Supporting Information For:

Reductive Silylation of a Uranyl Dibenzoylmethanate Complex: An Example of Controlled Uranyl Oxo Ligand Cleavage

Elizabeth A. Pedrick,[1] Guang Wu,[1] Nikolas Kaltsoyannis,[2] and Trevor W. Hayton*,[1]

1. Department of Chemistry and Biochemistry, University of California Santa Barbara, Santa Barbara, CA 93106

2. Christopher Ingold Laboratories, Department of Chemistry, University College London, 20 Gordon Street, London WC1H 0AJ, United Kingdom

*To whom correspondence should be addressed. Email: hayton@chem.ucsb.edu

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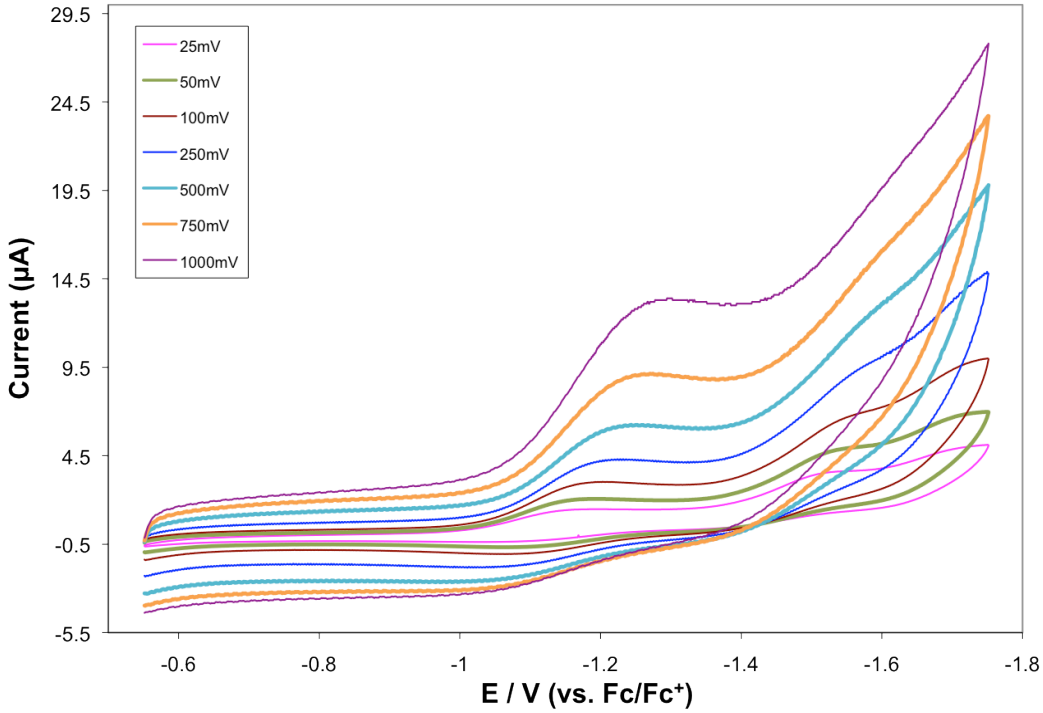

Figure S1. Room temperature cyclic voltammogram of $UO_2(dbm)_2(THF)$. Measured in CH_2Cl_2 with 0.1 M $[NBu_4][PF_6]$ as supporting electrolyte.

Table S1. Electrochemical parameters for $UO_2(dbm)_2(THF)$ in CH_2Cl_2 (vs. Fc/Fc^+, $[NBu_4][PF_6]$ as supporting electrolyte).

Reduction feature	**Scan rate, V/s**	$\mathbf{E_{p,c}}$**, V**		
	0.025	-1.167		
	0.05	-1.154		
	0.1	-1.189		
	0.25	-1.206		
	0.5	-1.230		
	0.75	-1.248		
	1	-1.283		
Ferrocene	**Scan rate, V/s**	$\mathbf{E_{p,a}}$**, V**	$\mathbf{\Delta E_p}^a$	$\boldsymbol{i_{p,c}/i_{p,a}}$
	0.025	0.052	0.089	1.06
	0.05	0.062	0.094	1.06
	0.1	0.051	0.109	1.05
	0.25	0.059	0.132	1.07
	0.5	0.072	0.160	1.09
	0.75	0.082	0.155	1.13
	1	0.086	0.200	1.15

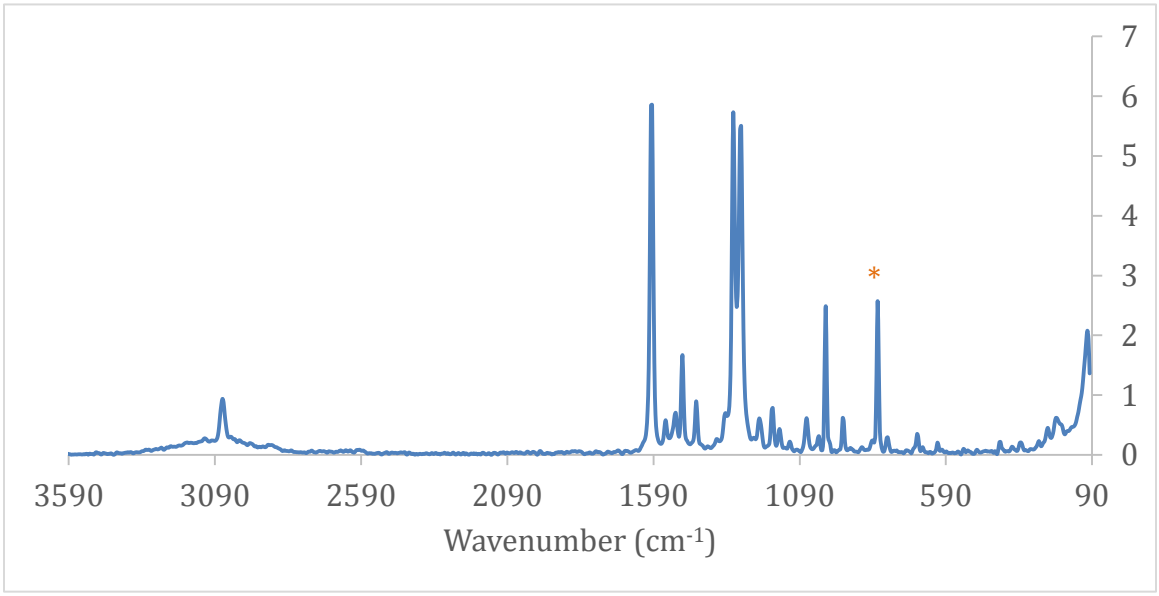

Figure S2. Solid state Raman spectrum of $UO_2(dbm)_2(THF)$. U=O ν_{sym} stretch is observed at 823 cm^{-1} (*).

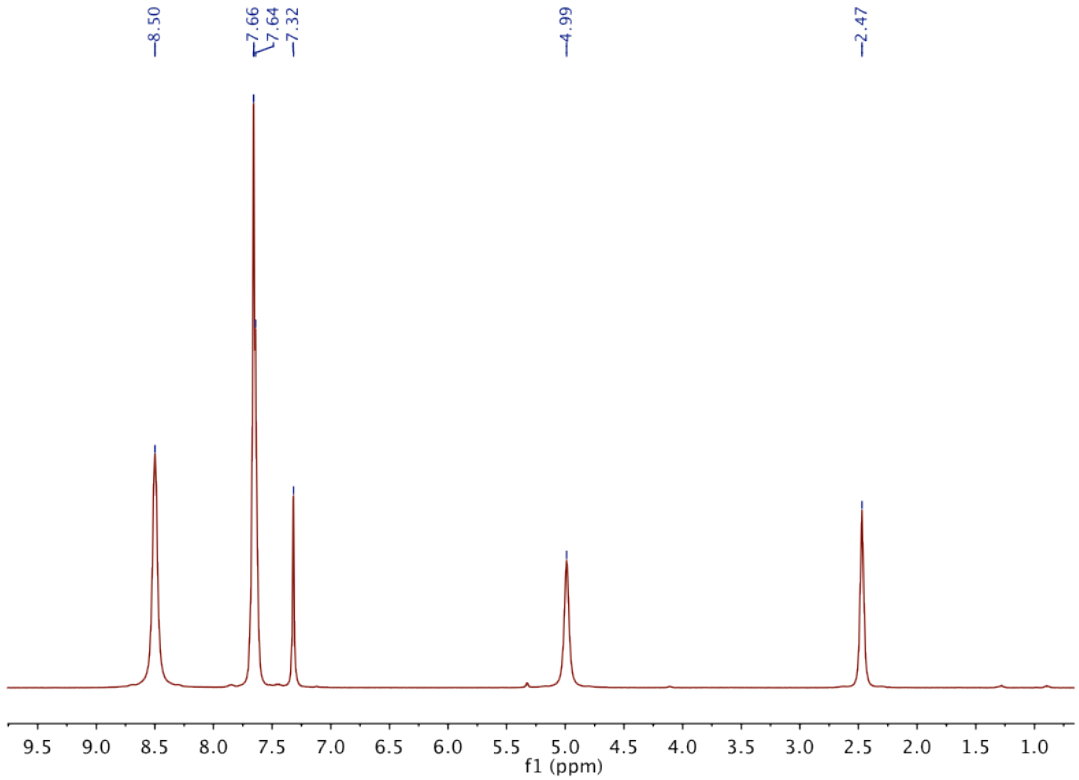

Figure S3. ^{1}H NMR spectrum of $UO_2(dbm)_2(THF)$ in CD_2Cl_2 at 25 °C.

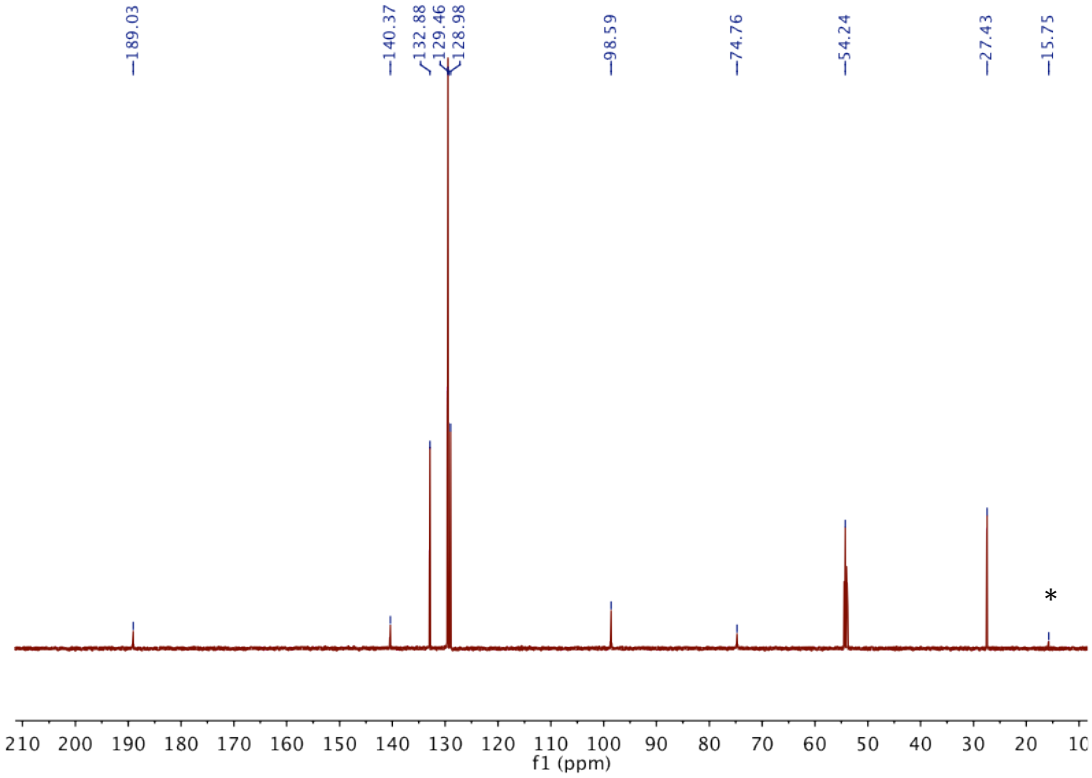

Figure S4. $^{13}C\{^{1}H\}$ NMR spectrum of $UO_2(dbm)_2(THF)$ in CD_2Cl_2 at 25 °C. Asterisk indicates the presence of hexanes.

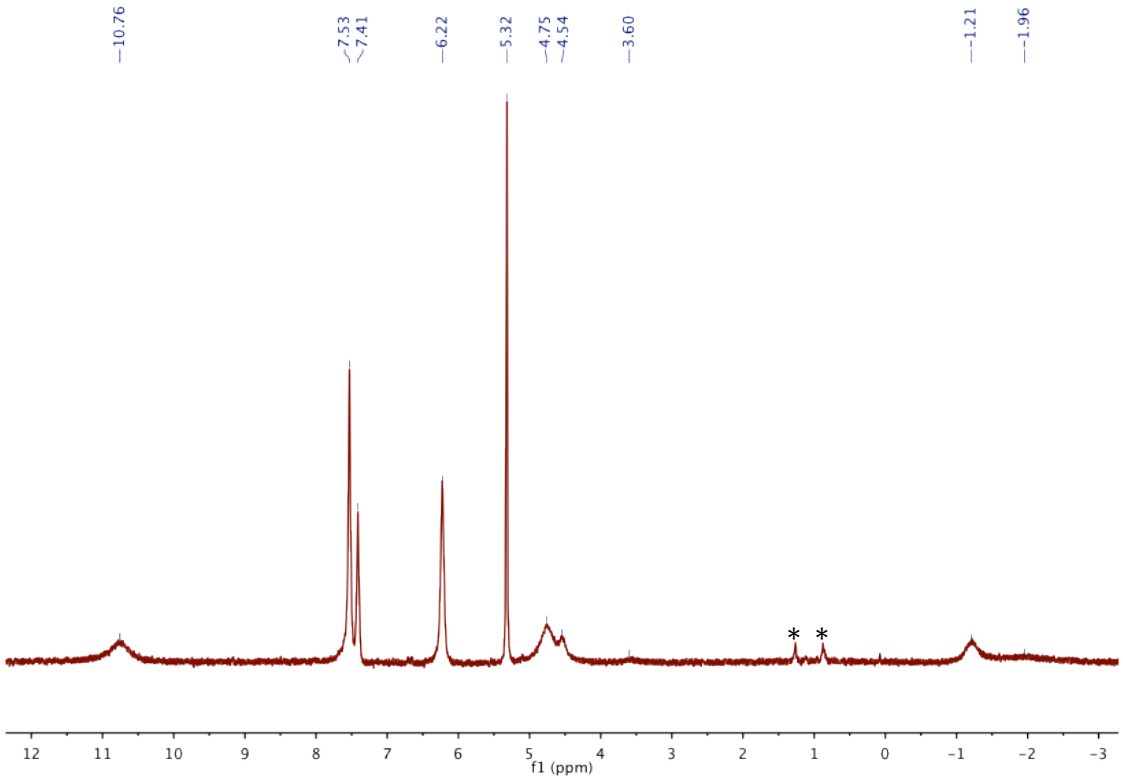

Figure S5. ^{1}H NMR spectrum of **1** in CD_2Cl_2 at 25 °C. Asterisks indicate the presence of hexanes.

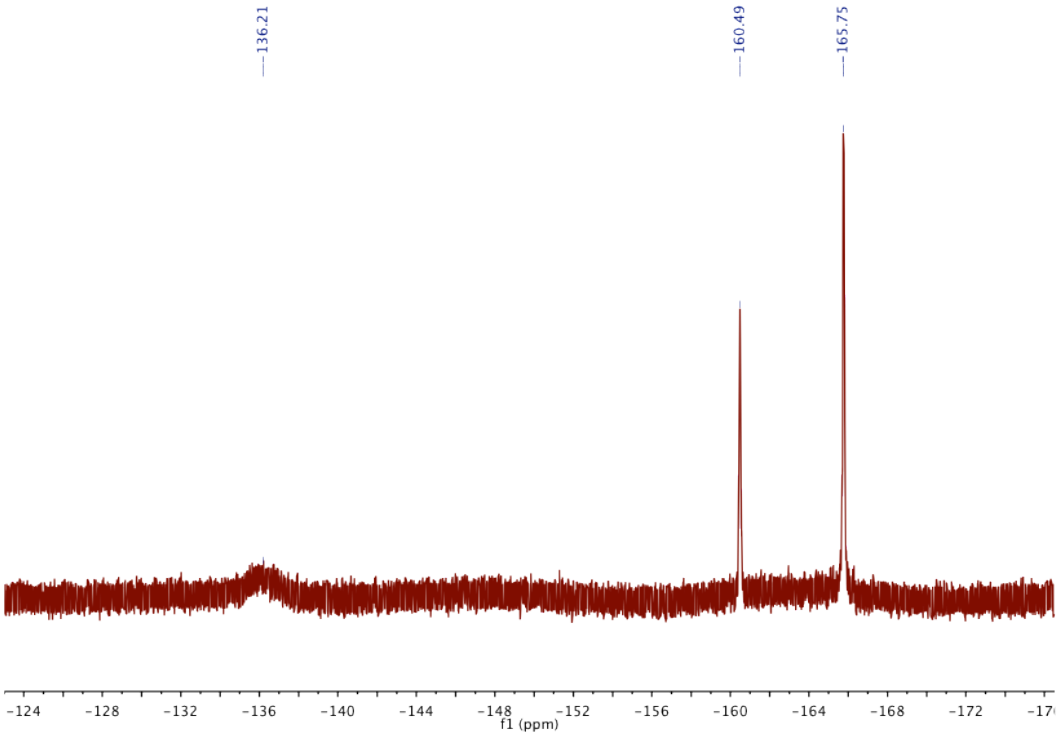

Figure S6. $^{19}F\{^{1}H\}$ NMR spectrum of **1** in CD_2Cl_2 at 25 °C.

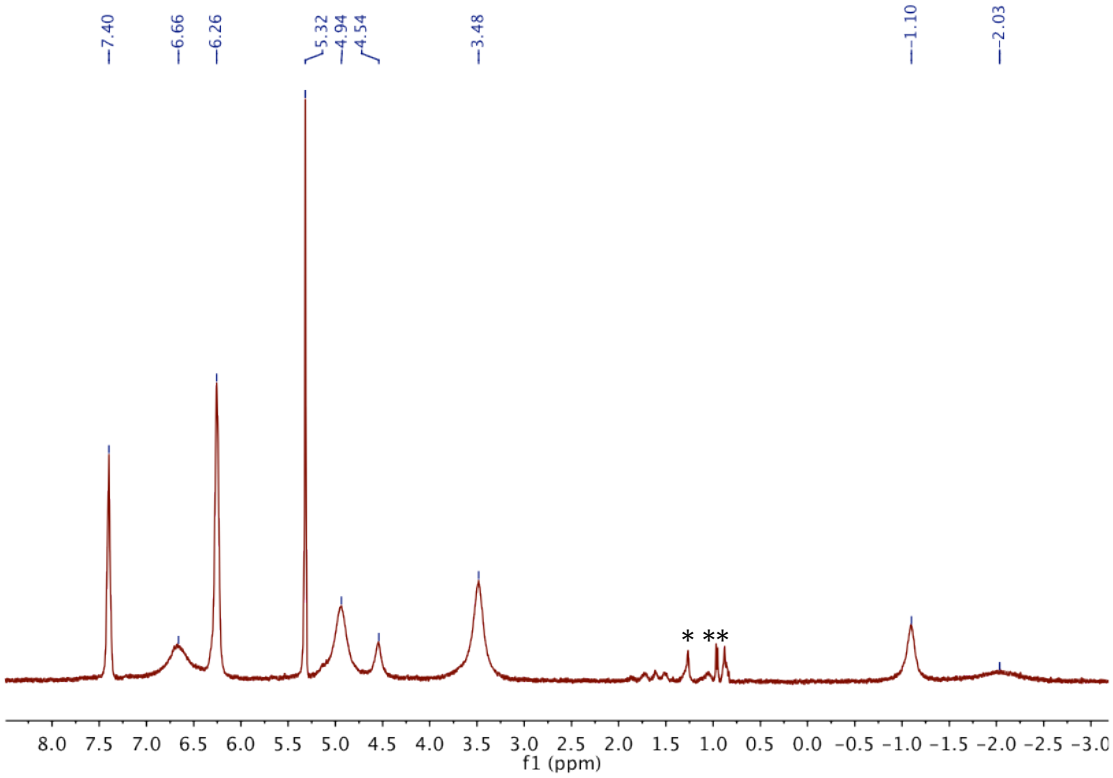

Figure S7. ^{1}H NMR spectrum of **2** in CD_2Cl_2 at 25 °C. Asterisks indicate the presence of hexanes.

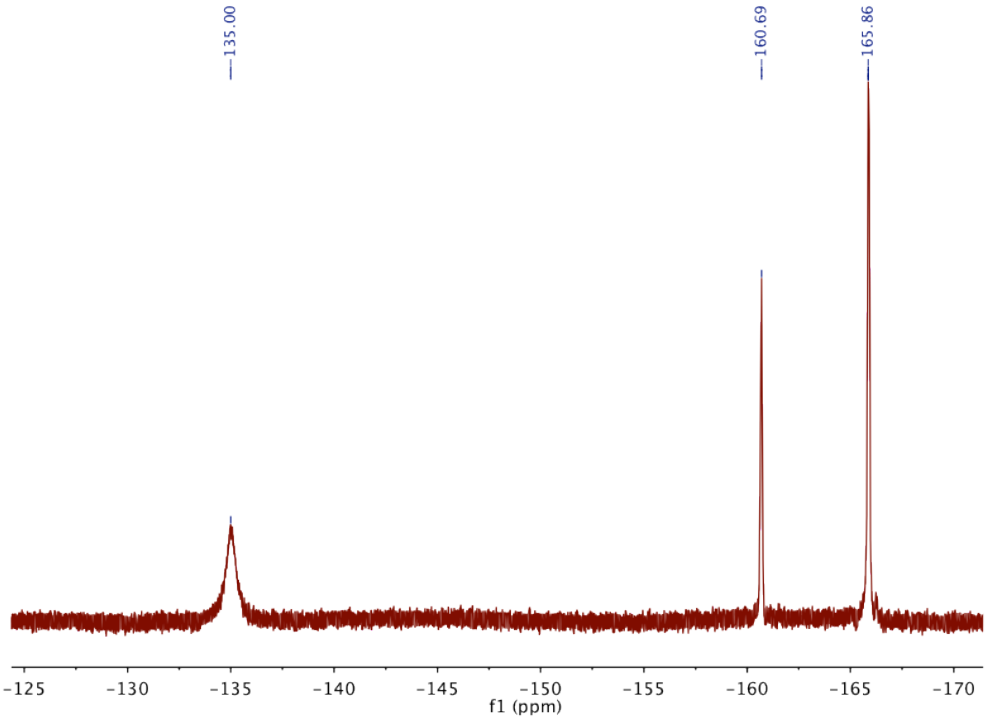

Figure S8. $^{19}F\{^{1}H\}$ NMR spectrum of **2** in CD_2Cl_2 at 25 °C.

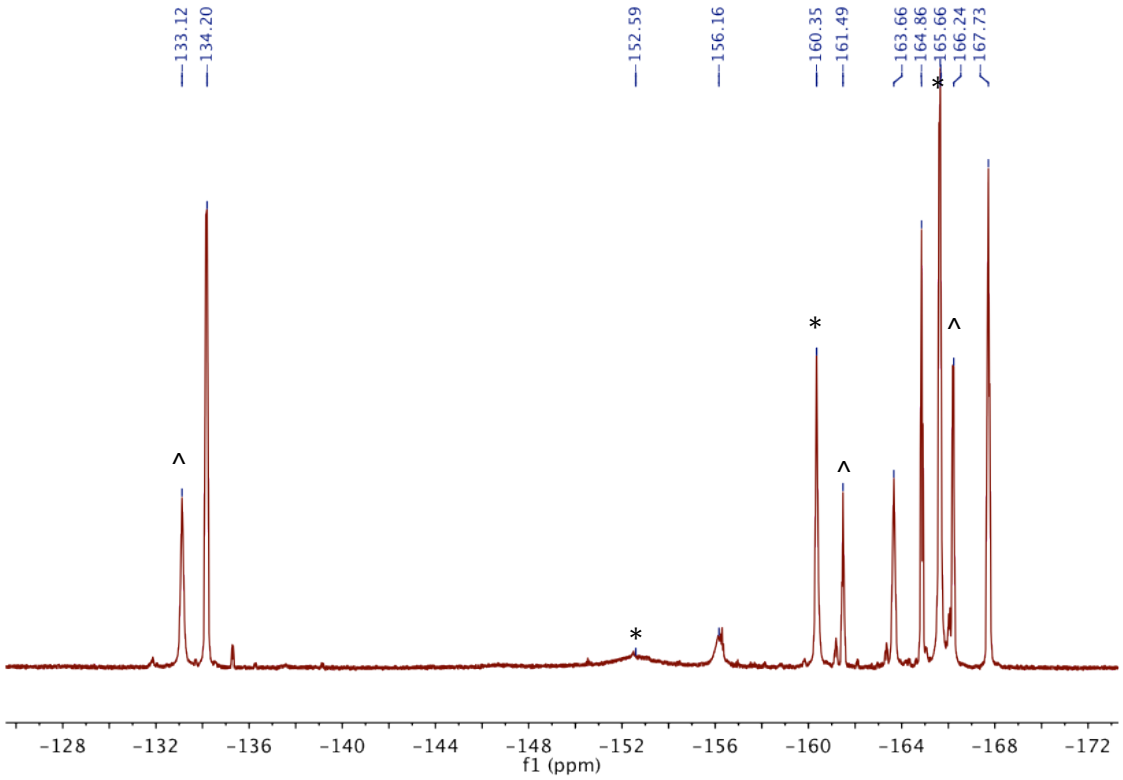

Figure S9. $^{19}F\{^{1}H\}$ NMR spectrum of the *in situ* reaction of $UO_2(dbm)_2(THF)$ with 1 equiv of $B(C_6F_5)_3$ and 2 equiv $HSiEt_3$ in CD_2Cl_2; after 24 h at 25 °C. **Experimental Details:** An orange CD_2Cl_2 solution (1 mL) containing $UO_2(dbm)_2(THF)$ (24.1 mg, 0.030 mmol) was sealed in a J. Young NMR tube, and the ^{1}H and $^{19}F\{^{1}H\}$ NMR spectra were recorded. Then a colorless CD_2Cl_2 solution (0.75 mL) of $B(C_6F_5)_3$ (16.0 mg, 0.031 mmol) and $HSiEt_3$ (10 µL, 0.061 mmol) was added drop-wise, resulting in a color change to deep red. The tube was sealed, and the ^{1}H and $^{19}F\{^{1}H\}$ NMR spectra were recorded after standing at room temperature for 24 h (^{19}F spectrum shown above). These spectra revealed the formation of **2** and **3**, in a 1:2 ratio, which was determined by comparing the integrations of the *meta* C–F resonances in the ^{19}F NMR spectrum. Asterisks indicate resonances assignable to complex **3**, while ^ indicates resonances assignable to complex **2**. Several other ^{19}F resonances are observed that were not assignable to any known species.

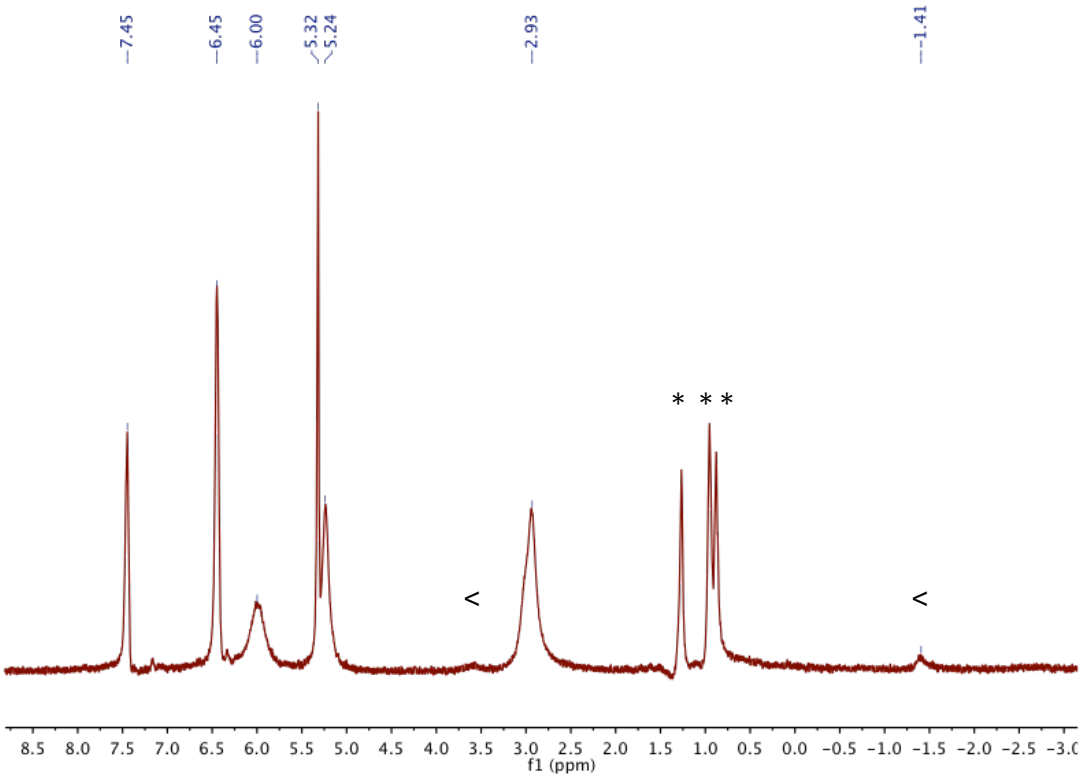

Figure S10. ^{1}H NMR spectrum of **3** in CD_2Cl_2 at 25 °C. < indicates resonances assignable to complex **2**. Asterisks indicate the presence of hexanes.

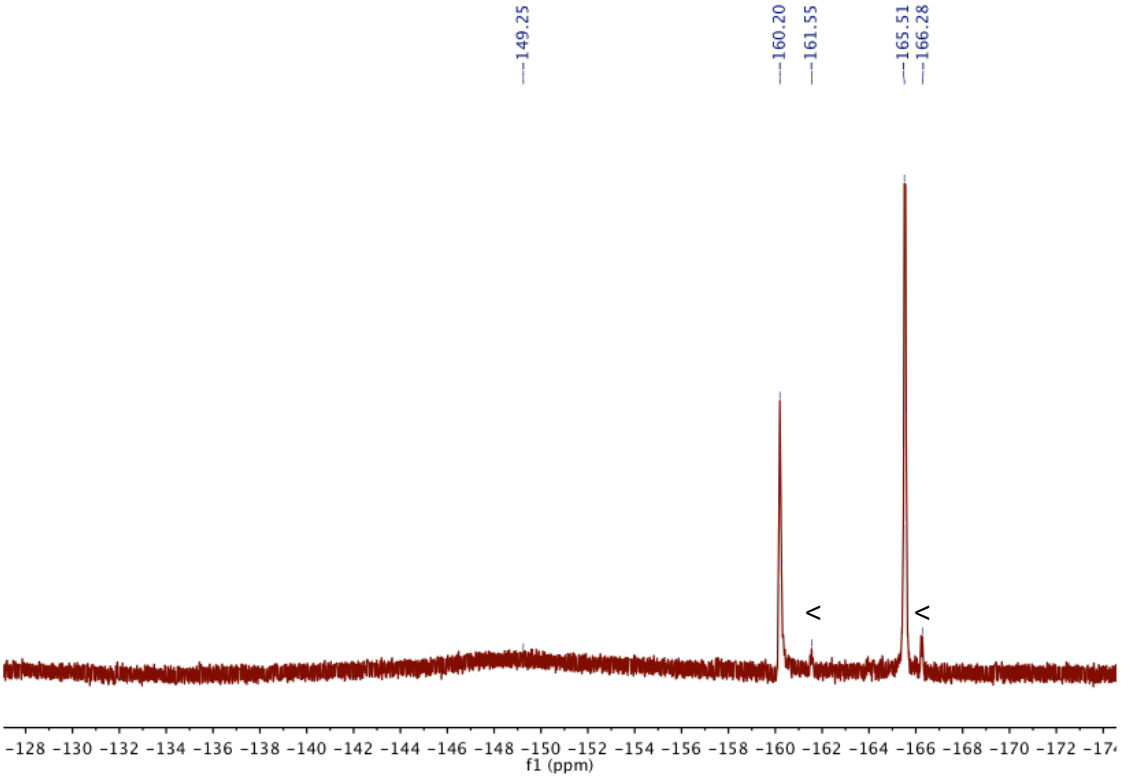

Figure S11. $^{19}F\{^{1}H\}$ NMR spectrum of **3** in CD_2Cl_2 at 25 °C. < indicates resonances assignable to complex **2**.

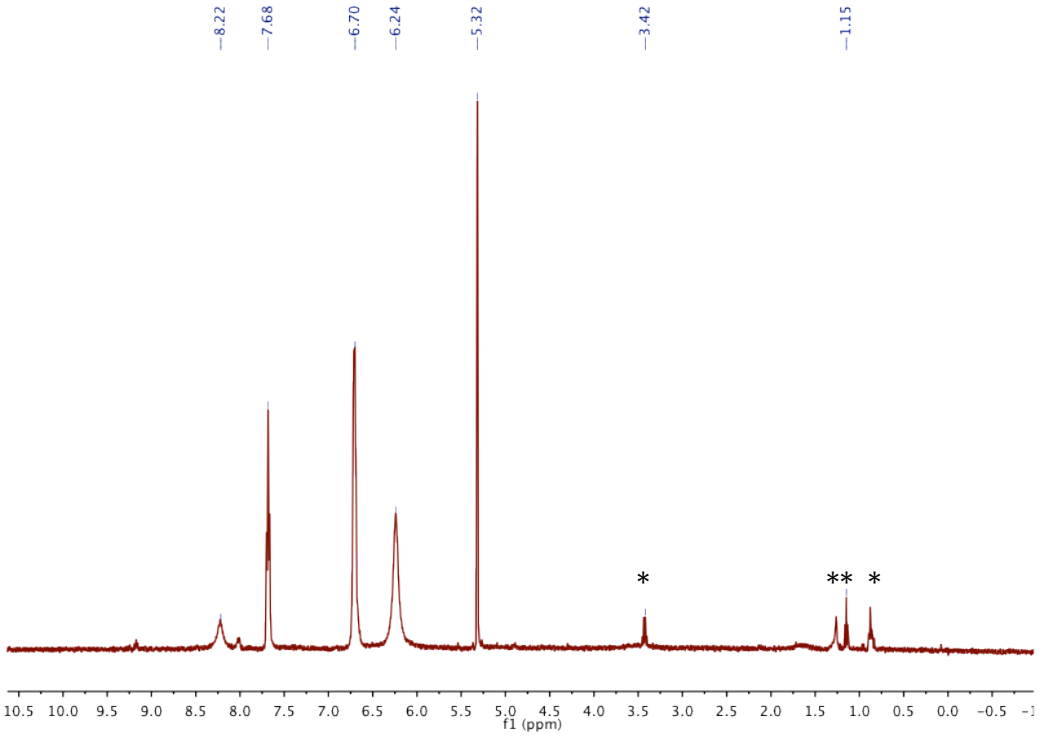

Figure S12. ^{1}H NMR spectrum of **4** in CD_2Cl_2 at 25 °C. Asterisks indicate the presence of hexanes and Et_2O.

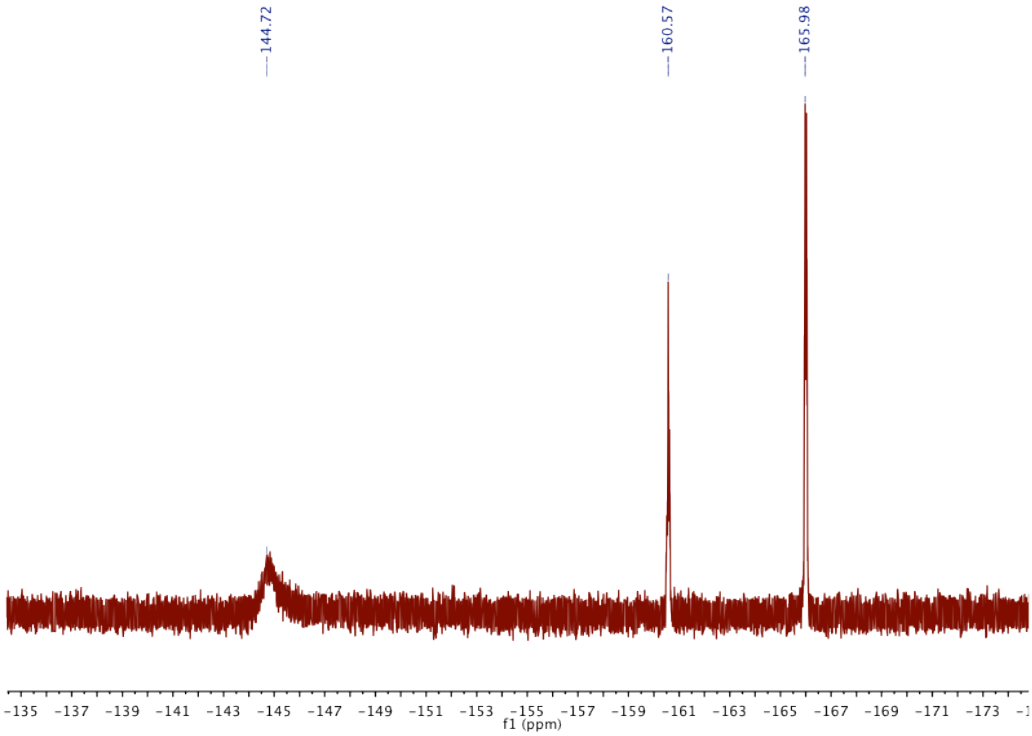

Figure S13. $^{19}F\{^{1}H\}$ NMR spectrum of **4** in CD_2Cl_2 at 25 °C.

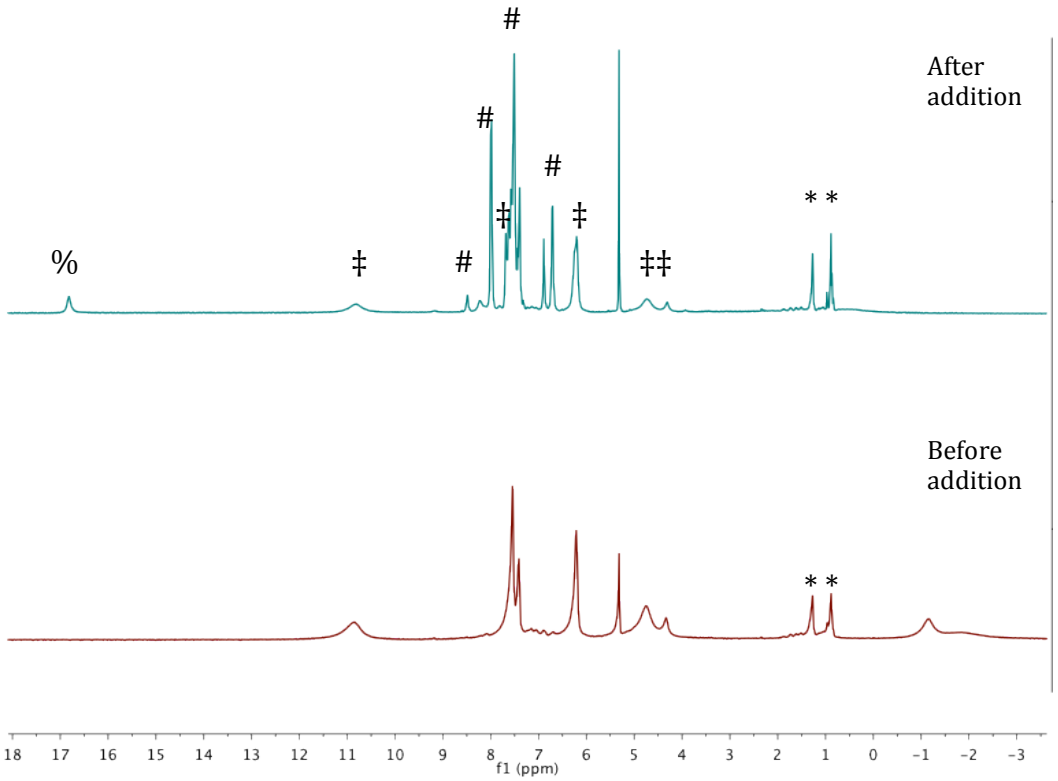

Figure S14. ^{1}H NMR spectra of the in situ formation of **4** from **1** in CD_2Cl_2 at 25 °C. **Experimental details:** A red orange CD_2Cl_2 solution (1 mL) containing **1** (15.1 mg, 0.010 mmol) was sealed in a J. Young NMR tube, and the ^{1}H and ^{19}F{^{1}H} NMR spectra were recorded (bottom spectrum). Then a colorless CD_2Cl_2 solution (0.5 mL) of H(dbm) (3.3 mg, 0.014 mmol) was added drop-wise, resulting in a color change to deep red. The tube was sealed, and the ^{1}H and ^{19}F{^{1}H} NMR spectra were re-recorded (top spectrum). These spectra revealed the presence of **1** and **4**, in a 3:2 ratio, according to the integrations of the *ortho* C–F resonances in the ^{19}F NMR spectrum (Figure S15). ‡ indicates resonances assignable to complex **1**, while # indicates resonances assignable to complex **4**, and % indicates resonances assignable to H(dbm). Asterisks indicate the presence of hexanes.

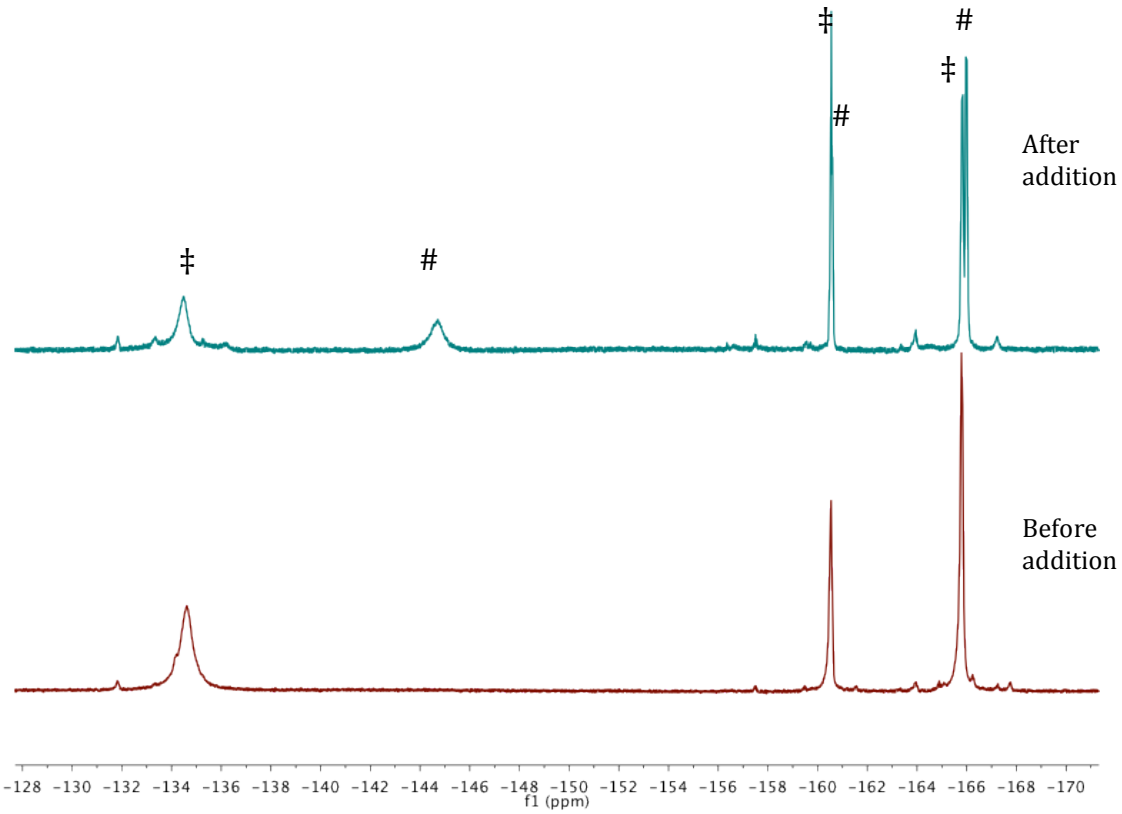

Figure S15. $^{19}F\{^{1}H\}$ NMR spectra of the in situ formation of **4** from **1** in CD_2Cl_2 at 25 °C. ‡ indicates resonances assignable to complex **1**, while # indicates resonances assignable to complex **4**.

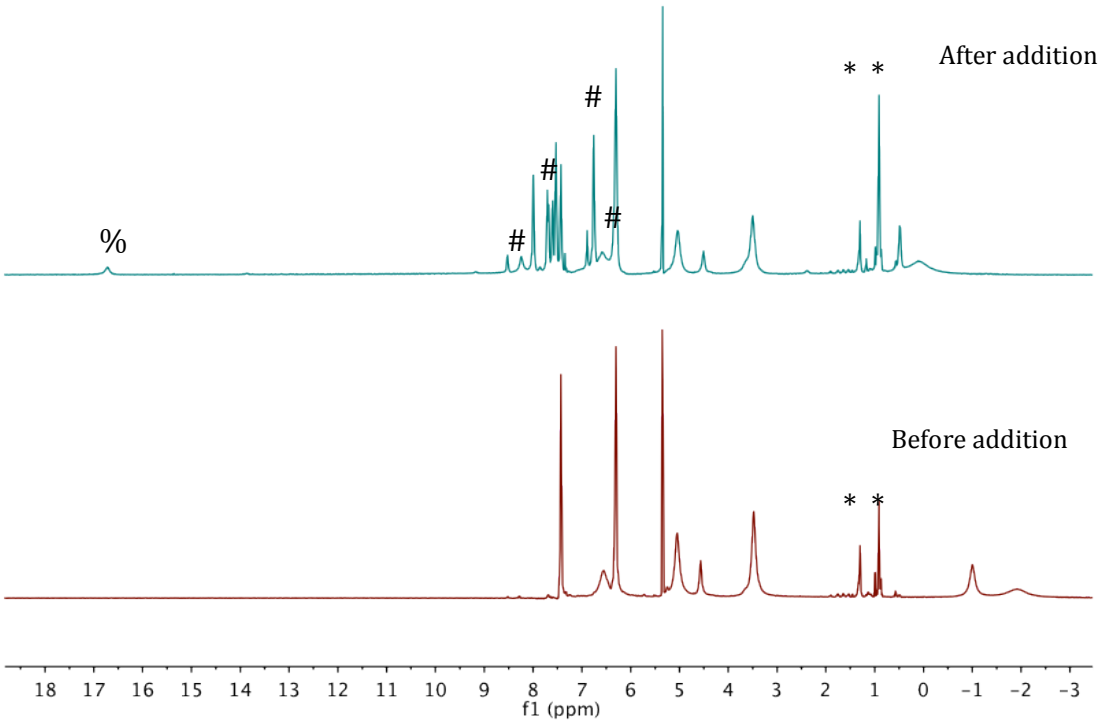

Figure S16. ^{1}H NMR spectra of the in situ formation of **4** from **2** in CD_2Cl_2 at 25 °C (500 MHz). **Experimental details:** A red orange CD_2Cl_2 solution (1 mL) containing **2** (29.2 mg, 0.021 mmol) was sealed in a J. Young NMR tube, and the ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra were recorded (bottom spectrum). Then a colorless CD_2Cl_2 solution (0.5 mL) of H(dbm) (4.9 mg, 0.022 mmol) was added drop-wise, resulting in a color change to deep red. The tube was sealed, and the ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra were re-recorded. These spectra revealed the presence of **2** and **4**, in a 3:2 ratio, according to the integration of the ^{1}H NMR spectrum. # indicates resonances assignable to complex **4**, and % indicates resonances assignable to H(dbm). Asterisks indicate the presence of hexanes.

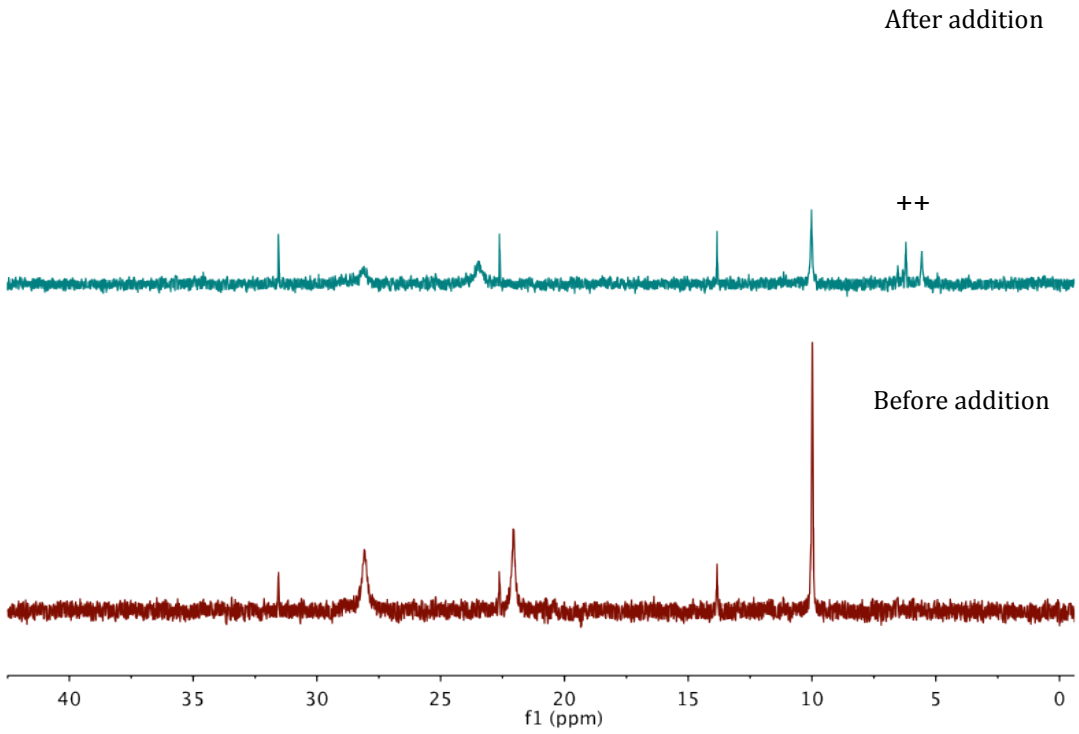

Figure S17. $^{13}C\{^{1}H\}$ NMR spectra of the in situ formation of **4** from **2** in CD_2Cl_2 at 25 °C (500 MHz). + indicates resonances assignable to $HOSiEt_3$.

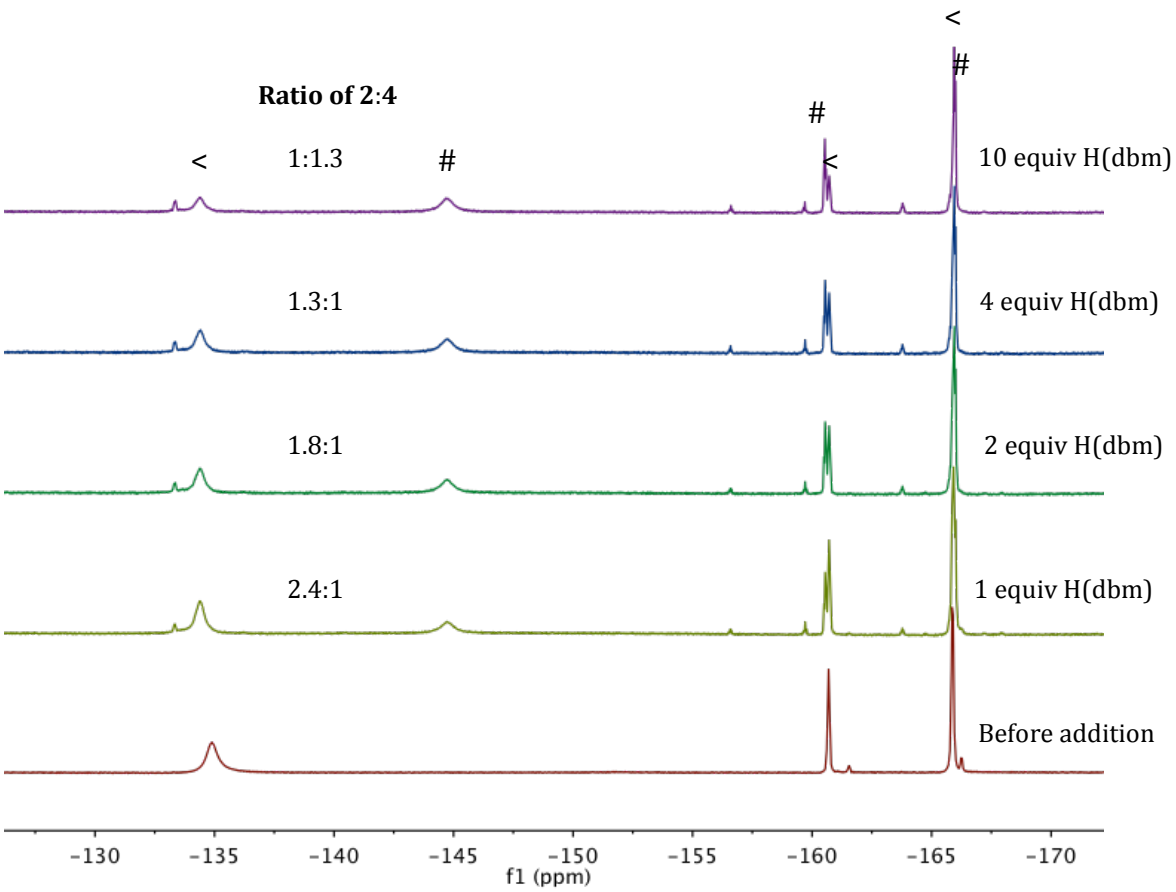

Figure S18. $^{19}F\{^{1}H\}$ NMR spectrum of the in situ formation of **4** from **2** in CD_2Cl_2 at 25 °C. **Experimental details:** A red orange CD_2Cl_2 solution (1 mL) containing **2** (24.5 mg, 0.017 mmol) was sealed in a J. Young NMR tube, and the ^{1}H and $^{19}F\{^{1}H\}$ NMR spectra were recorded. Then a colorless CD_2Cl_2 solution (0.5 mL) of H(dbm) (4.5 mg, 0.020 mmol) was added drop-wise, resulting in a color change to deep red. The tube was sealed, and the ^{1}H and $^{19}F\{^{1}H\}$ NMR spectra were re-recorded ($^{19}F\{^{1}H\}$ spectrum shown above). These spectra revealed the presence of **2** and **4**, in a 2.4:1 ratio, as determined by comparing the integrations of the *ortho* C–F resonances in the ^{19}F NMR spectrum. A second aliquot of H(dbm) (4.6 mg, 0.020 mmol) was added as a CD_2Cl_2 solution (0.5 mL), at which point the ^{1}H and $^{19}F\{^{1}H\}$ NMR spectra were re-recorded. These spectra revealed the presence of **2** and **4**, in a 1.8:1 ratio. A third aliquot of H(dbm) (8.7 mg, 0.039 mmol) was added as a CD_2Cl_2 solution (0.5 mL), which resulted in the formation of **2** and **4**, in a 1.3:1 ratio. A fourth aliquot of H(dbm) (23.4 mg, 0.105 mmol) was added as a CD_2Cl_2 solution (0.5 mL), which resulted in the formation of **2** and **4**, in a 1:1.3 ratio. < indicates resonances assignable to complex **2**, while # indicates resonances assignable to complex **4**.

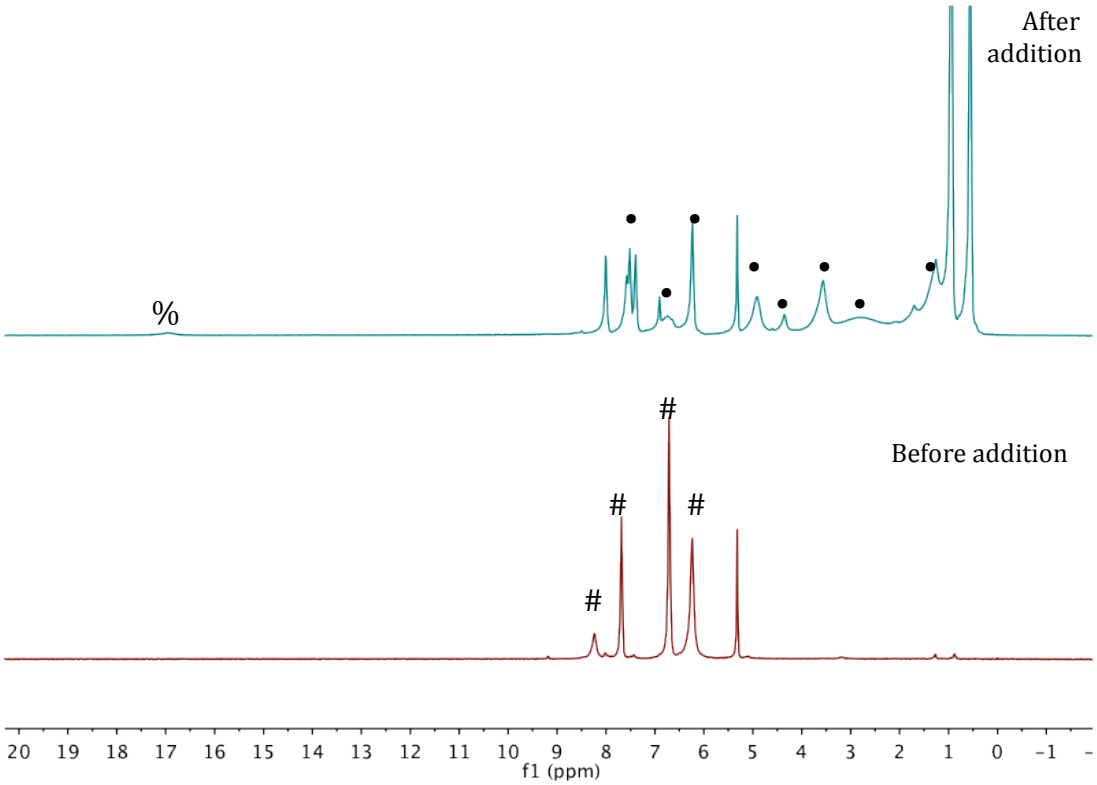

Figure S19. ^{1}H NMR spectra of the in situ formation of **2** from **4** in CD_2Cl_2 at 25 °C. **Experimental details.** A dark red CD_2Cl_2 solution (1 mL) containing **4** (9.8 mg, 0.007 mmol) was sealed in a J. Young NMR tube, and the ^{1}H and ^{19}F{^{1}H} NMR spectra were recorded (bottom spectrum). Then $HOSiEt_3$ (3 µL, 0.020 mmol) was added, resulting in a color change to red-orange. After standing for 1 h at room temperature, THF (2 µL, 0.025 mmol) was added to the reaction mixture and ^{1}H and ^{19}F{^{1}H} NMR spectra were re-recorded (top spectrum). These spectra revealed the formation of complex **2** and H(dbm), along with complete consumption of complex **4**. • indicates resonances assignable to complex **2**, while # indicates resonances assignable to complex **4**, and % indicates resonances assignable to H(dbm).

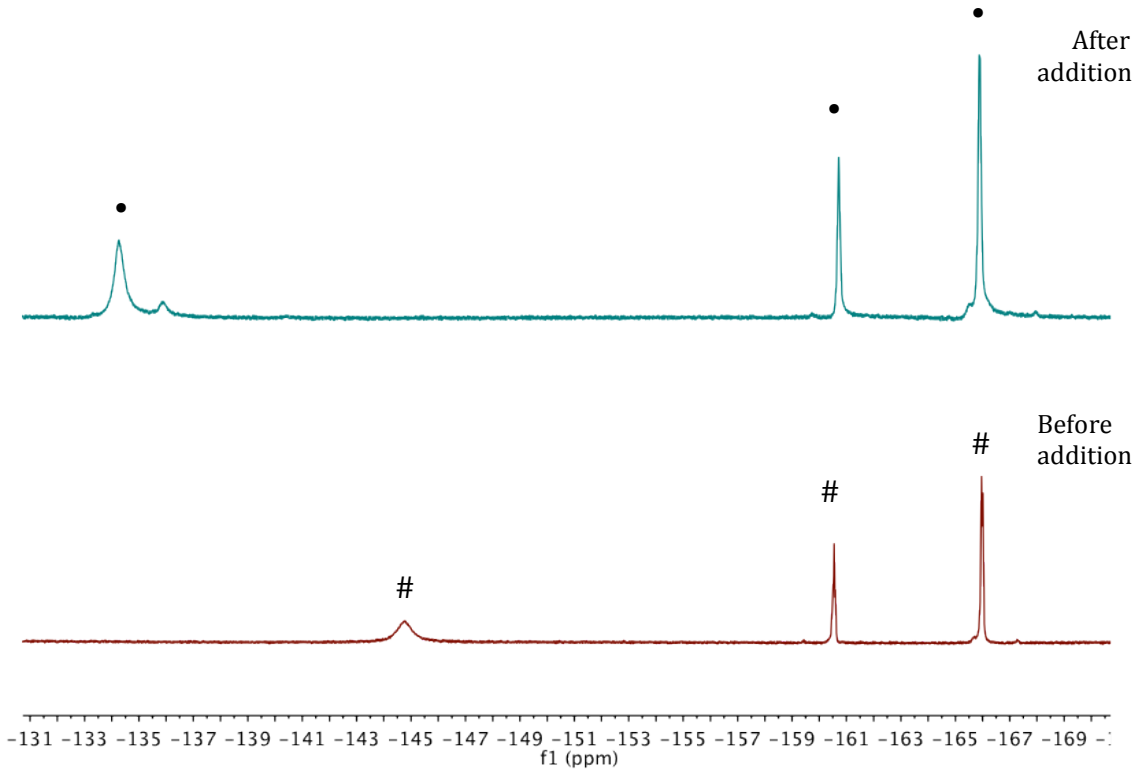

Figure S20. $^{19}F\{^{1}H\}$ NMR spectra of the in situ formation of **2** from **4** in CD_2Cl_2 at 25 °C. • indicates resonances assignable to complex **2**, while # indicates resonances assignable to complex **4**.

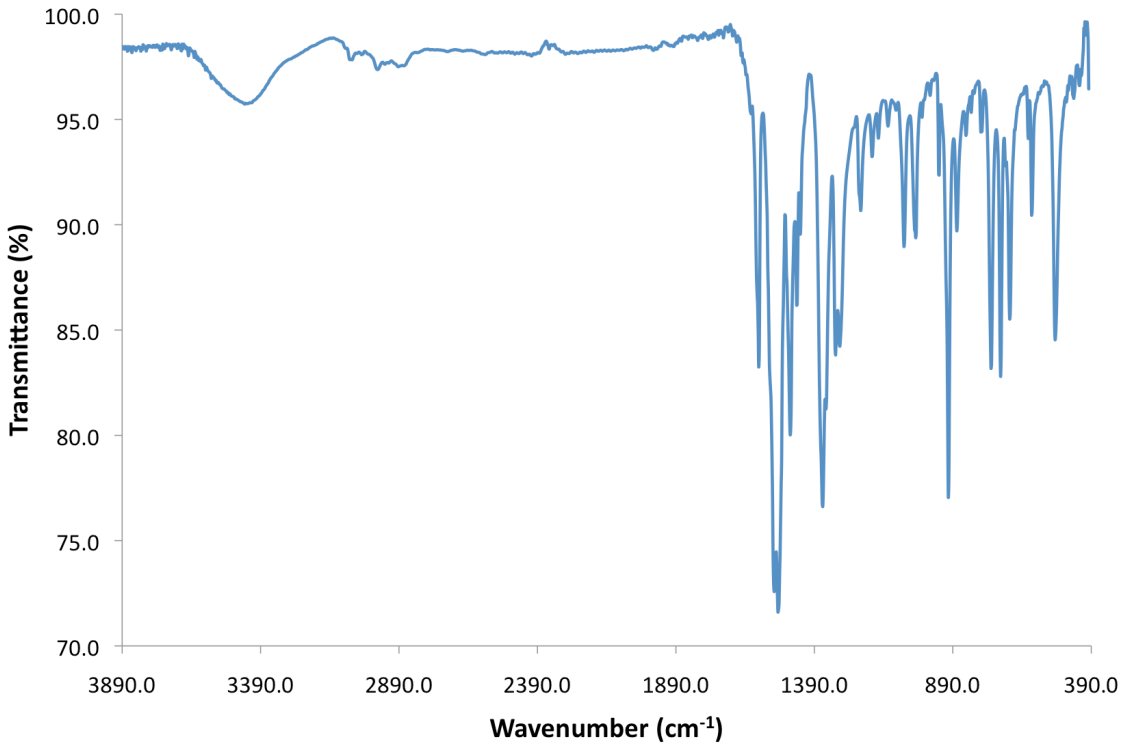

Figure S21. IR spectrum of $UO_2(dbm)_2(THF)$ (as KBr pellet).

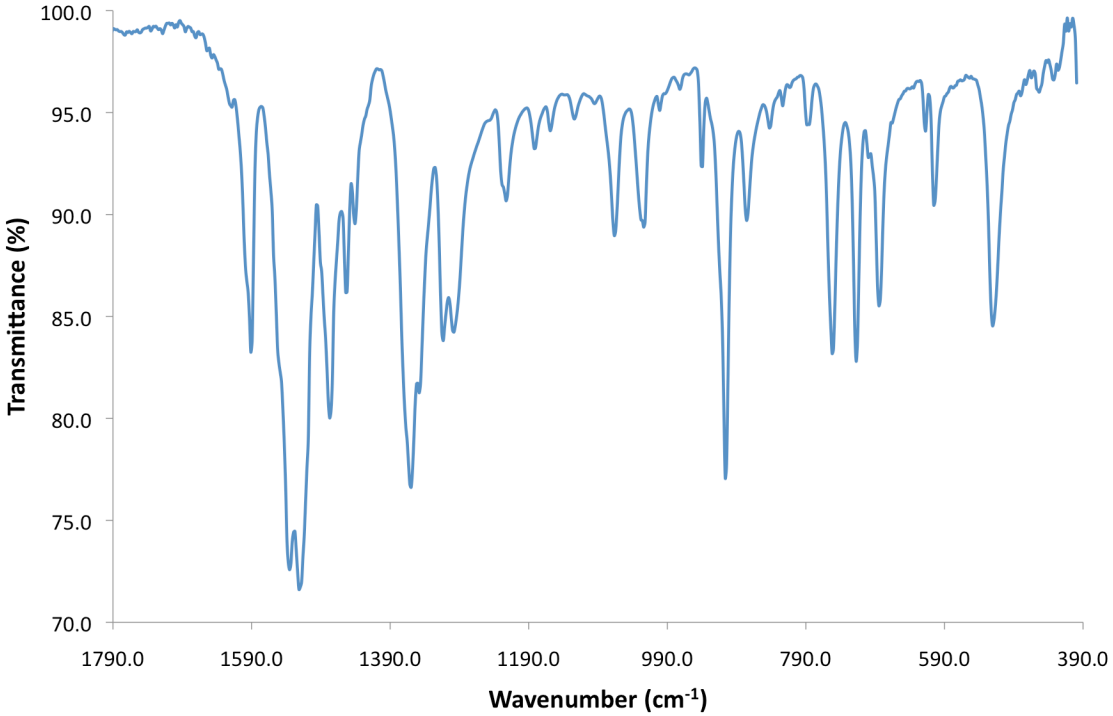

Figure S22. Partial IR spectrum of $UO_2(dbm)_2(THF)$ (as KBr pellet).

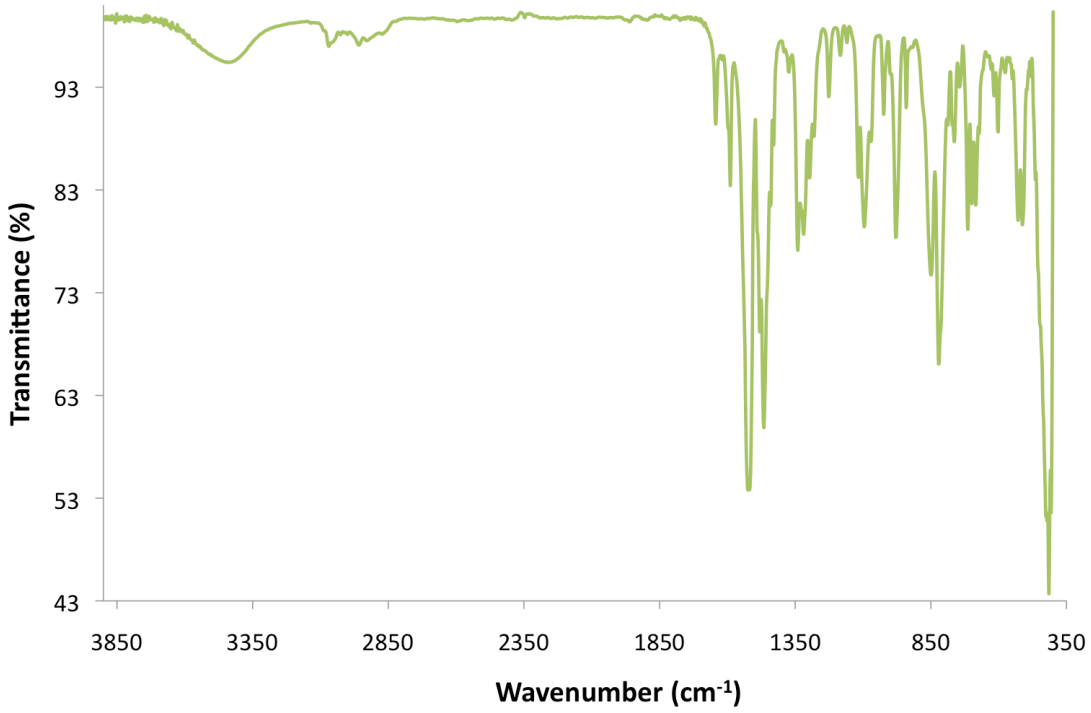

Figure S23. IR spectrum of complex **1** (as KBr pellet).

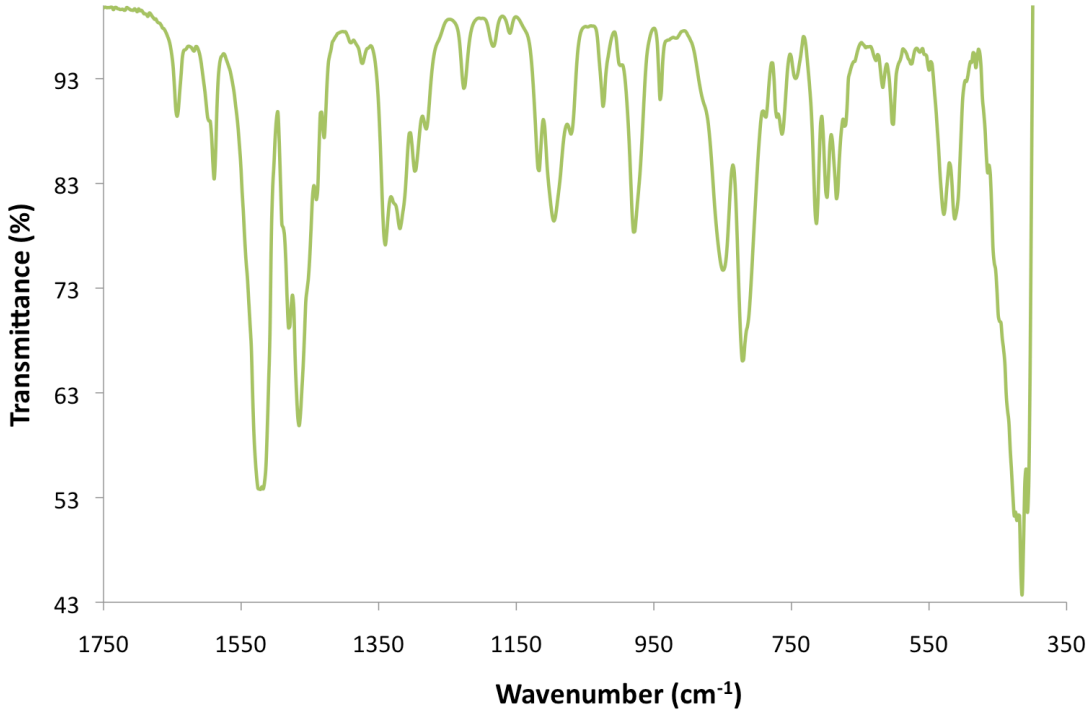

Figure S24. Partial IR spectrum of complex **1** (as KBr pellet).

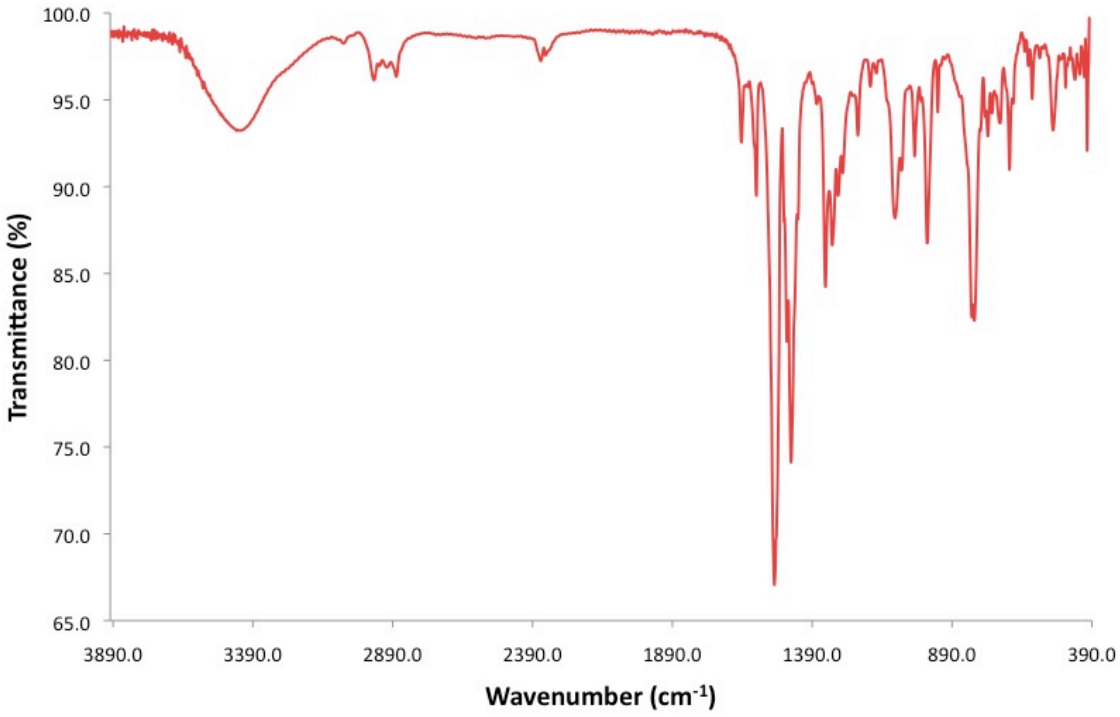

Figure S25. IR spectrum of complex **2** (as KBr pellet).

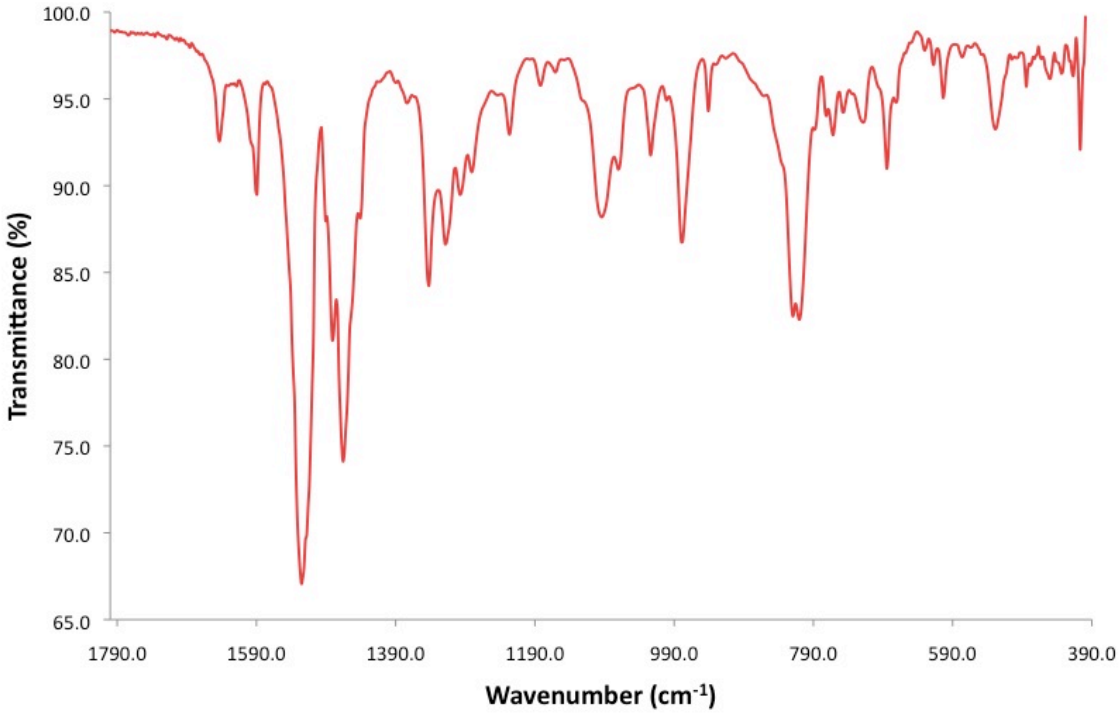

Figure S26. Partial IR spectrum of complex **2** (as KBr pellet).

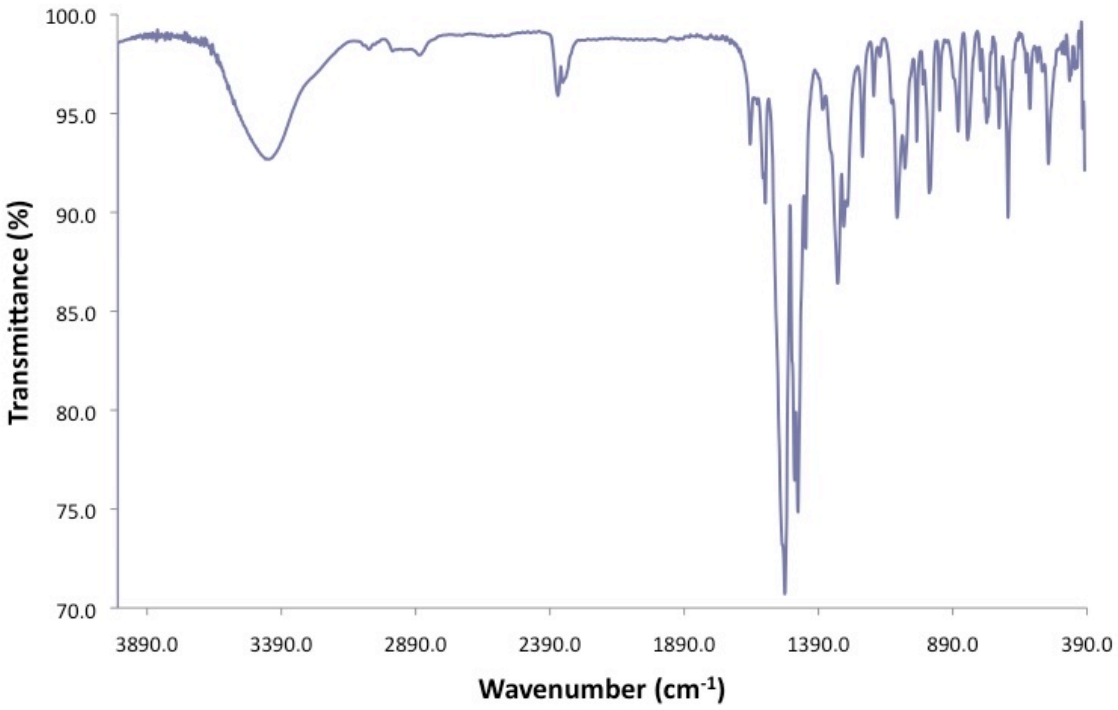

Figure S27. IR spectrum of complex **4** (as KBr pellet).

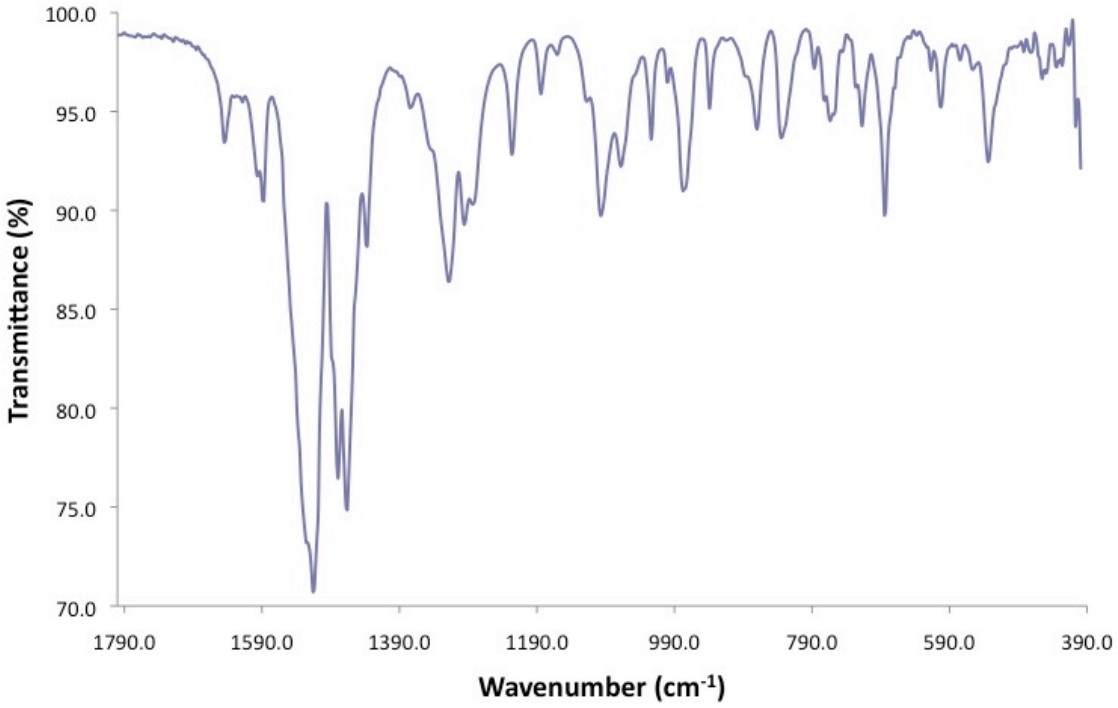

Figure S28. Partial IR spectrum of complex **4** (as KBr pellet).

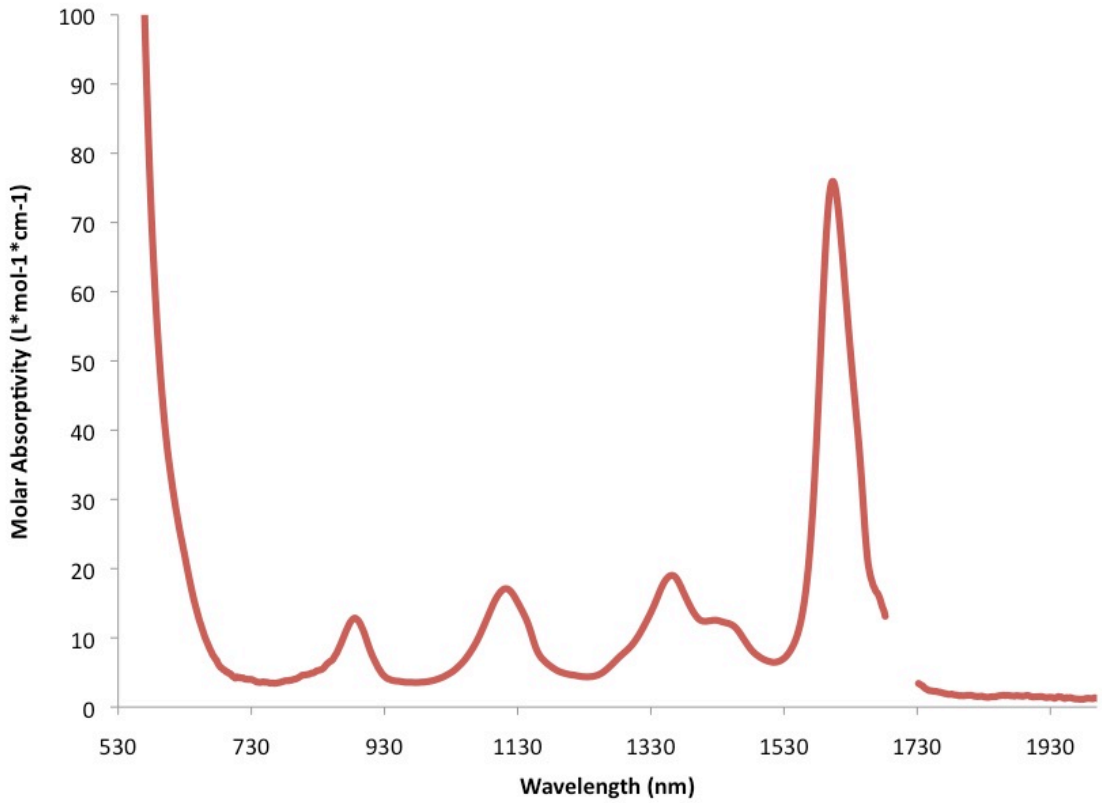

Figure S29. UV-vis/NIR spectrum of **1** (CH_2Cl_2, 3.85×10^{-3} M). Solvent absorption has been removed for clarity.

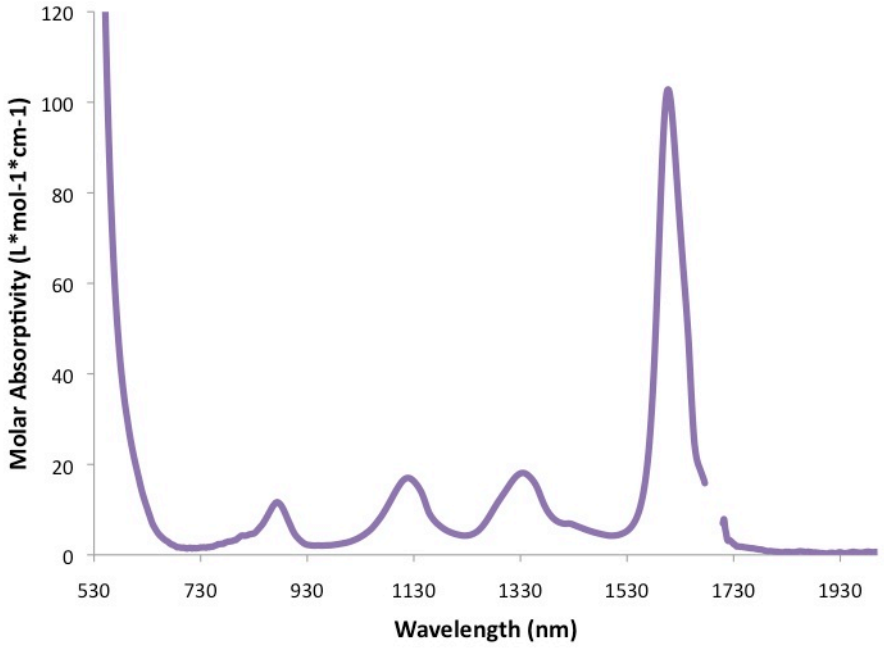

Figure S30. UV-vis/NIR spectrum of **2** (CH_2Cl_2, 4.15×10^{-3} M). Solvent absorption has been removed for clarity.

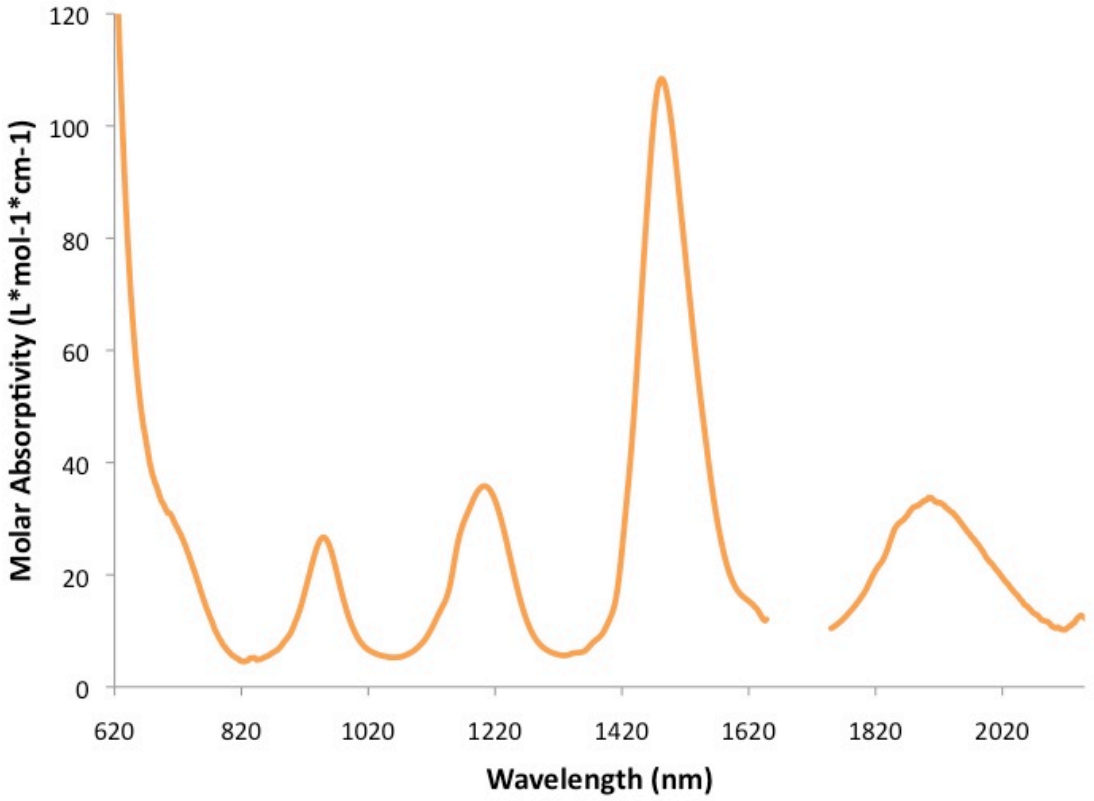

Figure S31. UV-vis/NIR spectrum of **4** (CH_2Cl_2, 2.75 × 10^{-3} M). Solvent absorption has been removed for clarity.

Table S2. X-ray Crystallographic Data for Complexes 1 – 4

	1·C_6H_{14}	**2**·C_7H_8·0.5C_6H_{14}	**3**	**4**·2C_7H_8·C_6H_{14}
empirical formula	$UO_7BF_{15}SiC_{76}H_{59}$	$UO_7BF_{15}SiC_{68}H_{60}$	$UO_6BF_{15}SiC_{54}H_{37}$	$UO_7BF_{15}C_{73}H_{48}$
Crystal habit, color	plate, red-orange	plate, red	plate, red-orange	plate, red
crystal size (mm)	0.35 × 0.30 × 0.30	0.40 × 0.30 × 0.10	0.10 × 0.08 × 0.05	0.20 × 0.15 × 0.10
crystal system	triclinic	triclinic	triclinic	triclinic
space group	*P*-1	*P*-1	*P*-1	*P*1
vol (Å^3)	3411.96(16)	3202.79(11)	2555.2(2)	3157.04(16)
a (Å)	13.6767(4)	12.8552(3)	12.0721(6)	15.1204(4)
b (Å)	15.7946(4)	15.7463(3)	12.2867(7)	16.1764(5)
c (Å)	16.3191(4)	16.5535(3)	17.8840(11)	16.4479(5)
α (deg)	102.448(2)	100.009(1)	89.672(4)	112.966(2)
β (deg)	93.042(2)	103.592(1)	80.120(4)	96.391(2)
γ (deg)	96.154(2)	90.593(1)	78.024(4)	115.286(2)
Z	2	2	2	2
fw (g/mol)	1646.16	1551.09	1343.77	1570.95
density (calcd) (Mg/m^3)	1.602	1.608	1.747	1.653
abs coeff (mm^{-1})	2.493	2.650	3.305	2.672
F_{000}	1634.0	1540.0	1310.0	1548.0
Total no. reflections	35645	31034	30650	32024
Unique reflections	13946	15762	12728	24983
final R indices [I > 2σ(I)]	R_1 = 0.0266 wR_2 = 0.0647	R_1 = 0.0281 wR_2 = 0.0783	R_1 = 0.0388 wR_2 = 0.1047	R_1 = 0.0468 wR_2 = 0.1062
largest diff peak and hole (e·Å^{-3})	1.960 and -1.180	2.493 and -0.716	6.198 and -1.785	1.486 and -2.212
GOF	1.032	1.097	1.047	0.975

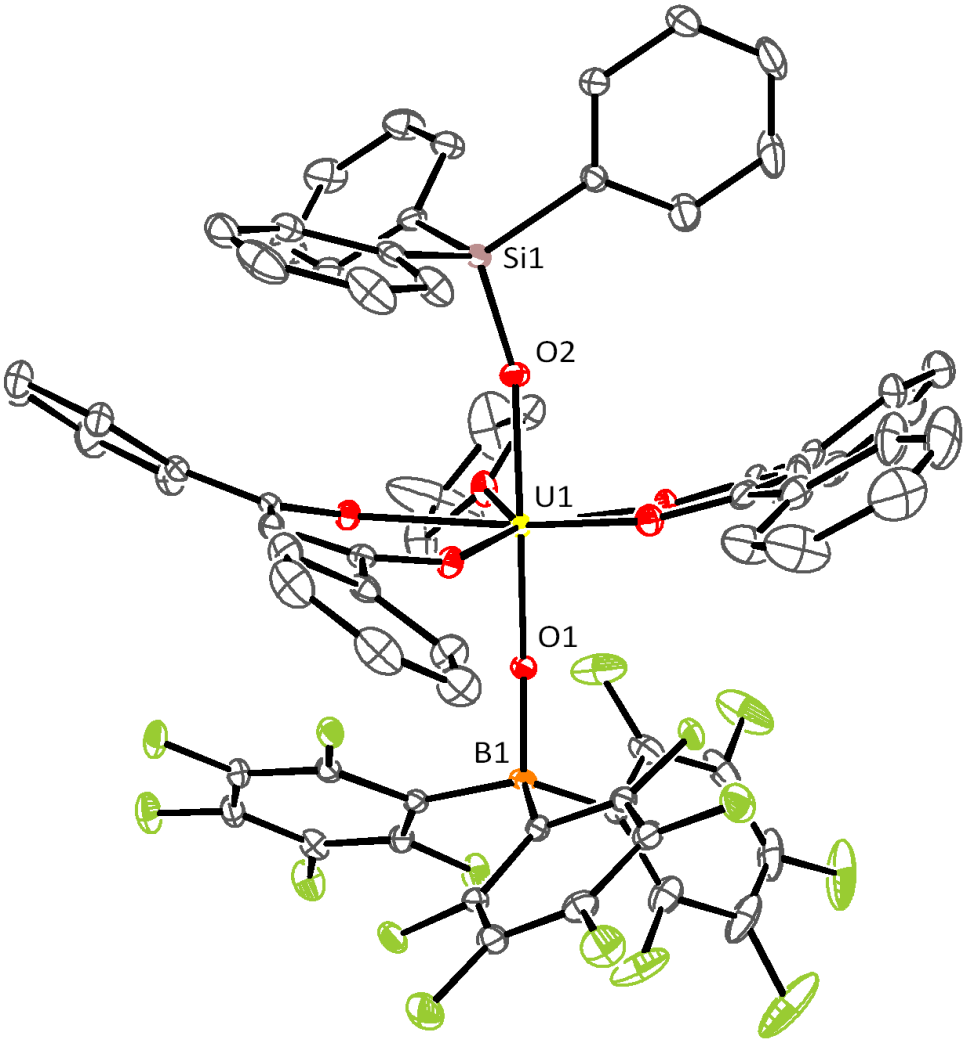

Figure S32. Solid-state molecular structure of $U(OB\{C_6F_5\}_3)(OSiPh_3)(dbm)_2(THF)\cdot C_6H_{14}$ (**1**$\cdot C_6H_{14}$) with 50% probability ellipsoids. Solvate molecule and hydrogen atoms have been omitted for clarity

Converged Cartesian coordinates and total SCF energies

Complex 4 (PBE)
-4942.3498465 H

B 2.153260 -0.908788 -0.097940
C -4.218138 1.471202 0.038070
C -4.848018 0.248072 -0.245077
H -5.927259 0.252060 -0.420554
C -4.134068 -0.974438 -0.361885
C -4.807089 -2.266590 -0.679619
C -3.999131 -3.412407 -0.875219
H -2.909305 -3.317462 -0.780222
C -4.579876 -4.647474 -1.184232
H -3.933969 -5.524755 -1.334805
C -5.975416 -4.763122 -1.298545
H -6.432592 -5.733927 -1.540158
C -6.787502 -3.633805 -1.100099
H -7.880607 -3.719370 -1.183261
C -6.210260 -2.395312 -0.793683
H -6.865190 -1.527660 -0.634944
C -4.984003 2.741399 0.161071
C -6.380360 2.763226 0.382997
H -6.935935 1.822426 0.500551
C -7.063478 3.980154 0.492514
H -8.147771 3.981575 0.675331
C -6.366397 5.194659 0.378214
H -6.905949 6.149398 0.461707
C -4.978373 5.184353 0.163706
H -4.427351 6.131797 0.074386
C -4.290095 3.969664 0.063200
H -3.204770 3.950030 -0.104244
C -0.030336 2.482421 -2.279706
C -0.064505 1.550416 -3.340999
H 0.215748 1.875904 -4.346837
C -0.527465 0.227290 -3.175673
C -0.571617 -0.730777 -4.312313
C 0.282792 -0.605298 -5.431108
H 1.044316 0.185444 -5.460394
C 0.213937 -1.531763 -6.478807
H 0.896741 -1.434712 -7.335120
C -0.708275 -2.589992 -6.428625
H -0.760927 -3.314121 -7.254875
C -1.551635 -2.729955 -5.313514
H -2.269337 -3.561829 -5.265011
C -1.477926 -1.814511 -4.257698

H -2.125628 -1.919124 -3.376503
C 0.409920 3.892901 -2.471620
C 0.251791 4.803487 -1.400516
H -0.189853 4.439332 -0.462775
C 0.657082 6.136393 -1.532603
H 0.524775 6.832461 -0.691343
C 1.237482 6.582353 -2.731526
H 1.562274 7.628131 -2.833921
C 1.413025 5.683650 -3.796488
H 1.883692 6.020272 -4.731191
C 1.001164 4.351759 -3.671100
H 1.173359 3.661597 -4.507474
C -1.098138 -0.485109 3.405299
C -0.454634 0.668344 3.895085
H -0.118576 0.680614 4.936420
C -0.161367 1.786645 3.078465
C -1.416958 -1.644106 4.279164
C -1.674714 -2.897995 3.678320
H -1.611669 -2.981786 2.585084
C -1.977637 -4.011908 4.468958
H -2.163162 -4.984885 3.991351
C -2.039557 -3.890815 5.867316
H -2.279882 -4.766957 6.487339
C -1.794486 -2.647186 6.472961
H -1.850600 -2.545185 7.566358
C -1.482780 -1.531849 5.686420
H -1.314239 -0.559991 6.170881
C 0.530629 2.983727 3.630291
C 1.307190 3.783888 2.760567
H 1.407473 3.485642 1.708284
C 1.975928 4.912254 3.249891
H 2.594879 5.514601 2.568994
C 1.865368 5.268931 4.604401
H 2.388241 6.158405 4.985624
C 1.087482 4.485314 5.472850
H 0.990412 4.765757 6.531722
C 0.429383 3.346217 4.992158
H -0.193910 2.750257 5.673966
C 3.034463 -1.013180 1.289726
C 2.436147 -1.554534 2.438766
C 3.076595 -1.669812 3.679073
C 4.411733 -1.261000 3.792110
C 5.069664 -0.751215 2.665746
C 4.378519 -0.639399 1.448541
C 1.879510 -2.451493 -0.596721
C 2.963438 -3.249360 -1.001515
C 2.847910 -4.591132 -1.385708

C 1.585592 -5.202844 -1.366119
C 0.475742 -4.457395 -0.955003
C 0.649197 -3.117982 -0.576790
C 2.782194 0.108105 -1.225964
C 3.044068 1.437814 -0.849962
C 3.464875 2.438889 -1.733010
C 3.639713 2.117681 -3.085590
C 3.384193 0.812032 -3.514427
C 2.956806 -0.157317 -2.591886
F -0.510331 -2.496541 -0.165480
F 6.359941 -0.368732 2.763321
F 5.057956 -1.364645 4.969615
F 2.429177 -2.171933 4.753163
F 1.156330 -2.019500 2.378849
F 2.861316 1.822189 0.442943
F 3.669174 3.702835 -1.307878
F 4.000396 3.067990 -3.972889
F 3.488714 0.512034 -4.832600
F 2.665341 -1.373619 -3.119690
F 4.205717 -2.707053 -1.037674
F 3.926608 -5.299167 -1.775284
F 1.445351 -6.490742 -1.733533
F -0.751168 -5.032296 -0.919717
F 5.094769 -0.144094 0.409065
O 0.820556 -0.250154 0.236214
O -2.921840 1.580231 0.190525
O -2.857314 -1.022703 -0.208588
O -1.448561 -0.601527 2.155373
O -0.460340 1.829700 1.819946
O -0.979125 -0.213864 -2.038695
O -0.403656 2.160787 -1.078341
U -1.037249 0.358769 0.158682

Complex 4 (PBE0)
-4942.4450355 H

B 1.994428 -1.148358 0.253380
C -3.982355 1.809286 -0.607562
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C -4.866163 -1.879663 -1.055999
C -4.170141 -3.098957 -1.060485
H -3.097339 -3.095913 -0.867635
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H -4.281721 -5.230490 -1.306531
C -6.213486 -4.286490 -1.546766
H -6.740735 -5.223382 -1.738617
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H -7.990901 -3.072255 -1.725476
C -6.247811 -1.885098 -1.297252
H -6.817510 -0.955498 -1.292835
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C -6.012645 3.309651 -0.523849
H -6.657122 2.445861 -0.355348
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H -6.210653 6.695694 -0.796934
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H -3.746038 6.417993 -1.019959
C -3.816926 4.276544 -0.819451
H -2.738541 4.143697 -0.910573
C 0.577990 2.253602 -2.438079
C 0.582147 1.255502 -3.423691
H 1.033269 1.460065 -4.389169
C -0.062379 0.024366 -3.238381
C -0.071195 -1.005215 -4.303632
C 0.934559 -1.076397 -5.277340
H 1.783081 -0.392463 -5.244390
C 0.892498 -2.064237 -6.255665
H 1.690631 -2.123339 -6.997803
C -0.154772 -2.984694 -6.278034
H -0.186309 -3.757029 -7.049396
C -1.153048 -2.927078 -5.305214
H -1.969777 -3.651446 -5.314247
C -1.106404 -1.950983 -4.316680
H -1.873495 -1.902532 -3.542832
C 1.205722 3.580324 -2.662587
C 0.992425 4.588317 -1.710363

H 0.374408 4.362662 -0.840568
C 1.564712 5.844973 -1.871440
H 1.387781 6.620953 -1.124012
C 2.368946 6.110232 -2.979450
H 2.825266 7.094496 -3.103347
C 2.598954 5.110858 -3.924311
H 3.242006 5.306453 -4.784068
C 2.019980 3.856172 -3.770522
H 2.234176 3.083528 -4.508855
C -1.566532 0.048793 3.191702
C -0.827400 1.142324 3.650543
H -0.622259 1.230011 4.713093
C -0.296327 2.111114 2.779128
C -2.158169 -0.940219 4.120196
C -2.529022 -2.195459 3.616530
H -2.355254 -2.410133 2.561854
C -3.085867 -3.152381 4.456820
H -3.359031 -4.130887 4.057425
C -3.290970 -2.865346 5.806257
H -3.730378 -3.617016 6.465345
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C -2.369522 -0.659582 5.477444
H -2.113440 0.320447 5.882046
C 0.456610 3.273994 3.308122
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H 1.617786 3.458168 1.502446
C 2.155365 4.963079 2.957286
H 2.922203 5.410612 2.321983
C 1.915307 5.474243 4.232850
H 2.486974 6.331020 4.595800
C 0.945523 4.888707 5.046470
H 0.748476 5.292104 6.041532
C 0.224490 3.789790 4.590526
H -0.545196 3.348560 5.225956
C 2.644647 -1.194400 1.757705
C 1.831188 -1.550915 2.831393
C 2.263933 -1.604857 4.149844
C 3.593891 -1.323734 4.433491
C 4.455817 -0.999485 3.394903
C 3.973727 -0.943186 2.090105
C 1.628322 -2.692225 -0.141582
C 2.655761 -3.621647 -0.298125
C 2.447775 -4.966852 -0.569841
C 1.146319 -5.442131 -0.690155
C 0.088784 -4.560482 -0.528773
C 0.349895 -3.221875 -0.254628

C 2.888709 -0.330596 -0.846004
C 3.251021 0.984825 -0.553135
C 3.910537 1.827403 -1.436362
C 4.236484 1.352580 -2.700427
C 3.892378 0.055409 -3.044838
C 3.226065 -0.754206 -2.127529
F -0.758802 -2.454995 -0.094691
F 5.737251 -0.740486 3.657512
F 4.038779 -1.372041 5.687425
F 1.423619 -1.926848 5.135696
F 0.545287 -1.882323 2.614211
F 2.940653 1.510133 0.643686
F 4.208470 3.081847 -1.097253
F 4.836201 2.147698 -3.586771
F 4.155347 -0.389684 -4.279842
F 2.883046 -1.969833 -2.575653
F 3.926584 -3.213258 -0.191400
F 3.472794 -5.804401 -0.718611
F 0.919182 -6.726995 -0.952630
F -1.171359 -5.001228 -0.632128
F 4.874148 -0.629906 1.149926
O 0.718371 -0.336087 0.326460
O -2.706856 1.817593 -0.378775
O -2.860273 -0.785840 -0.548827
O -1.777462 -0.160353 1.938563
O -0.417030 2.048124 1.510198
O -0.709923 -0.264855 -2.170386
O 0.015137 2.086227 -1.300057
U -0.981438 0.475107 -0.048871

$[UOCl_5]^-$ (PBE0)

-2852.8912231

U	0.000000	0.000000	0.162153
Cl	0.000000	0.000000	-2.315518
O	0.000000	0.000000	1.913049
Cl	0.000000	2.547269	0.134431
Cl	0.000000	-2.547269	0.134431
Cl	2.547269	0.000000	0.134431
Cl	-2.547269	0.000000	0.134431