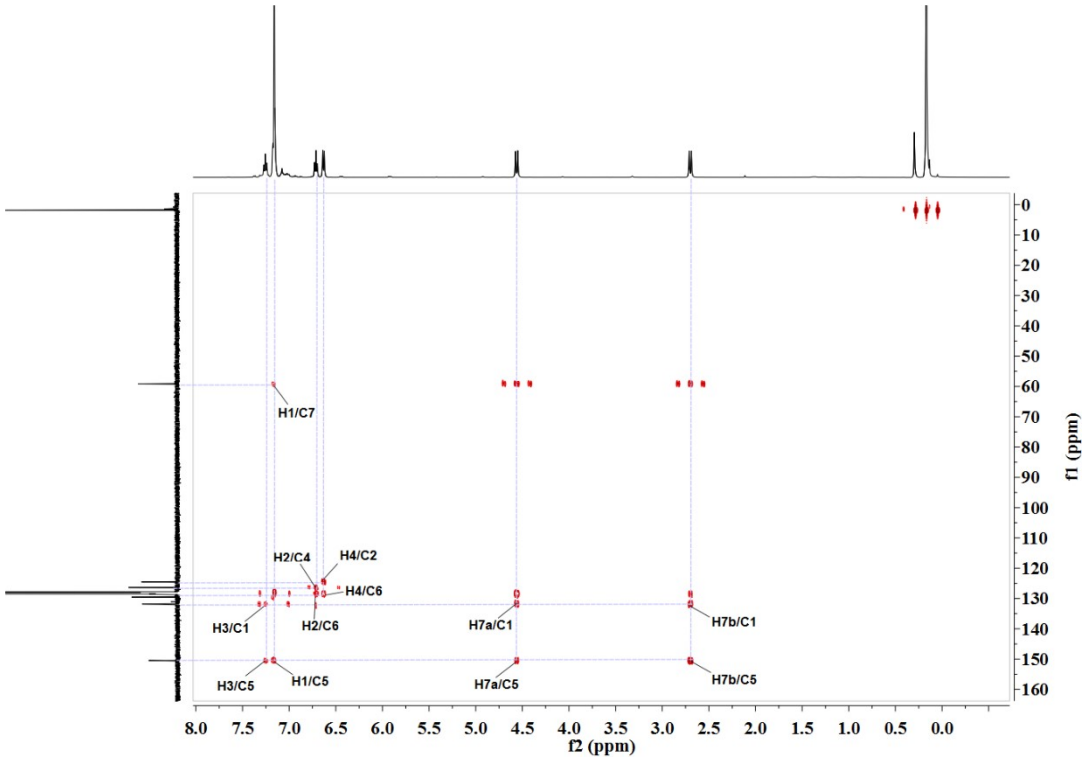

Figure S13. ^{1}H-^{13}C HMBC (C_6D_6, 298 K) spectrum of 1Ce.

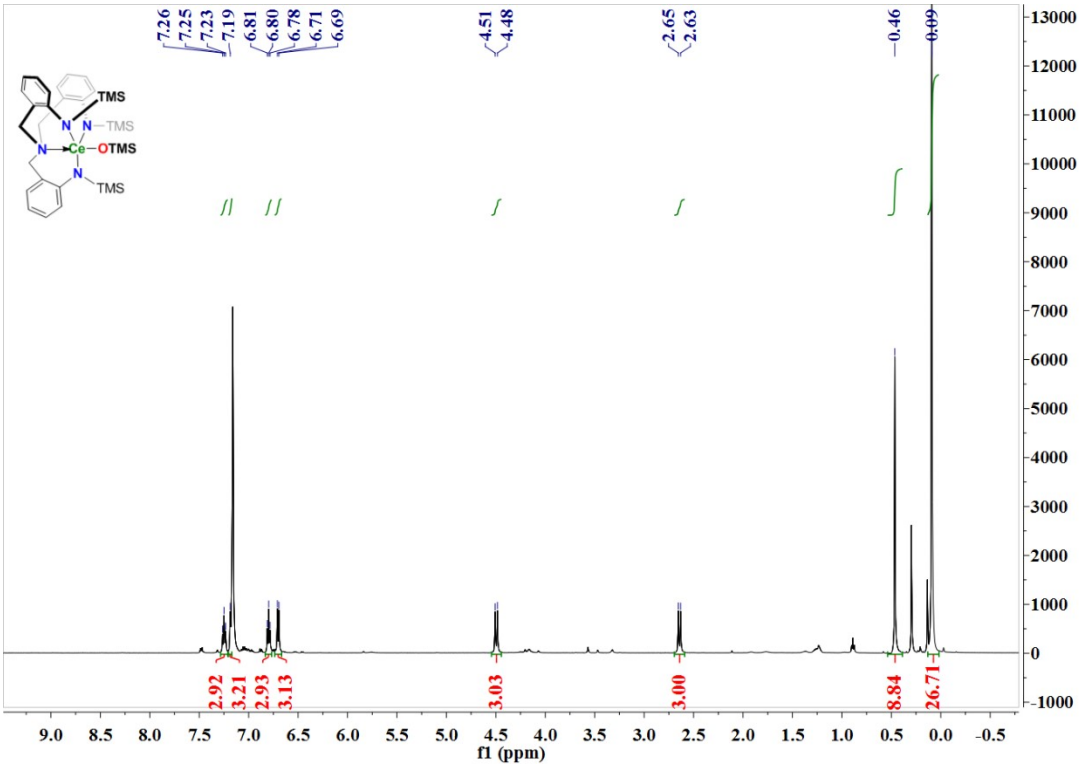

Figure S14. ^{1}H NMR (500 MHz, 298 K) spectrum of 2Ce in benzene-d_6.

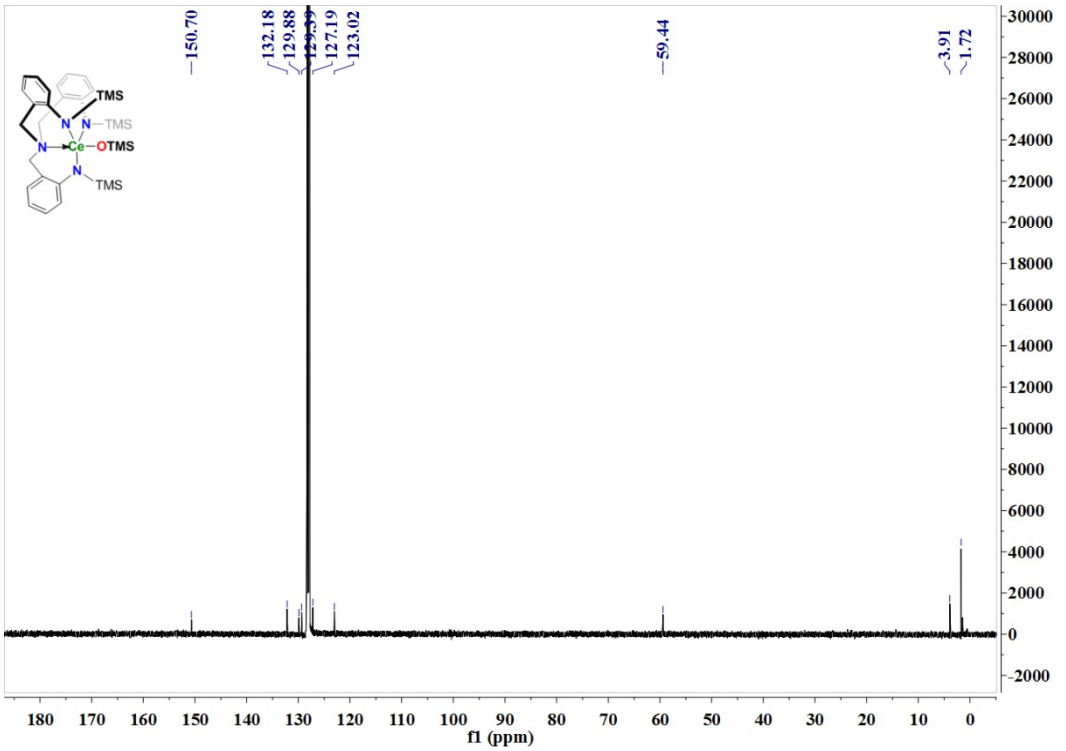

Figure S15. ^{13}C {^{1}H} NMR (125 MHz, 298 K) spectrum of 2Ce in benzene-d_6.

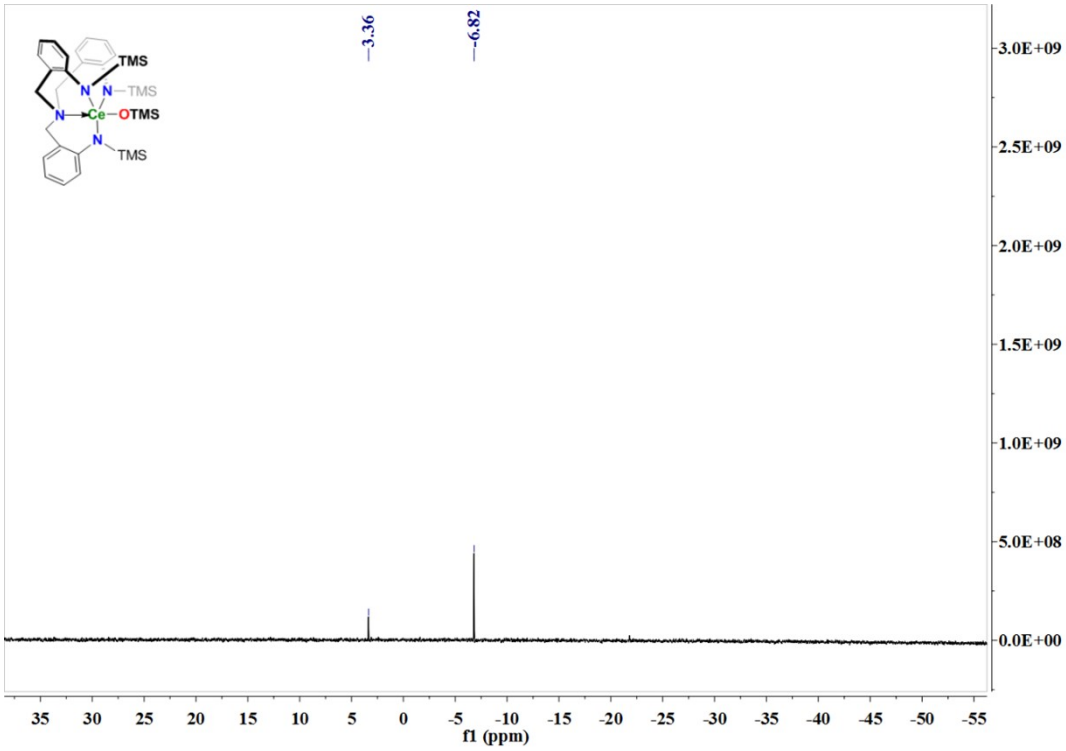

Figure S16. ^{29}Si {^{1}H} NMR (99 MHz, 298 K) spectrum of 2Ce in benzene-d_6.

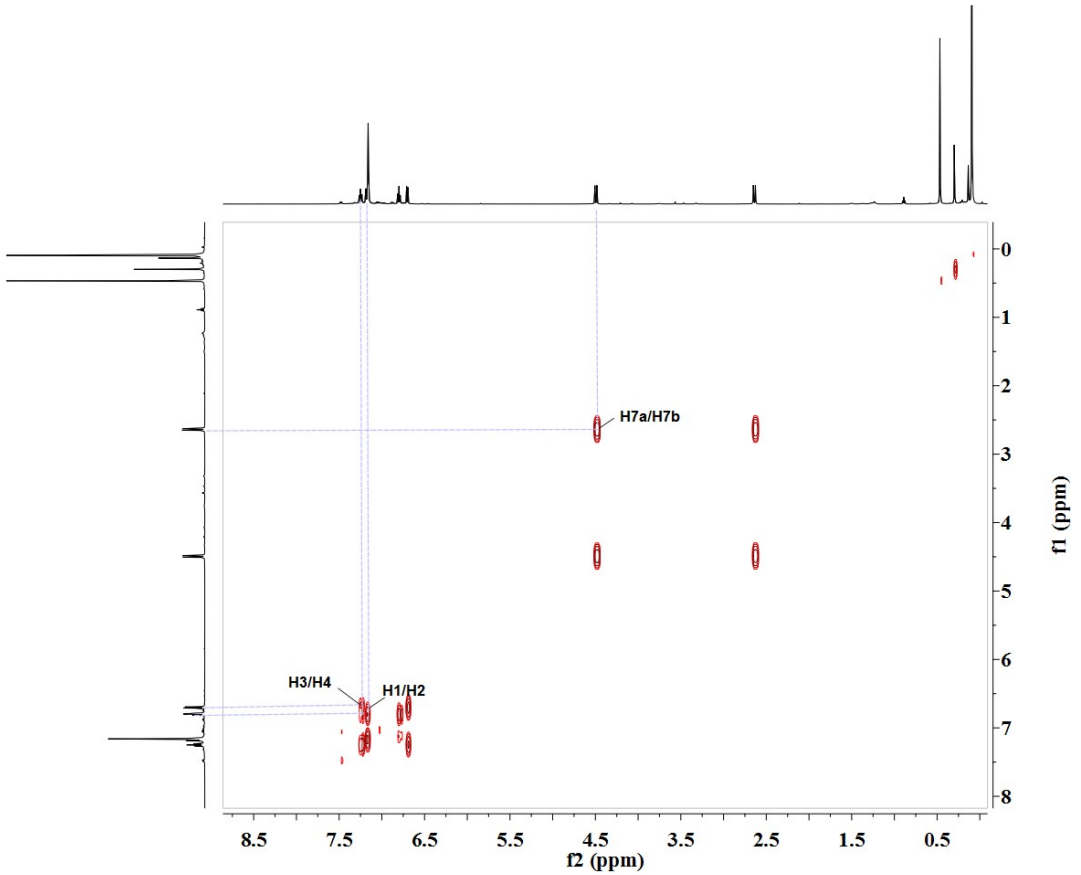

Figure S17. ^{1}H-^{1}H COSY (C_6D_6, 298 K) spectrum of 2Ce.

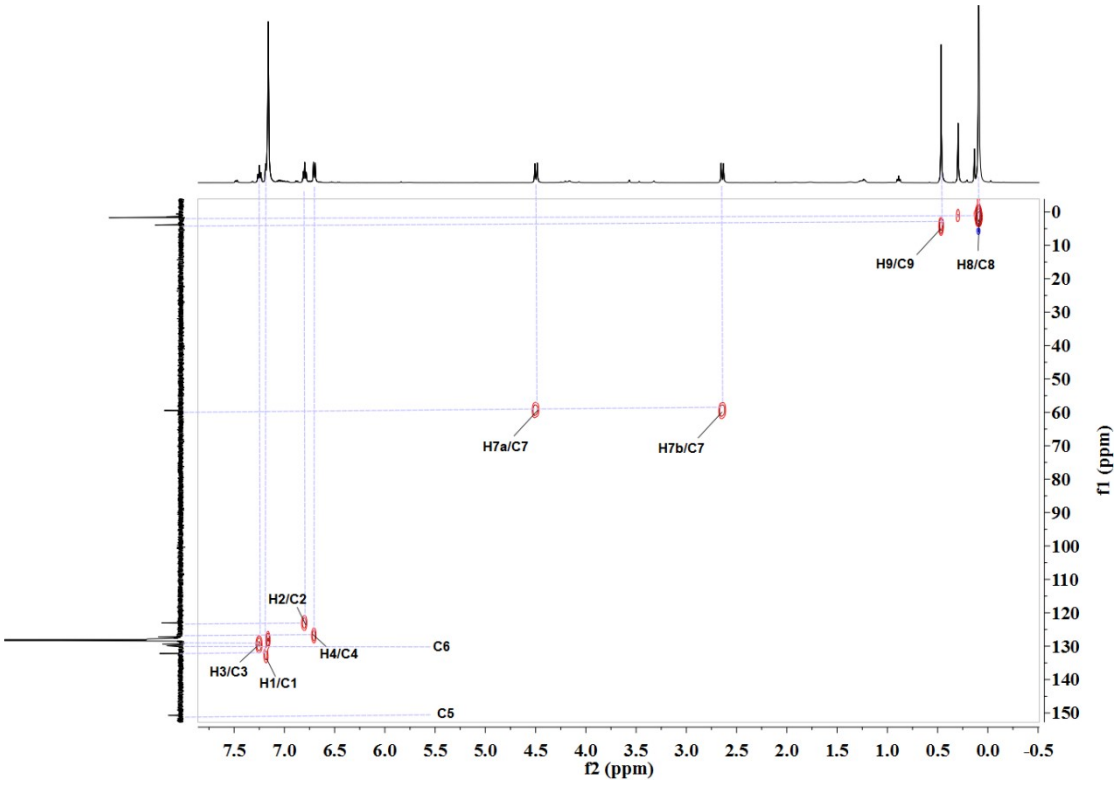

Figure S18. ^{1}H-^{13}C HSQC (C_6D_6, 298 K) spectrum of 2Ce.

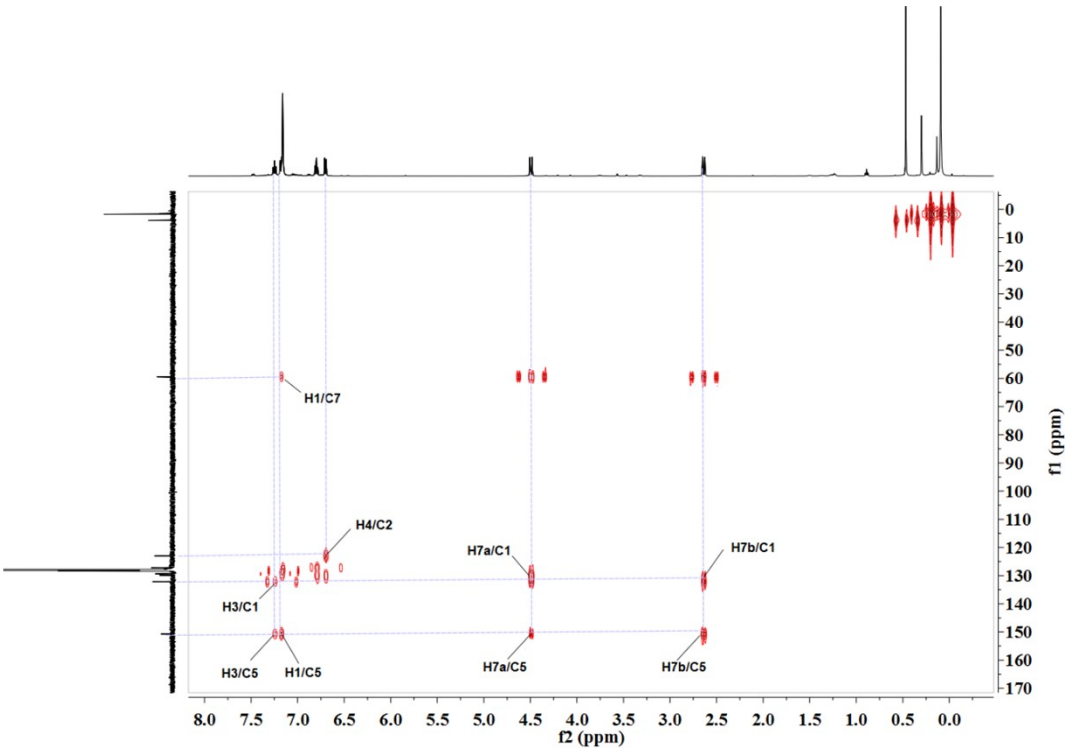

Figure S19. ^{1}H-^{13}C HMBC (C_6D_6, 298 K) spectrum of 2Ce.

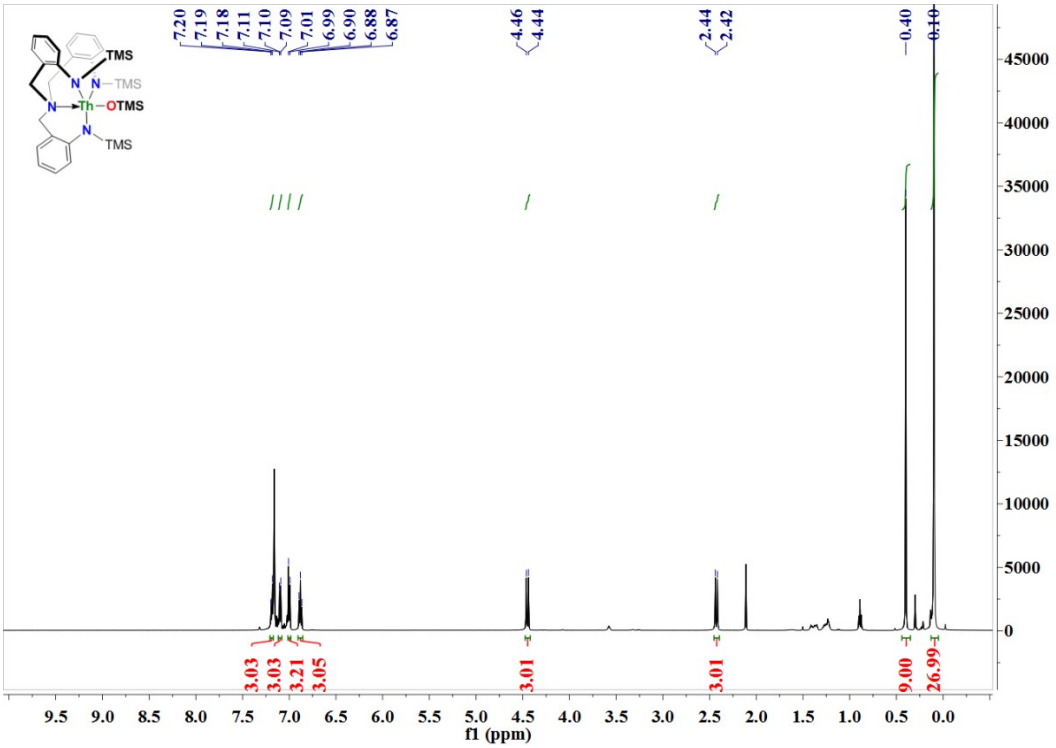

Figure S20. ^{1}H NMR (500 MHz, 298 K) spectrum of 2Th in benzene-d_6.

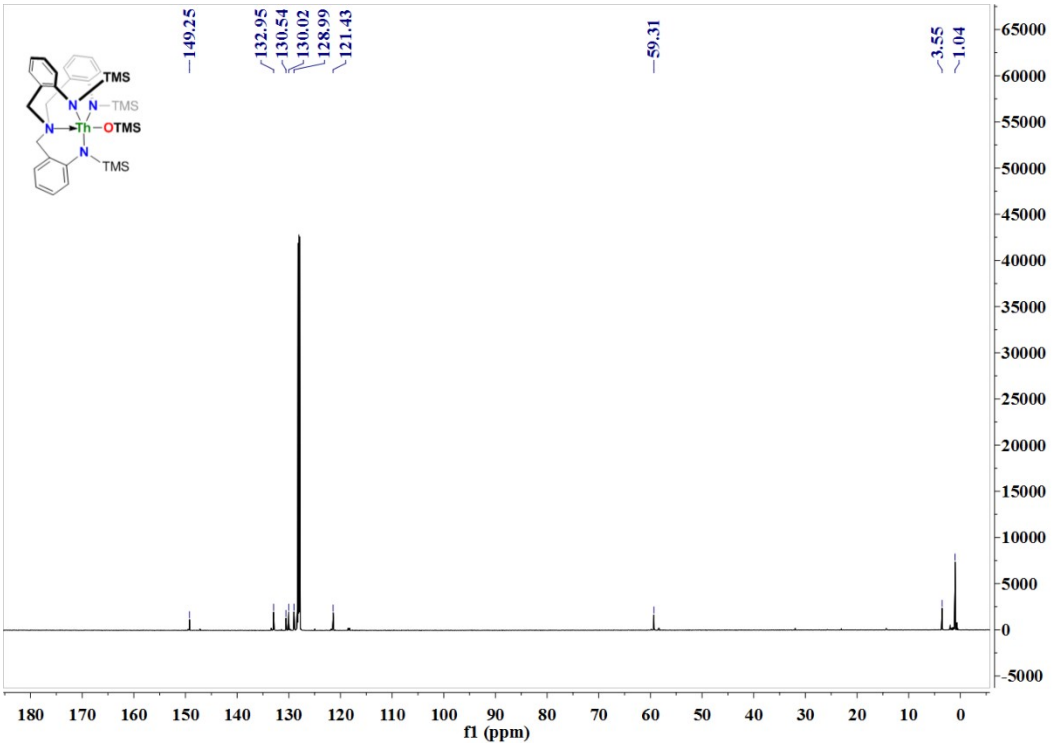

Figure S21. ^{13}C {^{1}H} NMR (125 MHz, 298 K) spectrum of 2Th in benzene-d_6.

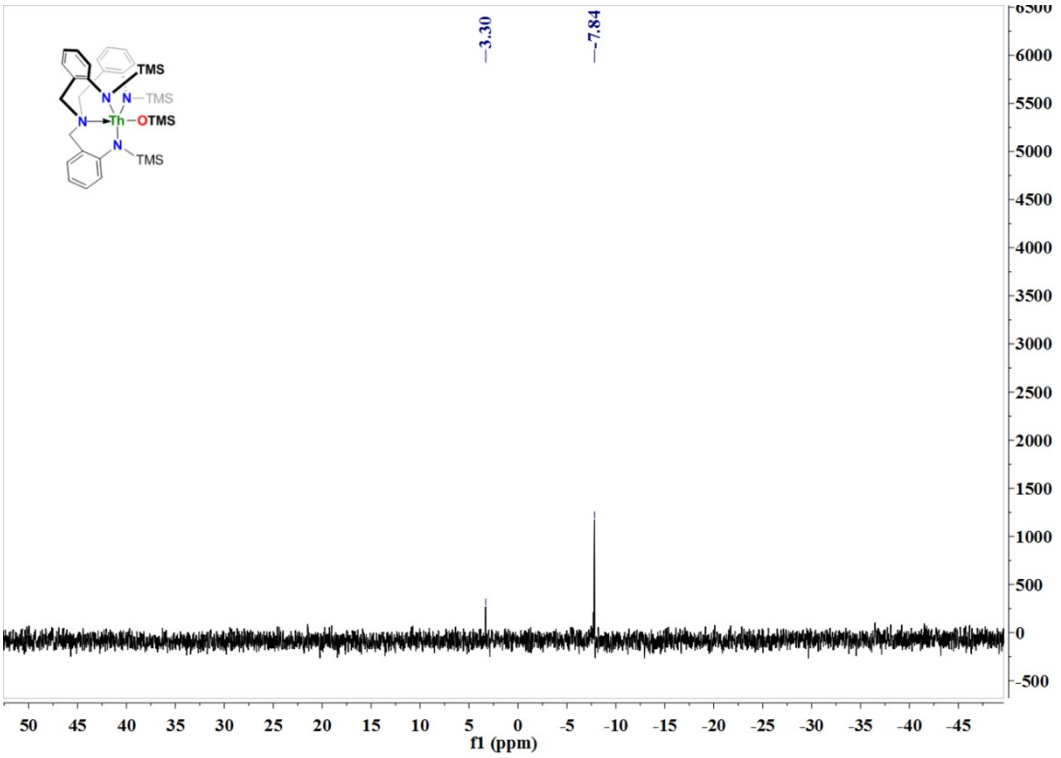

Figure S22. ^{29}Si {^{1}H} NMR (99 MHz, 298 K) spectrum of 2Th in benzene-d_6.

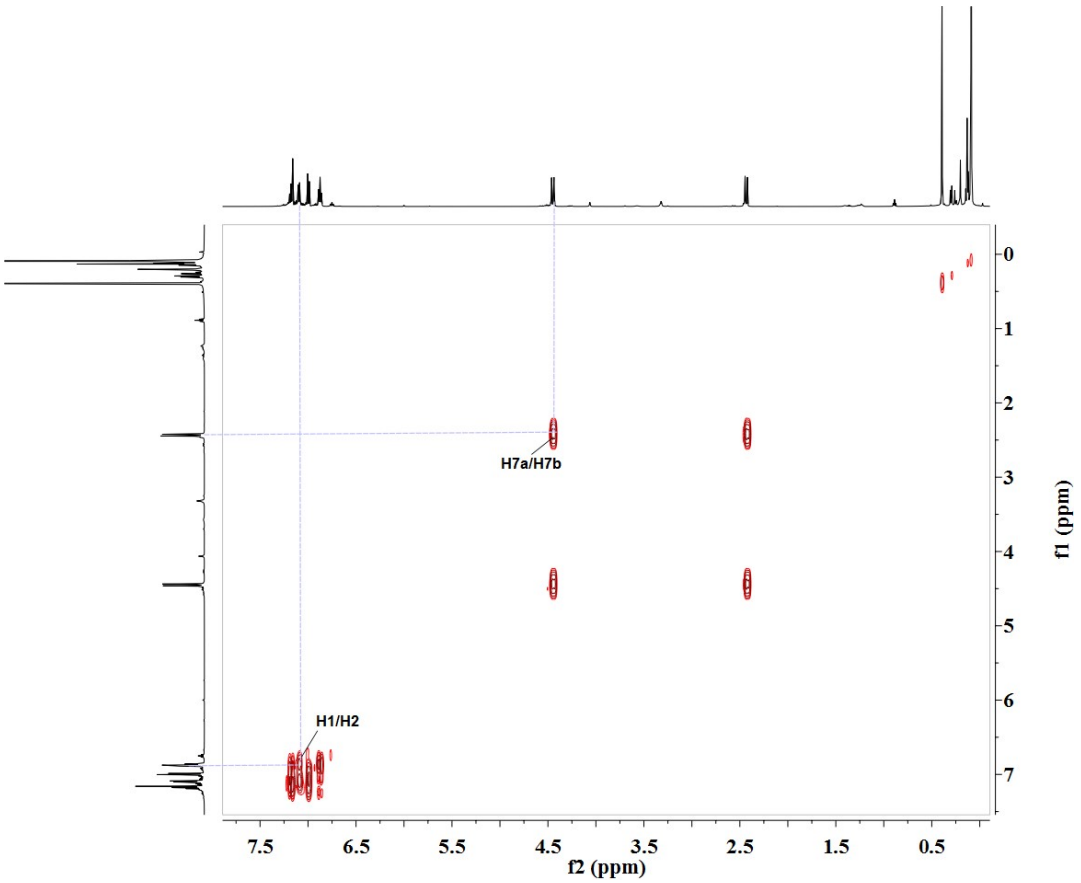

Figure S23. ^{1}H-^{1}H COSY (C_6D_6, 298 K) spectrum of 2Th.

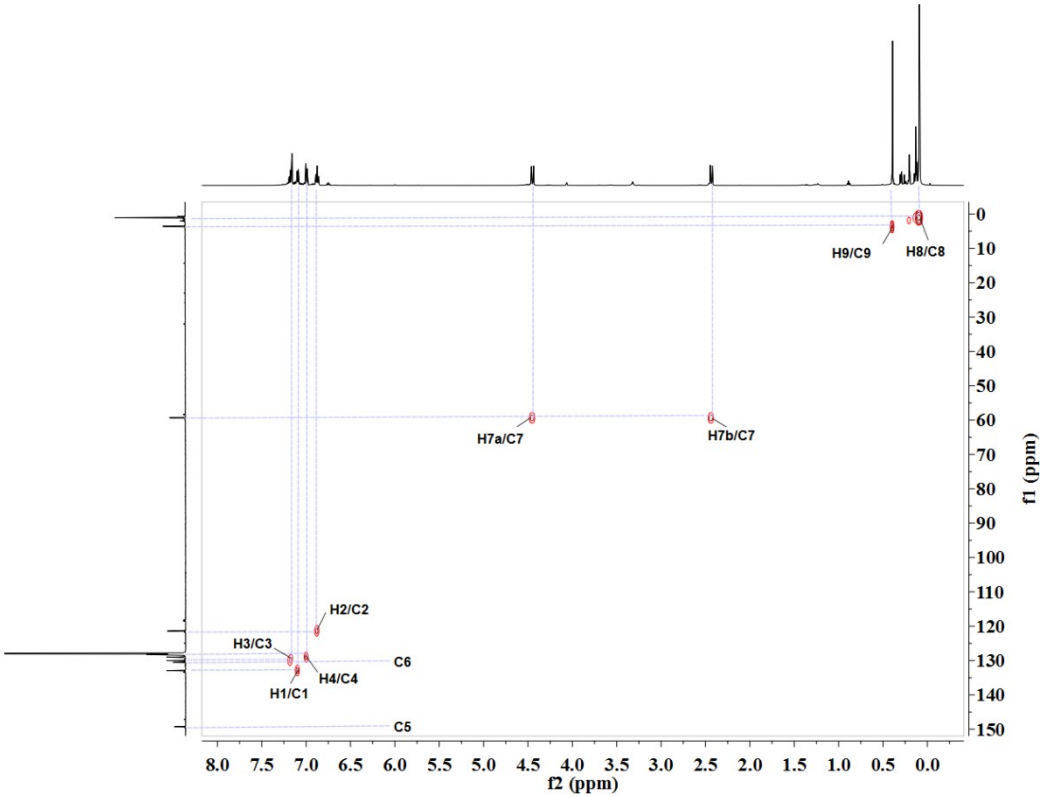

Figure S24. ^{1}H-^{13}C HSQC (C_6D_6, 298 K) spectrum of 2Th.

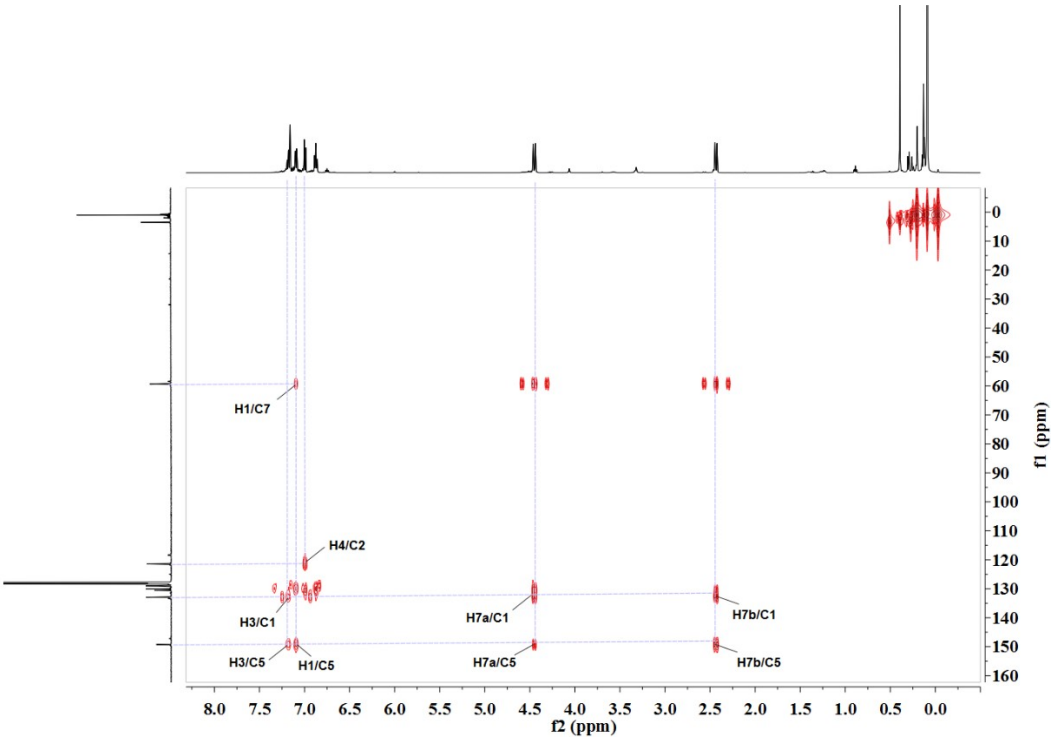

Figure S25. ^{1}H-^{13}C HMBC (C_6D_6, 298 K) spectrum of 2Th.

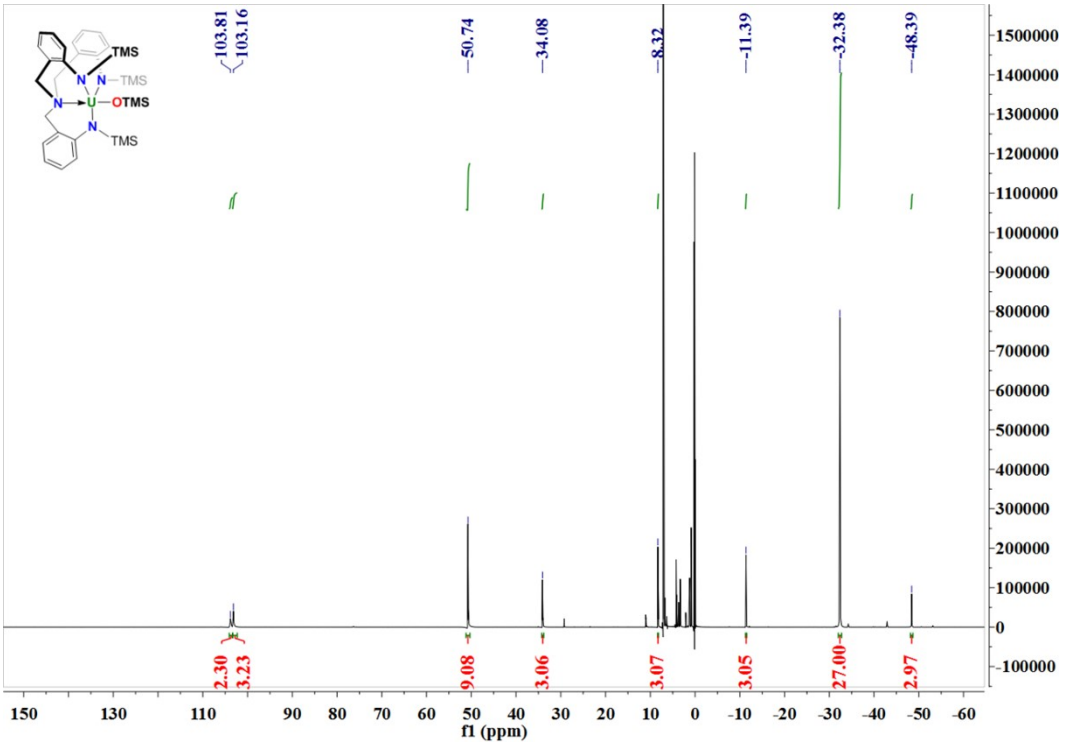

Figure S26. ^{1}H NMR (500 MHz, 298 K) spectrum of 2U in benzene-d_6.

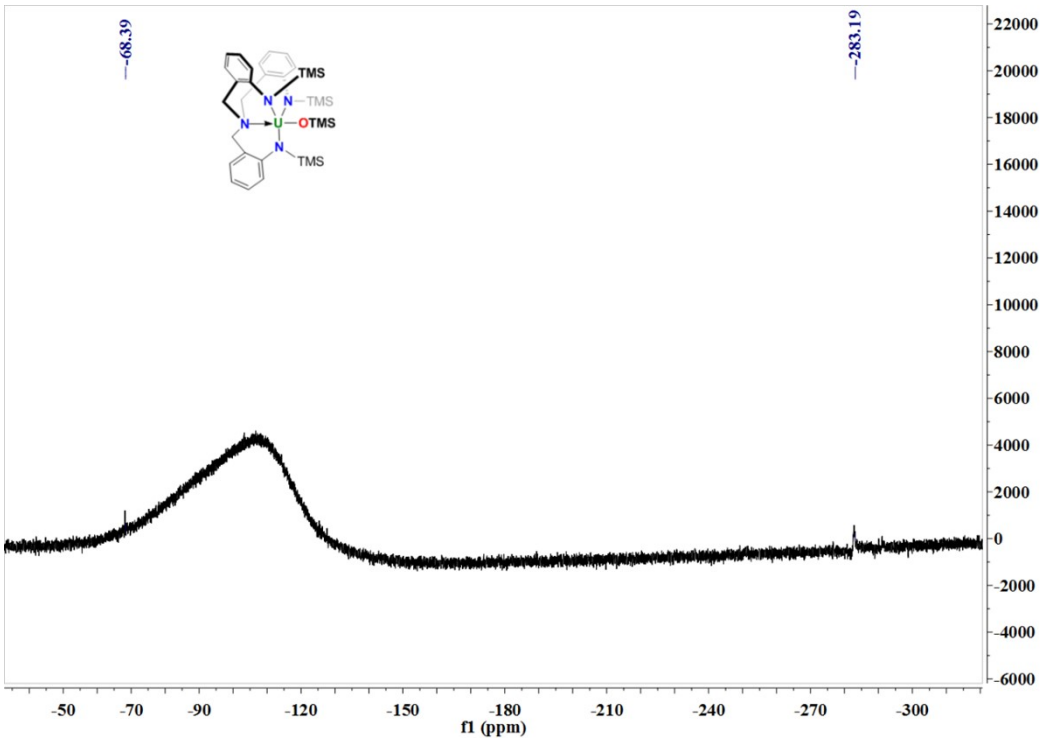

Figure S27. ^{29}Si {^{1}H} NMR (99 MHz, 298 K) spectrum of 2Th in benzene-d_6.

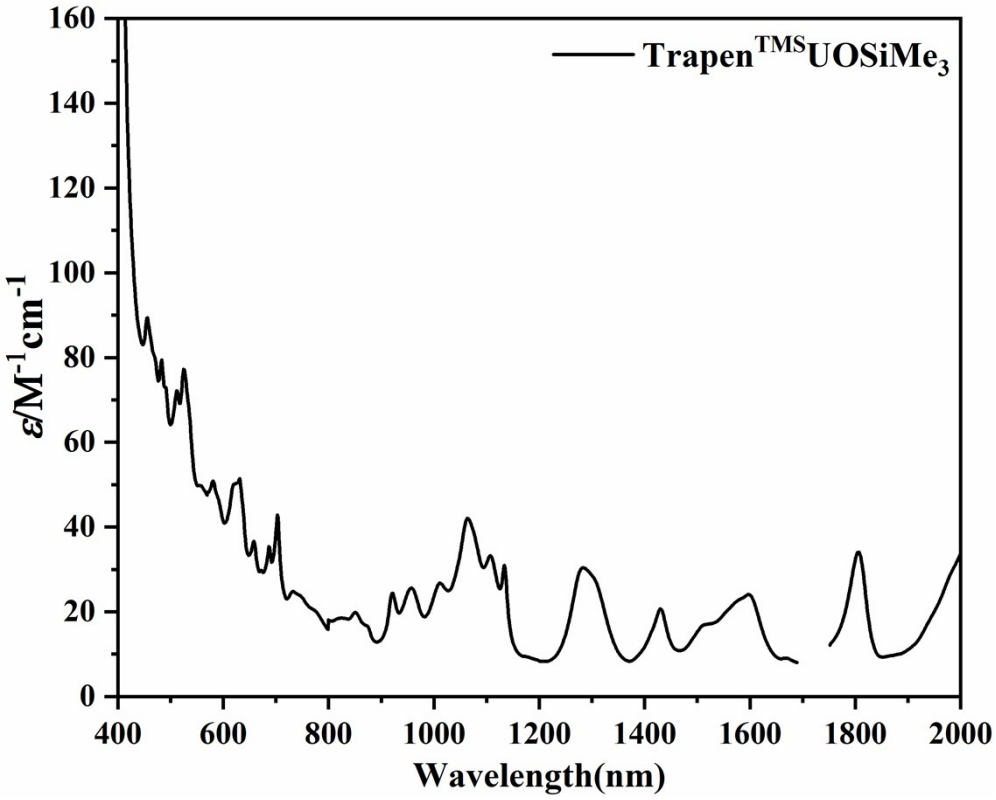

Figure S28. UV-Vis-NIR of 2U (2.75 mM) in THF at 298 K.

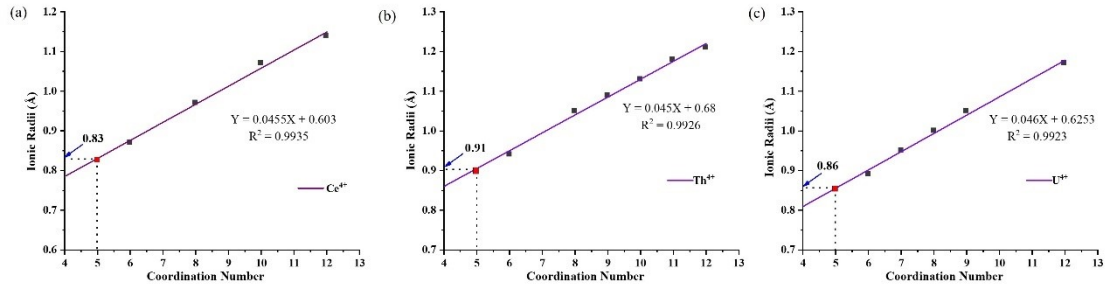

Figure S29. Ionic radius linear fitting diagram of 5-coordinated M^{4+} (M = Ce, Th and U) according to reference 64.

The coordination numbers of Ce^{4+} are provided in reference 64, which are 6, 8, 10 and 12, respectively. Linear regression analysis was performed for the ionic radius of Ce^{4+} using the least square method, where R^2 value exceeds 0.99. It can be reasonably deduced that the ionic radius of 5-coordinated Ce^{4+} is 0.83 Å (see Figure S29). Similarly, the calculated ionic radius values for 5-coordinated U^{4+} and Th^{4+} are 0.86 Å, and 0.91 Å, respectively.

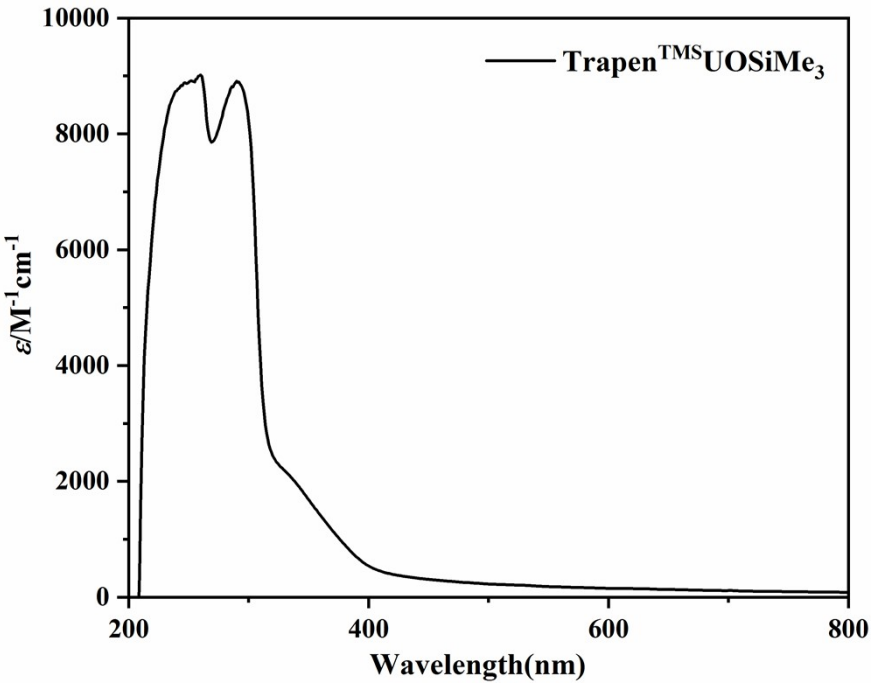

Figure S30. UV-Vis spectrum of 2U (0.4 mM) in THF at 298 K.

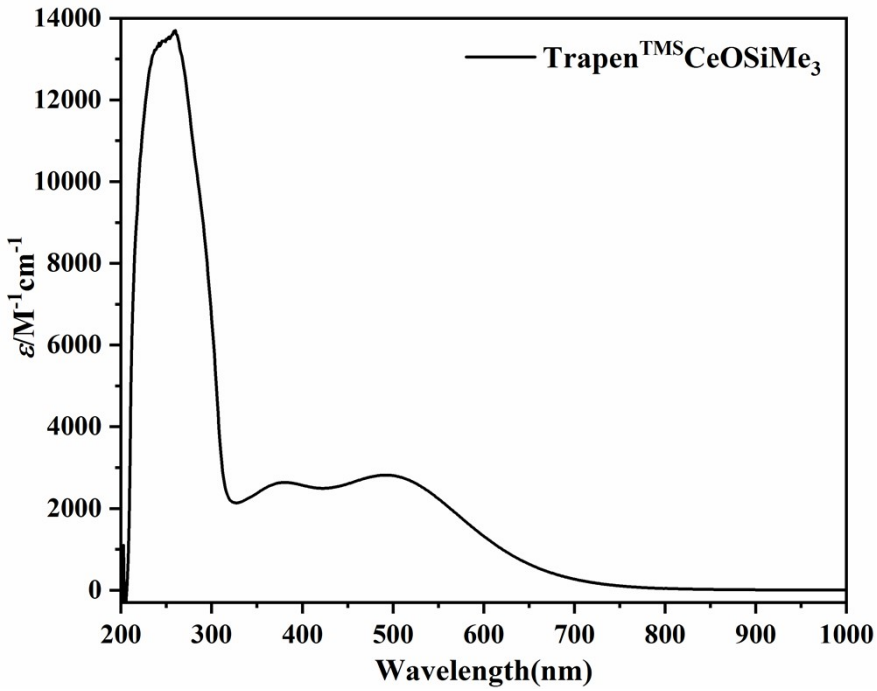

Figure S31. UV-Vis spectrum of 2Ce (0.29 mM) in THF at 298 K.

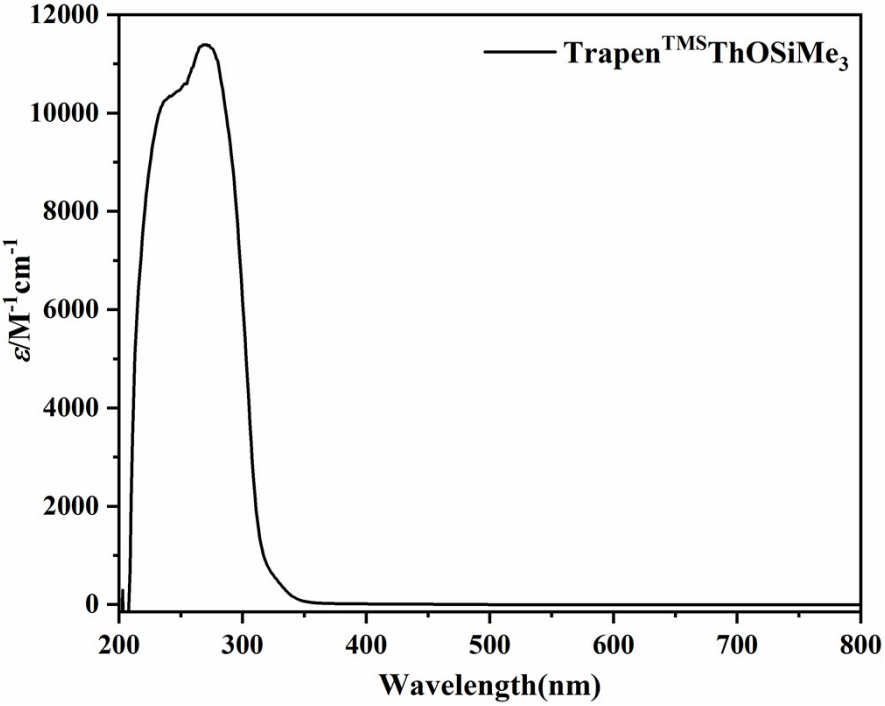

Figure S32. UV-Vis spectrum of 2Th (0.35 mM) in THF at 298 K.

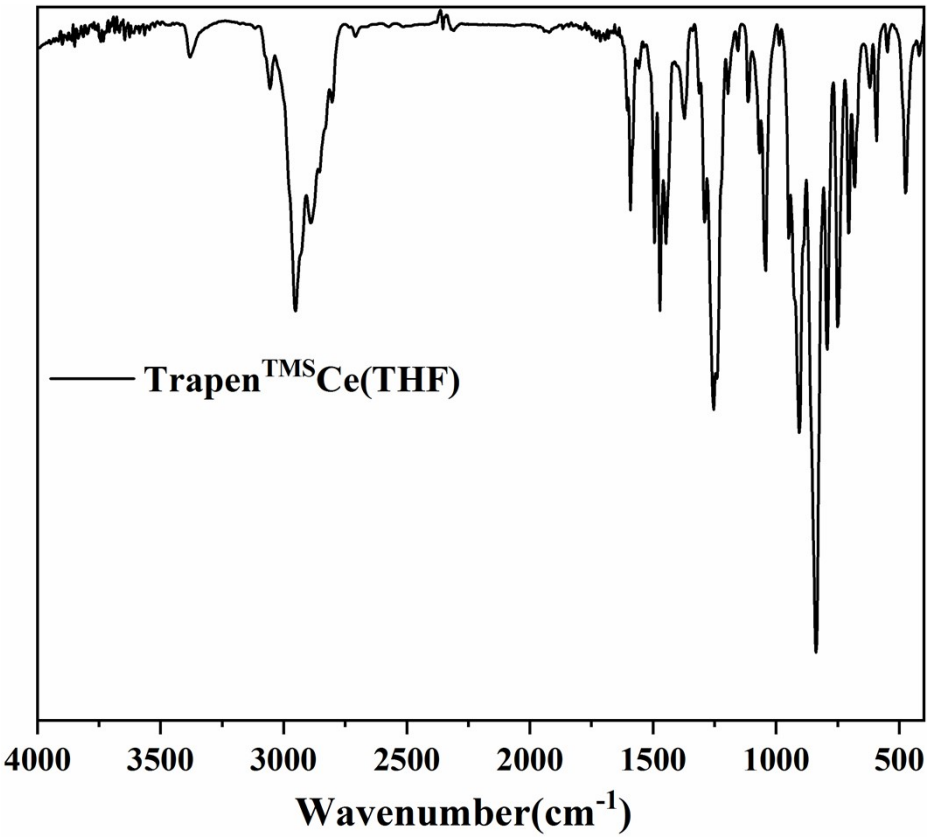

Figure S33. FT-IR of B.

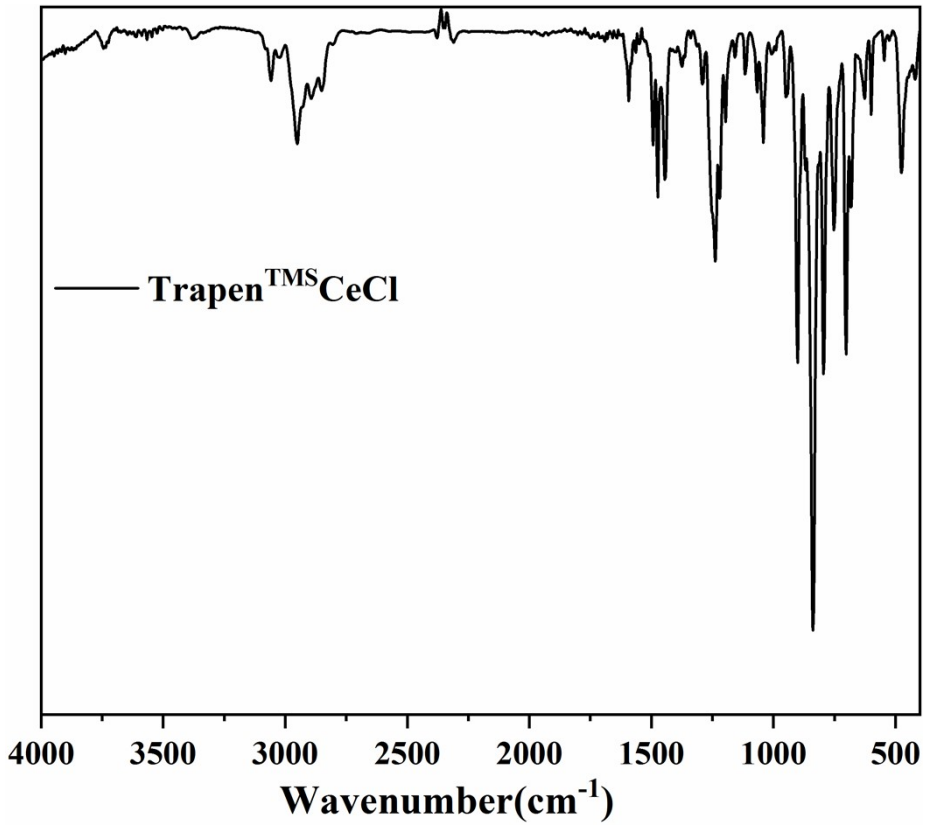

Figure S34. FT-IR of 1Ce.

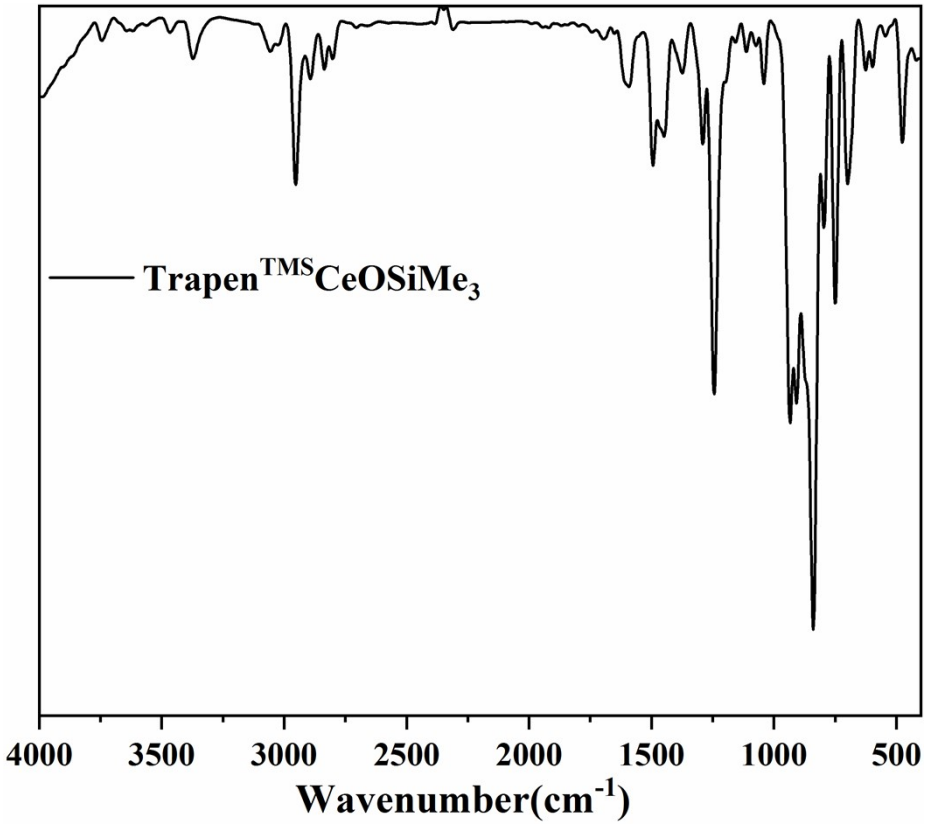

Figure S35. FT-IR of 2Ce.

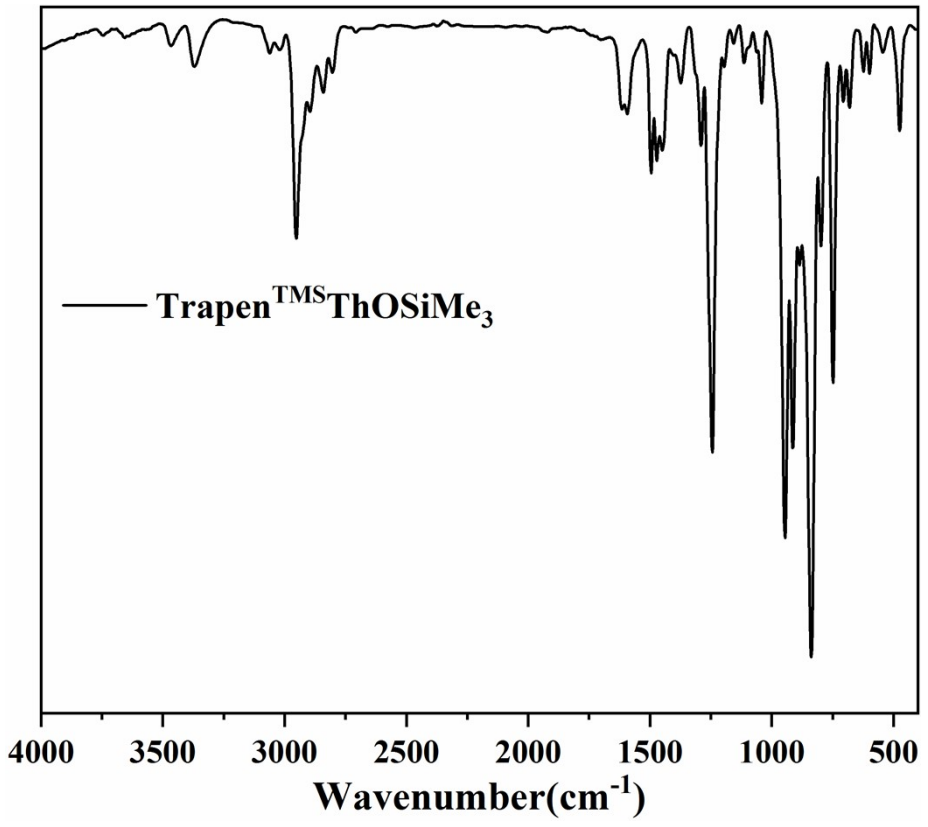

Figure S36. FT-IR of 2Th.

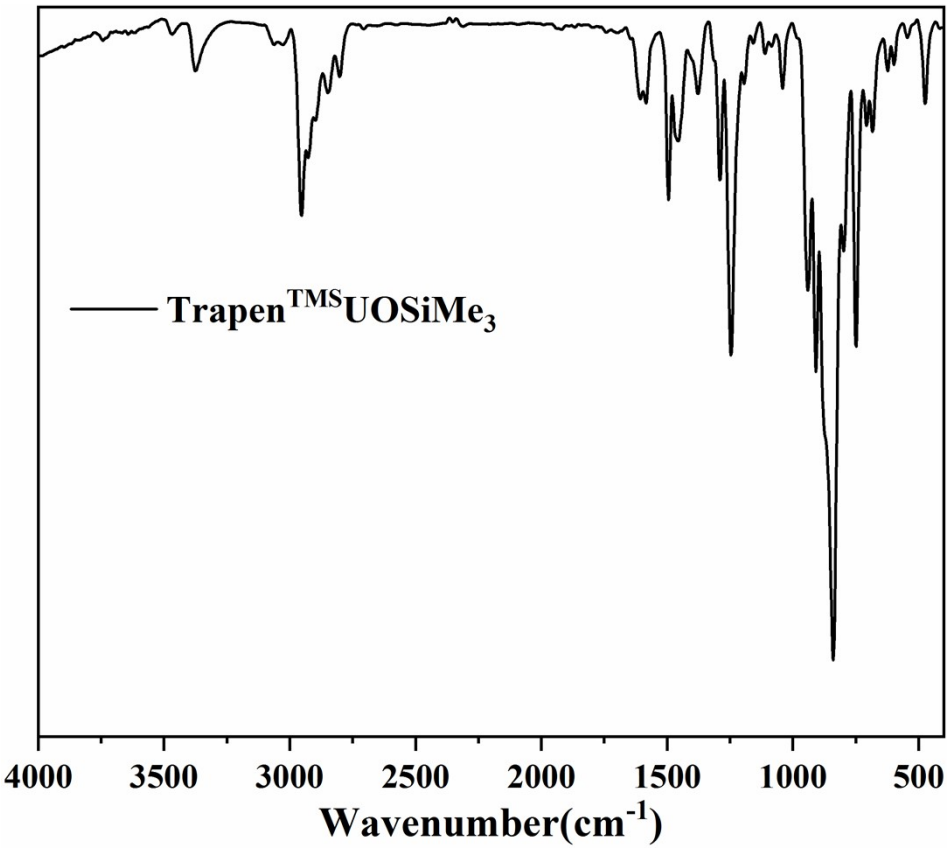

Figure S37. FT-IR of 2U.

Table S1. Crystal data and structural refinement for complexes B and 1Ce.

Complex	**B**	**1Ce**
Empirical formula	$C_{68}H_{106}Ce_2N_8O_2Si_6$	$C_{30}H_{45}CeClN_4Si_3$
Formula weight (amu)	1516.38	721.54
Wavelength (Å)	0.71073	0.71073
Crystal system	monoclinic	monoclinic
Space group	$P2_1$	$P2_1/c$
a (Å)	10.1162(3)	11.3841(4)
b (Å)	19.3047(5)	16.7664(7)
c (Å)	19.5448(5)	19.1613(7)
α (°)	90	90
β (°)	101.6510(10)	106.4920(10)
γ (°)	90	90
V (Å^3)	3738.26(18)	3506.9(2)
Z	2	4
ρ_{calcd} (g/cm^3)	1.347	1.367
μ (mm^{-1})	1.344	1.501
F000 (e$^-$)	1572.0	1480.0

Theta min/max (°)	2.498/27.527	2.671/27.512
Reflections collected	50498	68583
Independent reflections	17044	8041
R_{int}	0.0218	0.0198
Data/restr./param.	17044/7/793	8041/0/362
GOF	1.007	1.089
$R_1/wR_2{}^a(I > 2\sigma(I))$	0.0161/0.0353	0.0155/0.0386
$R_1/wR_2{}^a$(all data)	0.0172/0.0356	0.0164/0.0393
Res.peak/hole($e^- \cdot Å^{-3}$)	0.34/-0.23	0.44/-0.29

Table S2. Crystal data and structural refinement for complexes 2Ce, 2Th and 2U.

Complex	**2Ce**	**2Th**	**2U**
Empirical formula	$C_{33}H_{54}CeN_4OSi_4$	$C_{33}H_{54}N_4OSi_4Th$	$C_{33}H_{54}N_4OSi_4U$
Formula weight (amu)	775.28	867.20	873.19
Wavelength (Å)	0.71073	0.71073	0.71073
Crystal system	trigonal	trigonal	trigonal
Space group	*R*3*c*	*R*3*c*	*R*3*c*
a (Å)	16.9979(6)	17.113(4)	17.171(4)
b (Å)	16.9979(6)	17.113(4)	17.171(4)
c (Å)	23.6994(10)	24.012(5)	23.790(8)
α (°)	90	90	90
β (°)	90	90	90
γ (°)	120	120	120
V ($Å^3$)	5930.1(5)	6090(3)	6075(3)
Z	6	6	6
ρ_{calcd} (g/cm^3)	1.303	1.419	1.432
μ (mm^{-1})	1.302	3.819	4.155
*F*000 (e^-)	2412.0	2604.0	2616.0
Theta min/max (°)	3.258/29.310	3.231/27.472	2.193/27.496
Reflections collected	9847	44299	28533
Independent reflections	2472	3054	3101
R_{int}	0.0637	0.0272	0.0564
Data/restr./param.	2472/1/134	3054/1/133	3101/121/134
GOF	1.050	1.102	0.892
$R_1/wR_2{}^a(I > 2\sigma(I))$	0.0327/0.0830	0.0109/0.0240	0.0144/0.0326
$R_1/wR_2{}^a$(all data)	0.0368/0.074	0.0149/0.0256	0.0212/0.0336
Res.peak/hole($e^- \cdot Å^{-3}$)	0.43/-0.47	0.21/-0.20	0.20/-0.63

Table S3. Selected bond lengths (Å) and angles (o) for complex B.

Bond Lengths (Å)					
Ce1-N1	2.373(2)	Ce1-N2	2.351(2)	Ce1-N3	2.350(2)
Ce1-N4	2.630(2)	Ce1-O1	2.5839(19)		
Bond angles (°)					
N1-Ce1-N2	121.96(7)	N1-Ce1-N3	115.12(7)	N2-Ce1-N3	114.77(7)
O1-Ce1-N4	170.62(6)	N1-Ce1-N4	80.37(7)	N2-Ce1-N4	81.09(7)
N3-Ce1-N4	79.81(7)				

Table S4. Selected bond lengths (Å) and angles (o) for complex 1Ce.

Bond Lengths (Å)					
Ce1-Cl1	2.6561(4)	Ce1-N1	2.2273(11)	Ce1-N2	2.1991(11)
Ce1-N3	2.2251(11)	Ce1-N4	2.6347(11)		
Bond angles (°)					
N1-Ce1-N2	116.26(4)	N1-Ce1-N3	113.47(4)	N2-Ce1-N3	121.53(4)
Cl1-Ce1-N4	172.02(3)	N1-Ce1-N4	80.90(4)	N2-Ce1-N4	79.12(4)
N3-Ce1-N4	80.30(4)				

Table S5. Selected bond lengths (Å) and angles (o) for complex 2Ce.

Bond Lengths (Å)					
Ce1-O1	2.092(12)	Ce1-N1	2.246(5)	Ce1-N2	2.246(5)
Ce1-N3	2.246(5)	Ce1-N4	2.675(13)		
Bond angles (°)					
N1-Ce1-N2	116.41(9)	N1-Ce1-N3	116.41(9)	N2-Ce1-N3	116.41(9)
O1-Ce1-N4	180.0	N1-Ce1-N4	78.94(14)	N2-Ce1-N4	78.94(14)
N3-Ce1-N4	78.94(14)				

Table S6. Selected bond lengths (Å) and angles (o) for complex 2Th.

Bond Lengths (Å)					
Th1-O1	2.173(4)	Th1-N1	2.327(2)	Th1-N2	2.327(2)
Th1-N3	2.327(2)	Th1-N4	2.738(5)	Si4-O1	1.626(4)
Bond angles (°)					
N1-Th1-N2	115.44(4)	N1-Th1-N3	115.44(4)	N2-Th1-N3	115.44(4)
O1-Th1-N4	180.0	N1-Th1-N4	77.49(6)	N2-Th1-N4	77.49(6)
N3-Th1-N4	77.49(6)	O1-Th1-Si4	180.0		

Table S7. Selected bond lengths (Å) and angles (o) for complex 2U.

Bond Lengths (Å)					
U1-O1	2.114(5)	U1-N1	2.264(3)	U1-N2	2.264(3)
U1-N3	2.264(3)	U1-N4	2.677(7)	Si4-O1	1.621(6)
Bond angles (°)					
N1-U1-N2	116.48(5)	N1-U1-N3	116.48(5)	N2-U1-N3	116.48(5)
O1-U1-N4	180.0	N1-U1-N4	79.05(8)	N2-U1-N4	79.05(8)
N3-U1-N4	79.05(8)	O1-U1-Si4	180.0		

Table S8. Shape analysis for the metal centers of 2M.

ML_5	PP-5	vOC-5	TBPY-5	SPY-5	JTBPY-5
2Ce	37.234	7.633	**0.689**	6.057	2.304
2Th	37.346	7.800	**0.877**	6.227	2.502
2U	37.234	7.629	**0.669**	6.037	2.345

PP-5: Pentagon
vOC-5: Vacant octahedron
TBPY-5: Trigonal bipyramid
SPY-5: Square pyramid

JTBPY-5: Johnson trigonal bipyramid

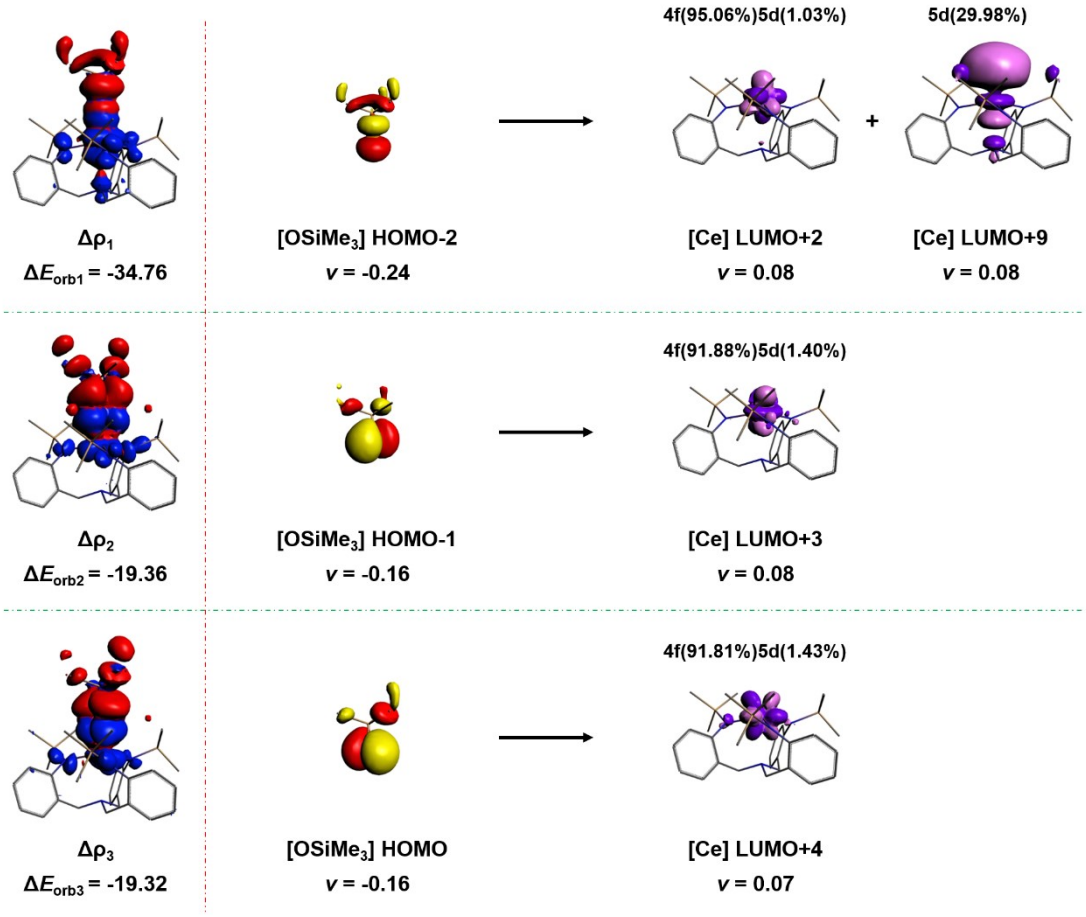

Figure S38. NOCV with larger deformation density (Δρ) of the main pairwise orbital interaction in **2Ce** complex between the [Ce] and [OTMS] fragments together with the associated interaction energies ΔE_{orb}. The charge eigenvalues (*v*) give an estimate of the relative size of the charge migration. The direction of the charge flow is red to blue, and hydrogen atoms have been omitted for clarity. The isodensity value is set to 0.0003 au.

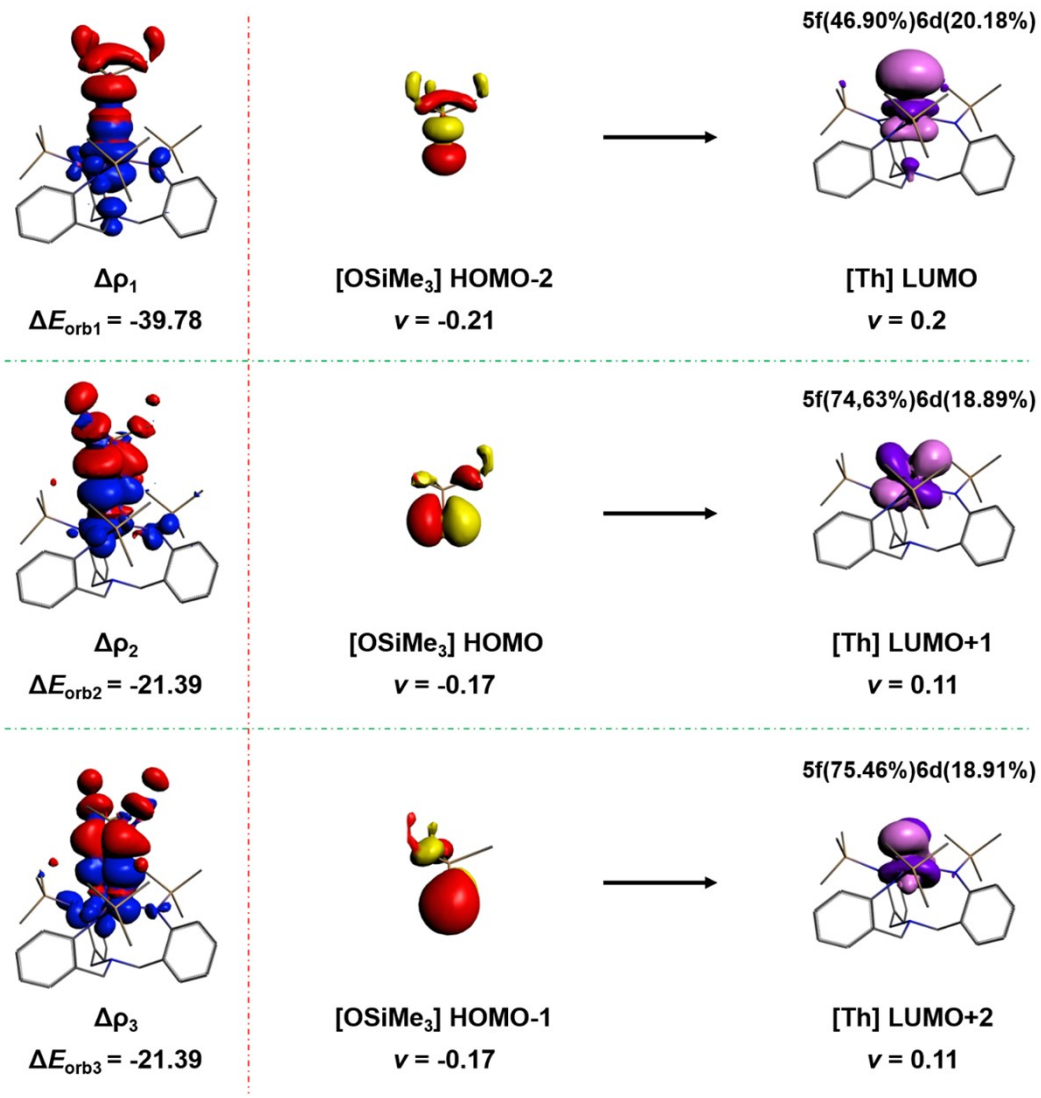

Figure S39. NOCV with larger deformation density (Δρ) of the main pairwise orbital interaction in **2Th** complex between the [Th] and [OTMS] fragments together with the associated interaction energies ΔE_{orb}. The charge eigenvalues (v) give an estimate of the relative size of the charge migration. The direction of the charge flow is red to blue, and hydrogen atoms have been omitted for clarity. The isodensity value is set to 0.0003 au.

Table S9. Final Coordinates of Geometry Optimized 2Ce.

Ce	-0.00153	-0.0019	0.29602
O	-0.01003	-0.01858	2.42908
Si	-0.01283	-0.02804	4.10822
N	0.00662	0.01401	-2.43925
N	-2.19027	-0.58945	-0.15639

N	1.60769	-1.59955	-0.15006
N	0.58261	2.19303	-0.1312
C	-1.34769	-0.38182	-2.93135
C	1.03084	-0.95806	-2.92819
C	0.34047	1.38989	-2.91714
Si	-3.65186	0.1496	0.53407
C	-2.29965	-1.72412	-0.98644
Si	1.69485	-3.23993	0.52872
C	2.65192	-1.1213	-0.96866
Si	1.95564	3.08494	0.56048
C	-0.34599	2.86321	-0.95453
C	1.59882	-0.80696	4.74497
C	-0.14918	1.75257	4.75668
C	-1.49151	-1.0411	4.73808
H	-1.32354	-0.45262	-4.04313
H	-2.03116	0.4413	-2.65979
C	-1.85663	-1.6799	-2.34843
H	1.09034	-0.8947	-4.03908
H	0.65672	-1.96309	-2.66685
C	2.40417	-0.75344	-2.33132
H	0.26512	1.41622	-4.02856
H	1.39562	1.56716	-2.64589
C	-0.52888	2.47298	-2.32114
C	-4.67729	-1.02453	1.63213
C	-3.10018	1.61645	1.60006
C	-4.77262	0.76628	-0.87428
C	-2.83196	-2.95718	-0.51122
C	3.21254	-3.54587	1.64185
C	0.13647	-3.50748	1.57359
C	1.74146	-4.50836	-0.88855
C	3.98143	-0.96675	-0.48067
C	1.45516	4.55526	1.6667
C	2.95465	1.87017	1.61837
C	3.0466	3.75434	-0.84721
C	-1.14855	3.93459	-0.46708
H	2.48328	-0.24456	4.39481
H	1.70459	-1.84982	4.39519
H	1.62556	-0.81979	5.85064
H	-1.0763	2.2394	4.4037
H	0.7031	2.36855	4.41712
H	-0.15901	1.77427	5.86249
H	-1.44708	-2.08445	4.37668
H	-2.44869	-0.60812	4.39545
H	-1.513	-1.06962	5.84358

C	-1.95582	-2.82894	-3.15627
C	3.45594	-0.26092	-3.12747
C	-1.47471	3.14221	-3.12137
H	-4.06744	-1.47045	2.43856
H	-5.1393	-1.84553	1.05616
H	-5.49727	-0.45478	2.10961
H	-2.6724	2.43006	0.98836
H	-2.34946	1.31861	2.35339
H	-3.97147	2.03107	2.14058
H	-5.03198	-0.05393	-1.56822
H	-4.27504	1.56246	-1.45687
H	-5.71863	1.17907	-0.47666
C	-2.92739	-4.0864	-1.33401
H	-3.16464	-3.00955	0.52995
H	3.28387	-2.80091	2.45488
H	4.16081	-3.52958	1.07638
H	3.12564	-4.54463	2.11081
H	-0.77379	-3.54334	0.94961
H	0.0066	-2.71324	2.32991
H	0.20944	-4.47222	2.10947
H	2.58906	-4.31542	-1.57115
H	0.81	-4.47441	-1.48196
H	1.85549	-5.53643	-0.49676
C	5.0142	-0.48042	-1.29194
H	4.18407	-1.23345	0.56115
H	0.76962	4.24658	2.47656
H	0.97005	5.36673	1.09629
H	2.36078	4.98072	2.13979
H	3.43704	1.09046	1.00318
H	2.32755	1.37249	2.37906
H	3.75663	2.41549	2.15012
H	2.46414	4.39267	-1.53632
H	3.4862	2.92857	-1.43525
H	3.87783	4.36534	-0.44822
C	-2.07913	4.59076	-1.28237
H	-1.02758	4.23716	0.57758
H	-1.62146	-2.76732	-4.20007
C	-2.48623	-4.0318	-2.66691
H	3.24465	0.00238	-4.17204
C	4.75833	-0.12033	-2.62574
H	-1.58823	2.83379	-4.16879
C	-2.25193	4.19679	-2.61993
H	-3.34487	-5.01575	-0.92892
H	6.02397	-0.37839	-0.87715

H	-2.67581	5.41185	-0.86779
H	-2.55763	-4.91055	-3.31663
H	5.56071	0.26034	-3.26661
H	-2.97744	4.70503	-3.26394

Table S10. Final Coordinates of Geometry Optimized 2Th.

Th	-0.00105	3.41E-04	0.32228
O	-0.00804	0.00128	2.49801
Si	-0.01291	0.00456	4.18006
N	-0.06995	2.29374	-0.1741
N	0.00708	-0.00247	-2.43854
N	-1.95085	-1.20829	-0.17579
N	2.02176	-1.08666	-0.16478
Si	-1.23379	3.45284	0.49851
C	0.96599	2.75631	-1.02495
C	-0.03253	1.40931	-2.94335
C	1.25205	-0.67331	-2.93799
C	-1.19397	-0.74459	-2.94484
Si	-2.37465	-2.79266	0.5028
C	-2.86646	-0.54633	-1.03275
Si	3.60416	-0.65819	0.51547
C	1.90948	-2.21384	-1.01797
C	0.51926	1.71588	4.80696
C	1.19937	-1.31154	4.81486
C	-1.76256	-0.38679	4.80478
C	-2.1399	4.3547	-0.90931
C	-2.48135	2.44281	1.51333
C	-0.46513	4.76679	1.64551
C	1.0485	2.3032	-2.37994
C	1.96809	3.65817	-0.57223
H	-1.02521	1.80817	-2.67144
H	0.03555	1.39261	-4.05476
H	2.09229	-0.01313	-2.66119
H	1.20905	-0.72261	-4.04968
C	1.48329	-2.05709	-2.37513
H	-1.04377	-1.80272	-2.66875
H	-1.20974	-0.68121	-4.05654
C	-2.51067	-0.25362	-2.3877
C	-0.87786	-3.36486	1.52193
C	-2.70113	-4.03367	-0.90068
C	-3.89874	-2.77874	1.64737
C	-4.15057	-0.12878	-0.58644
C	4.35244	-1.98142	1.66532
C	3.34835	0.92718	1.52927

C	4.84492	-0.3236	-0.88634
C	2.18804	-3.53298	-0.56559
H	-0.1675	2.50366	4.44771
H	1.53548	1.97324	4.45699
H	0.52531	1.7549	5.91222
H	0.91562	-2.32072	4.4649
H	1.22459	-1.33468	5.9203
H	2.22682	-1.11143	4.46044
H	-2.49272	0.3628	4.44927
H	-1.80183	-0.39526	5.91003
H	-2.10065	-1.3773	4.44998
H	-2.82478	5.12804	-0.51421
H	-2.73933	3.64878	-1.51224
H	-1.42466	4.85773	-1.58549
H	-3.19004	3.12952	2.01313
H	-1.99577	1.84308	2.30485
H	-3.07985	1.76511	0.87758
H	0.18406	5.47281	1.09791
H	0.13421	4.30583	2.45163
H	-1.26746	5.36135	2.12265
C	2.10152	2.74629	-3.20462
C	3.00234	4.09363	-1.41142
H	1.92099	4.00709	0.46441
C	1.34593	-3.18954	-3.20216
C	-3.4184	0.43302	-3.21828
H	-0.60077	-2.64133	2.31041
H	0.00851	-3.54832	0.88767
H	-1.11993	-4.31938	2.02585
H	-3.49363	-3.66826	-1.5791
H	-1.78945	-4.20214	-1.50204
H	-3.02893	-5.01199	-0.50234
H	-3.80012	-2.02648	2.45102
H	-4.01392	-3.76909	2.12784
H	-4.83376	-2.57094	1.09754
C	-5.04231	0.54519	-1.43149
H	3.65032	-2.26984	2.46866
H	5.26693	-1.58464	2.14612
H	4.64075	-2.89673	1.11862
H	3.06525	1.78465	0.89191
H	4.29475	1.19659	2.03462
H	2.5815	0.80737	2.31641
H	4.92721	-1.19463	-1.56188
H	5.8549	-0.11596	-0.48629
H	4.53543	0.548	-1.4911

C	2.05348	-4.64536	-1.40705
H	2.50839	-3.66761	0.4726
H	2.13967	2.39326	-4.24343
C	3.07937	3.63618	-2.73735
H	3.75525	4.79005	-1.02369
H	1.02696	-3.04488	-4.24261
C	1.62598	-4.48178	-2.73512
C	-4.67996	0.83585	-2.75719
H	-3.12827	0.63855	-4.25694
H	-6.02357	0.84965	-1.04855
H	2.27881	-5.64598	-1.01949
H	3.88562	3.97048	-3.39897
H	1.51672	-5.34631	-3.39858
H	-5.37057	1.3638	-3.42343
H	-4.43284	-0.3405	0.44994

Table S11. Final Coordinates of Geometry Optimized 2U.

U	-0.04167	-0.09436	0.26238
O	-0.20663	-0.62566	2.29889
Si	-0.28169	-1.02498	3.93421
N	0.12539	0.52879	-2.34943
N	-2.26942	-0.12102	-0.28746
N	1.43244	-1.702	-0.42177
N	0.95986	1.96905	0.33086
C	-1.25609	0.52942	-2.93244
C	0.95566	-0.51698	-3.03165
C	0.75006	1.87692	-2.5542
Si	-3.4475	-1.42388	0.01205
C	-2.72907	1.0598	-0.92492
Si	3.05128	-2.12134	0.17879
C	0.82415	-2.49173	-1.42994
Si	0.40804	3.36848	1.2855
C	2.14082	2.12076	-0.44236
C	-2.22753	1.43489	-2.21139
H	-1.61369	-0.5139	-2.89018
H	-1.18884	0.8249	-4.00374
C	0.53111	-1.93247	-2.7152
H	1.99504	-0.35354	-2.69903
H	0.91542	-0.34518	-4.13076
C	2.08419	2.04693	-1.86982
H	0.02756	2.61328	-2.1624
H	0.86052	2.05551	-3.64756
C	0.90305	0.09247	4.90871
C	-2.05495	-0.76813	4.55886

C	0.22004	-2.84191	4.15646
C	-2.51637	-2.89027	0.77114
C	-4.23004	-1.95964	-1.63739
C	-4.85417	-0.93873	1.20356
C	-3.6896	1.91633	-0.31963
C	3.40046	-1.02511	1.68506
C	4.34421	-1.79552	-1.17716
C	3.22407	-3.93908	0.72506
C	0.45428	-3.84757	-1.20355
C	-1.17022	2.87028	2.21218
C	0.02694	4.82448	0.12208
C	1.66966	3.96564	2.58403
C	3.41252	2.3453	0.15183
C	-2.68304	2.61813	-2.82492
C	-0.09964	-2.72288	-3.69746
C	3.26142	2.18481	-2.62933
H	1.94581	-0.02893	4.56442
H	0.87526	-0.14425	5.98874
H	0.63454	1.15804	4.79235
H	-2.37562	0.2815	4.43014
H	-2.13896	-1.016	5.63344
H	-2.77027	-1.40689	4.01028
H	-0.45619	-3.51555	3.59977
H	0.18757	-3.13777	5.22164
H	1.24682	-3.0217	3.78973
H	-3.23564	-3.69049	1.02846
H	-1.98351	-2.60796	1.6958
H	-1.7809	-3.31883	0.06724
H	-4.685	-1.10118	-2.16411
H	-5.02543	-2.71058	-1.47384
H	-3.47489	-2.40989	-2.30705
H	-5.5353	-0.18684	0.76769
H	-4.46377	-0.53711	2.15614
H	-5.46075	-1.83343	1.44133
C	-4.13436	3.08659	-0.94896
H	-4.07667	1.64481	0.66749
H	4.42691	-1.21012	2.0531
H	2.70162	-1.23933	2.51212
H	3.32908	0.04899	1.43967
H	4.10705	-2.36137	-2.09706
H	5.35441	-2.1046	-0.84907
H	4.38654	-0.72244	-1.43744
H	3.08875	-4.64613	-0.11224
H	2.49989	-4.20332	1.5171

H	4.23933	-4.10187	1.13449
C	-0.16061	-4.61903	-2.19728
H	0.66041	-4.28141	-0.22015
H	-1.50276	3.71583	2.84374
H	-1.00865	2.00187	2.87453
H	-1.99791	2.63074	1.52166
H	0.89872	5.06743	-0.51253
H	-0.23171	5.73438	0.69527
H	-0.82485	4.59109	-0.54217
H	2.5768	4.39667	2.12561
H	1.98118	3.14797	3.25927
H	1.20738	4.75515	3.2069
C	4.57287	2.48696	-0.62148
H	3.47395	2.40227	1.2431
H	-2.29102	2.8817	-3.81583
C	-3.6314	3.44852	-2.2096
H	-0.30475	-2.27733	-4.67952
C	-0.44538	-4.05935	-3.45516
H	3.19143	2.13018	-3.72361
C	4.50704	2.40596	-2.02213
H	-4.87523	3.72082	-0.44799
H	-0.42574	-5.66155	-1.9853
H	5.53469	2.65863	-0.12381
H	-3.97431	4.36147	-2.70805
H	-0.92755	-4.65676	-4.23632
H	5.40963	2.51529	-2.63276