Supporting Information

Uranium and Thorium Complexes of the Phosphaethynolate Ion

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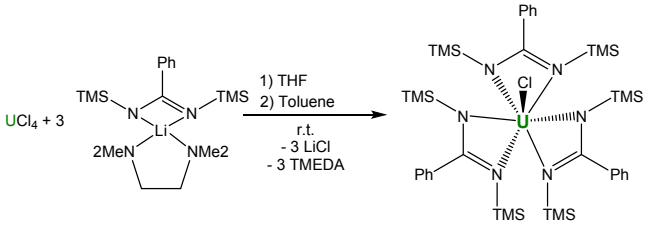
Content

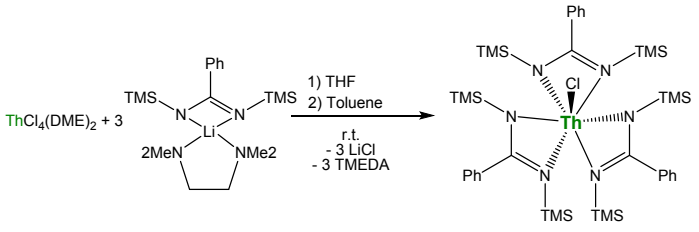
A. Experimental section

General Considerations. Unless otherwise noted, all reactions were performed either using standard Schlenk line techniques or in an MBraun inert atmosphere glovebox under an atmosphere of purified nitrogen (<1 ppm O_2/H_2O). Glassware and cannulae were stored in an oven at ~160 °C for at least 12 h prior to use. Hexanes, THF and toluene were purified by passage through a column of activated alumina, stored over 3 or 4 Å molecular sieves, and degassed prior to use. C_6D_6 was dried over sodium/benzophenone and then vacuum-transferred to a storage flask and freeze-pump-thaw degassed before being stored over activated molecular sieves in the drybox. UCl_4,[1] $ThCl_4(DME)_2$,[2] (amid)Li(TMEDA)[3] and $Na(OCP)(dioxane)_{2.9}$[4] were prepared using literature procedures. All other reagents were acquired from commercial sources and used as received. NMR spectra were recorded on Bruker AVQ-400, AVB-400, DRX-500, AV-500, and AV-600 spectrometers. Chemical shifts were measured relative to residual solvent peaks, which were assigned relative to an external TMS standard set at 0.00 ppm. ^{31}P chemical shifts were referenced to an external standard (Ph_3PO for ^{31}P set at 23 ppm). ^{1}H and ^{13}C NMR assignments were routinely confirmed by $^{1}H–^{1}H$ COSY and $^{1}H–^{13}C$ HSQC experiments. Infrared (IR) spectra were recorded with a Thermo Scientific Nicolet iS10 series FTIR spectrophotometer as a Nujol mull between KBr plates. The uncorrected melting points were determined using sealed capillaries prepared under nitrogen on an Optmelt SRS. Elemental analyses were performed at the School of Human Sciences, Science Center, London Metropolitan University. The X-ray structural determinations were performed at CHEXRAY, University of California, Berkeley on a Bruker SMART APEX II QUAZAR diffractometer. Solution magnetic moments were obtained by Evan's Method. Details concerning X-ray diffraction analyses and DFT computational studies are provided in the following sections.

Synthetic methods



1 green crystals, 88%



2 colorless crystals, 59%

$UCl(amid)_3$ (1)

This compound was prepared according to a modified published procedure.[5] A 50 mL THF solution of (amid)Li(TMEDA) (3.15 g, 8.13 mmol, 3 equiv.) was added to UCl_4 (1.03 g, 2.71 mmol, 1 equiv.) and the reaction mixture was vigorously stirred at room temperature for 15 h affording a green suspension. The THF solvent was then removed *in vacuo* and the residue was triturated with 2x10 mL toluene and taken to dryness. The green residue was then extracted with 3x30mL toluene and filtered. The resulting green filtrate was concentrated to 30 mL and allowed to crystallize at -40°C in a freezer for 24 h. This produced large bright green crystals that were recovered and dried *in vacuo* (2.55 g, 88 % yield). The crystal structure for **1** was previously reported by Edelmann and coworkers.[5] ^{1}H NMR (400 MHz, C_6D_6, 293 K) δ = 15.3 (br s, 3H, CH_{Ar}), 10.9 (br s, 3H, CH_{Ar}), 9.3 (br s, 6H, CH_{Ar}), 8.8 (t, 3H, CH_{Ar}), 1.3 (s, 27H, $SiMe_3$), -3.1 (s, 27H, $SiMe_3$). FT-IR (cm^{-1}) 2915 (s), 2851 (s), 1463 (s), 1386 (s), 1245 (s), 1157 (w), 1075 (w), 1000 (w), 973 (s), 920 (w), 841 (s), 784 (s), 759 (s), 704 (s), 477(s). M.p. 317(2)°C, decomp. Anal. calcd for $C_{39}H_{69Cl}N_6Si_6U$: C, 44.02; H, 6.54; N, 7.90. Found: C, 43.98; H, 6.47; N, 7.93.

$ThCl(amid)_3$ (2)

This compound was prepared in an analogous fashion to that previously stated for **1**. (amid)Li(TMEDA) (5.01 g, 12.9 mmol, 3 equiv.) and $ThCl_4(DME)_2$ (2.39 g, 4.3 mmol, 1 equiv.) yielded 2.71 g of **2** (59 % yield). Colorless crystals suitable for X-ray diffraction were grown from a concentrated toluene solution kept at -40 °C for 24 h. ^{1}H NMR (500 MHz, C_6D_6, 293 K) δ = 7.5 (br s, 6H, CH_{Ar}), 7.0 (m, 9H, CH_{Ar}), 0.4 (s, 27H, $SiMe_3$), 0.2 (s, 27H, $SiMe_3$). FT-IR (cm^{-1}) 2922 (s), 2853 (s), 1463 (s), 1246 (s), 1160 (w), 1025 (w), 1000 (w), 978 (s), 920 (w), 842 (s), 785 (m), 761 (s), 717 (s), 479 (s). M.p. 317(2)°C, decomp. Anal. calcd for $C_{39}H_{69}N_6Si_6ClTh$: C, 44.15; H, 6.84; N, 7.92. Found: C, 44.16; H, 6.71; N, 7.85.

$U(OCP)(amid)_3$ (3)

A 10 mL THF solution of $UCl(amid)_3$ (300 mg, 0.282 mmol, 1 equiv.) and $Na(OCP)(dioxane)_{2.9}$ (100 mg, 0.296 mmol, 1.05 equiv.) was stirred at room temperature for 24 h. The THF solvent was then removed *in vacuo* and the residue was extracted with 2 mL toluene and filtered. The green filtrate was allowed to crystallize at -40°C in a freezer for 48 h. This produced green block-shaped crystals that were recovered and dried *in vacuo* (234 mg, 76 % yield). Single crystals suitable for X-ray diffraction were obtained similarly. ^{1}H NMR (400 MHz, C_6D_6, 293 K) δ = 13.7 (br s, 3H, CH_{Ar}), 10.3 (br s, 3H, CH_{Ar}), 8.9 (t, 6H, CH_{Ar}), 8.4 (t, 3H, CH_{Ar}), 0.5 (s, 27H, $SiMe_3$), -2.6 (s, 27H, $SiMe_3$). ^{31}P NMR (243 MHz, C_6D_6, 293 K) δ = -285.2 (s, OC*P*). ^{13}C NMR (125.8 MHz, C_6D_6, 293 K) δ = 142.7 (*C*$_{Ar}$), 132.9 (*C*$_{Ar}$), 4.6 (Si*Me*$_3$), 1.8 (Si*Me*$_3$). FT-IR (cm^{-1}) 2955 (s), 2925 (s), 2852 (s), 1685 (s, PCO), 1463 (s), 1386 (s), 1247 (s), 1179 (w), 1157 (w), 1000 (w), 974 (s), 931 (w), 920 (w), 838 (s), 783 (s), 761 (s), 704 (s). M.p. 233(2)°C, decomp. μ_{eff} = 3.23 μ_B (C_6D_6, 293 K, Evans'method). Anal. calcd for $C_{40}H_{69}N_6OPSi_6U$: C, 44.18; H, 6.40; N, 7.73. Found: C, 43.83; H, 6.31; N, 7.62.

$Th(OCP)(amid)_3$ (4)

This compound was prepared in an analogous fashion to that previously stated for **3**. $ThCl(amid)_3$ (298 mg, 0.282 mmol, 1 equiv.) and $Na(OCP)(dioxane)_{2.9}$ (100 mg, 0.296 mmol, 1.05 equiv.) yielded 191 mg of **4** (63%). Colorless crystals suitable for X-ray diffraction were grown from a concentrated toluene solution kept at -40 °C for 24 h. ^{1}H NMR (400 MHz, C_6D_6, 293 K) δ = 7.3 (br s, 6H, CH_{Ar}), 7.0 (m, 9H, CH_{Ar}), 0.3 (s, 27H, $SiMe_3$), 0.1 (s, 27H, $SiMe_3$). ^{31}P NMR (243 MHz, C_6D_6, 293 K) δ = -334.4 (s, OC*P*). ^{13}C NMR (125.8 MHz, C_6D_6, 293 K) δ = 181.7 (N*C*N), 143.0 (*C*$_{Ar}$), 128.8 (*C*$_{Ar}$), 126.8 (*C*$_{Ar}$), 3.4 (Si*Me*$_3$), 2.7 (Si*Me*$_3$). FT-IR (cm^{-1}) 2923 (s), 2853 (s), 1683 (s, PCO), 1385 (s), 1248 (s), 978 (s), 839 (s), 785 (s), 761 (s), 703 (s). M.p. 277(2)°C, decomp. Anal. calcd for $C_{40}H_{69}N_6OPSi_6Th$: C, 44.42; H, 6.43; N, 7.77. Found: C, 44.35; H, 6.35; N, 7.69.

$U(NCO)(amid)_3$ (5)

A 5 mL THF suspension of $UCl(amid)_3$ (195 mg, 0.183 mmol, 1 equiv.) and sodium cyanate (13.7 mg, 0.211 mmol, 1.15 equiv.) was stirred at room temperature for 24 h. The THF solvent was then removed *in vacuo* and the residue was extracted with 1.5 mL toluene and filtered. The green filtrate was allowed to crystallize at -40°C in a freezer for 48 h. This produced green block-shaped crystals that were recovered and dried *in vacuo* (123 mg, 63 % yield). Single crystals suitable for X-ray diffraction were obtained similarly. ^{1}H NMR (400 MHz, C_6D_6, 293 K) δ = 13.2 (br s, 3H, CH_{Ar}), 10.1 (br s, 3H, CH_{Ar}), 8.8 (t, 6H, CH_{Ar}), 8.4 (t, 3H, CH_{Ar}), 0.5 (s, 27H, $SiMe_3$), -2.5 (s, 27H, $SiMe_3$). ^{13}C NMR (125.8 MHz, C_6D_6, 293 K) δ = 144.0 (*C*$_{Ar}$), 132.7 (*C*$_{Ar}$), 3.4 (Si*Me*$_3$), 1.9 (Si*Me*$_3$). FT-IR (cm^{-1}) 3063 (w), 2922 (s), 2853 (s), 2199 (s, OCN), 1398 (s), 1246 (s), 1157 (w), 1074 (w), 1000 (w), 973 (s), 920 (w), 847 (s), 784 (s), 758 (s), 706 (s). M.p. 288(2)°C, decomp. Anal. calcd for $C_{40}H_{69}N_7OSi_6U$: C, 44.88; H, 6.50; N, 9.16. Found: C, 44.72; H, 6.61; N, 9.06.

$Th(NCO)(amid)_3$ (6)

This compound was prepared in an analogous fashion to that previously stated for **5**, although a longer reaction time of 96 h and an excess of sodium cyanate were required. $ThCl(amid)_3$ (297 mg, 0.281 mmol, 1 equiv.) and sodium cyanate (40 mg, 0.615 mmol, 2.19 equiv.) yielded 120 mg of **6** (40%). Colorless crystals suitable for X-ray diffraction were grown from a concentrated toluene solution kept at -40 °C for 24 h. ^{1}H NMR (400 MHz, C_6D_6, 293 K) δ = 7.4 (br s, 6H, CH_{Ar}), 7.0 (m, 9H, CH_{Ar}), 0.3 (s, 27H, $SiMe_3$), 0.2 (s, 27H, $SiMe_3$). ^{13}C NMR (125.8 MHz, C_6D_6, 293 K) δ = 181.7 (N*C*N), 143.0 (*C*$_{Ar}$), 128.8 (*C*$_{Ar}$), 126.6 (*C*$_{Ar}$), 3.2 (Si*Me*$_3$), 2.3

(Si*Me*$_3$). FT-IR (cm^{-1}) 2923 (s), 2853 (s), 2200 (s), 1663 (w), 1463 (s), 1378 (s), 1246 (s), 1157 (w), 1074 (w), 1000 (w), 978 (s), 842 (s), 785 (w), 758 (m), 716 (m), 703 (m), 630 (w), 479 (s). M.p. 205(2)°C, decomp. Anal. calcd for $C_{40}H_{69}N_7OSi_6Th$: C, 45.15; H, 6.53; N, 9.21. Found: C, 44.93; H, 6.72; N, 9.15.

U(NCS)(amid)$_3$ (7)

A 5 mL THF suspension of UCl(amid)$_3$ (163 mg, 0.153 mmol, 1 equiv.) and potassium thiocyanate (17.1 mg, 0.176 mmol, 1.15 equiv.) was stirred at room temperature for 24 h. The THF solvent was then removed *in vacuo* and the residue was extracted with 1.5 mL toluene and filtered. The green filtrate was allowed to crystallize at -40°C in a freezer for 48 h. This produced green block-shaped crystals that were recovered and dried *in vacuo* (133 mg, 80 % yield). Single crystals suitable for X-ray diffraction were obtained similarly. ^{1}H NMR (500 MHz, C_6D_6, 293 K) δ = 15.6 (br s, 3H, C*H*$_{Ar}$), 11.1 (br s, 3H, C*H*$_{Ar}$), 9.5 (br s, 6H, C*H*$_{Ar}$), 8.9 (t, 3H, C*H*$_{Ar}$), 0.9 (s, 27H, SiMe$_3$), -3.4 (s, 27H, SiMe$_3$). ^{13}C NMR (125.8 MHz, C_6D_6, 293 K) δ = 151.1 (*C*$_{Ar}$), 133.7 (*C*$_{Ar}$), 4.6 (Si*Me*$_3$), 0.8 (Si*Me*$_3$). FT-IR (cm^{-1}) 3062 (w), 3024 (w), 2924 (s), 2854 (s), 2021 (s, SCN), 1386 (s), 1247 (s), 1179 (w), 1158 (w), 1000 (w), 973 (s), 922 (w), 834 (s), 783 (s), 761 (s), 704 (s). M.p. 288(2)°C, decomp. Anal. calcd for $C_{40}H_{69}N_7S_1Si_6U$: C, 44.21; H, 6.40; N, 9.02. Found: C, 44.19; H, 6.50; N, 8.98.

Th(NCS)(amid)$_3$ (8)

This compound was prepared in an analogous fashion to that previously stated for **7**. ThCl(amid)$_3$ (303 mg, 0.286 mmol, 1 equiv.) and potassium thiocyanate (34 mg, 0.350 mmol, 1.22 equiv.) yielded 201 mg of **8** (65%). Colorless crystals suitable for X-ray diffraction were grown from a concentrated toluene solution kept at -40 °C for 24 h. ^{1}H NMR (400 MHz, C_6D_6, 293 K) δ = 7.4 (br s, 6H, C*H*$_{Ar}$), 7.0 (m, 9H, C*H*$_{Ar}$), 0.3 (s, 27H, SiMe$_3$), 0.1 (s, 27H, SiMe$_3$). ^{13}C NMR (125.8 MHz, C_6D_6, 293 K) δ = 182.1 (N*C*N), 142.7 (*C*$_{Ar}$), 129.0 (*C*$_{Ar}$), 126.6 (*C*$_{Ar}$), 3.1 (Si*Me*$_3$), 2.3 (Si*Me*$_3$). FT-IR (cm^{-1}) 2921 (s), 2854 (s), 2018 (s), 1444 (s), 1382 (s), 1246 (s), 1179 (w), 1158 (w), 1001 (w), 978 (s), 921 (w), 846 (s), 784 (w), 760 (m), 702 (s), 604 (w), 479 (s). M.p. 308(2)°C, decomp. Anal. Calcd for $C_{40}H_{69}N_7S_1Si_6Th$: C, 44.46; H, 6.44; N, 9.07. Found: C, 44.51; H, 6.51; N, 8.89.

(amid)$_3$Th(μ-η^1(O):η^2(C,P)-OCP)Ni(COD) (9)

A 2 mL toluene solution of Th(OCP)(amid)$_3$ **4** (255 mg, 0.236 mmol, 1 equiv.) and *bis*(1,5-cyclooctadiene)nickel(0) (64.9 mg, 0.236 mmol, 1 equiv.) was stirred at room temperature for 12 h during which time the solution turned from pale yellow to dark brown within a few hours. Monitoring the reaction by ^{1}H and ^{31}P NMR showed that the reaction reaches equilibrium after approximatively 12h at room temperature. The solvent was then removed *in vacuo* and the residue was extracted with 0.5 mL hexane and filtered. The dark brown filtrate was allowed to crystallize at -40°C in a freezer for 72 h. This produced a dark brown crystalline material (122 mg) containing **9** as well as **4** and Ni(COD)$_2$. Despite several attempts, the purification of **9** from its starting materials by fractional recrystallization proved highly challenging since these species exhibit similar high-solubility in common solvents and limited stability. In one occurrence, few crystals of **9** (1% yield) were obtained upon 4 successive recrystallizations of the reaction materials in hexanes at -40°C. These were sufficient to get X-ray diffraction and NMR spectroscopy data. The latter revealed that **9** exhibits limited stability in C_6D_6 solution (Figure S17 and S18) and is converted back to **4** through the loss of free COD, Ni(COD)$_2$ and other non-identified Ni species. ^{1}H NMR (600 MHz, C_6D_6, 293 K) δ = 7.5 (3, 6H, C*H*$_{Ar}$), 7.0 (m, 12H, C*H*$_{Ar}$), 6.1 (m, 2H, C*H*=CH$_{COD}$), 5.5 (m, 2H, CH=C*H*$_{COD}$), 2.4 (m, 2H, C*H*$_{2COD}$), 2.2 (m, 2H, C*H*$_{2COD}$), 2.0 (m, 2H, C*H*$_{2COD}$), 1.9 (m, 2H, C*H*$_{2COD}$), 0.3 (s, 27H, SiMe$_3$). ^{31}P NMR (243 MHz, C_6D_6, 293 K) δ = -7.7 (s, OC*P*).

B. NMR and IR spectroscopic data

Figure S1. ^{1}H NMR spectrum for UCl_3 **1** (C_6D_6, 293K, 400MHz).

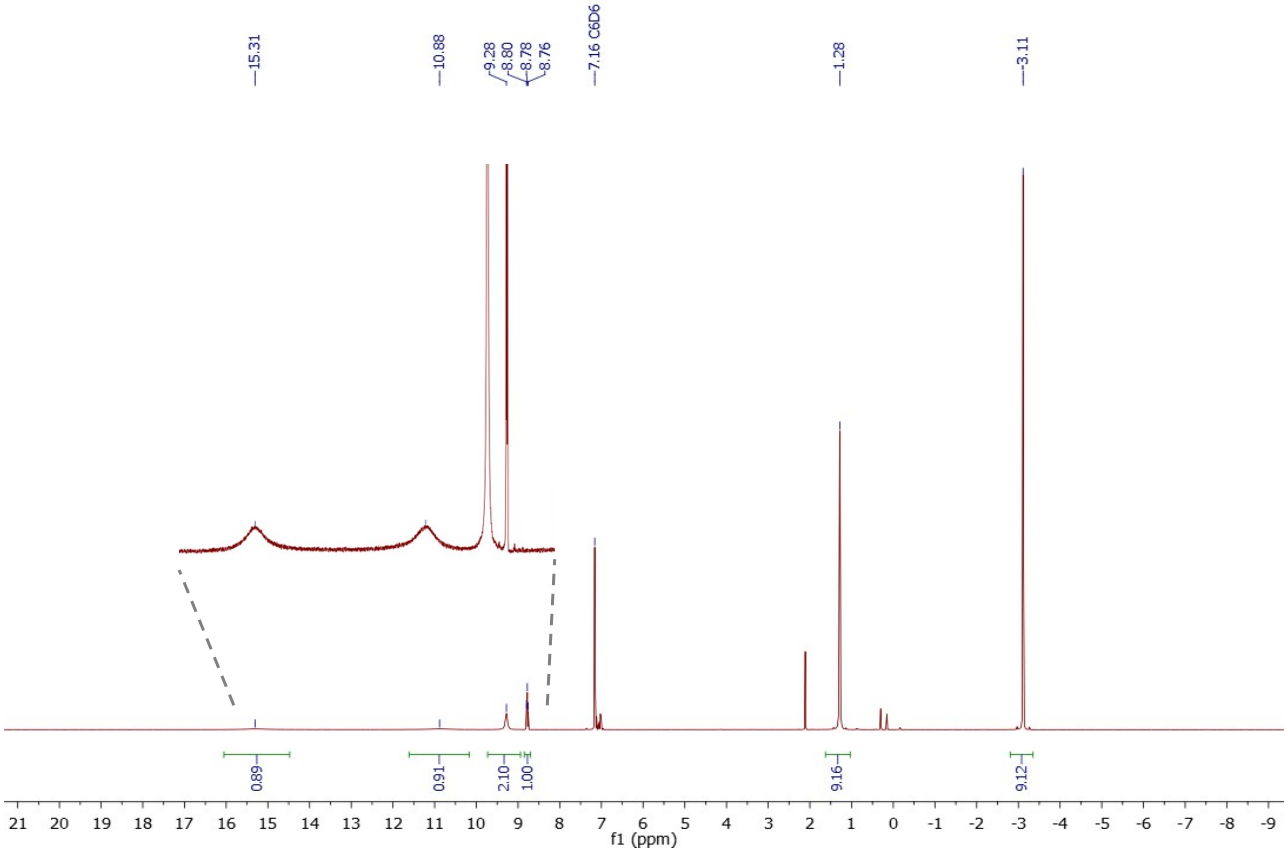


Figure S2. ^{1}H NMR spectrum for $ThCl_3$ **2** (C_6D_6, 293K, 400MHz).

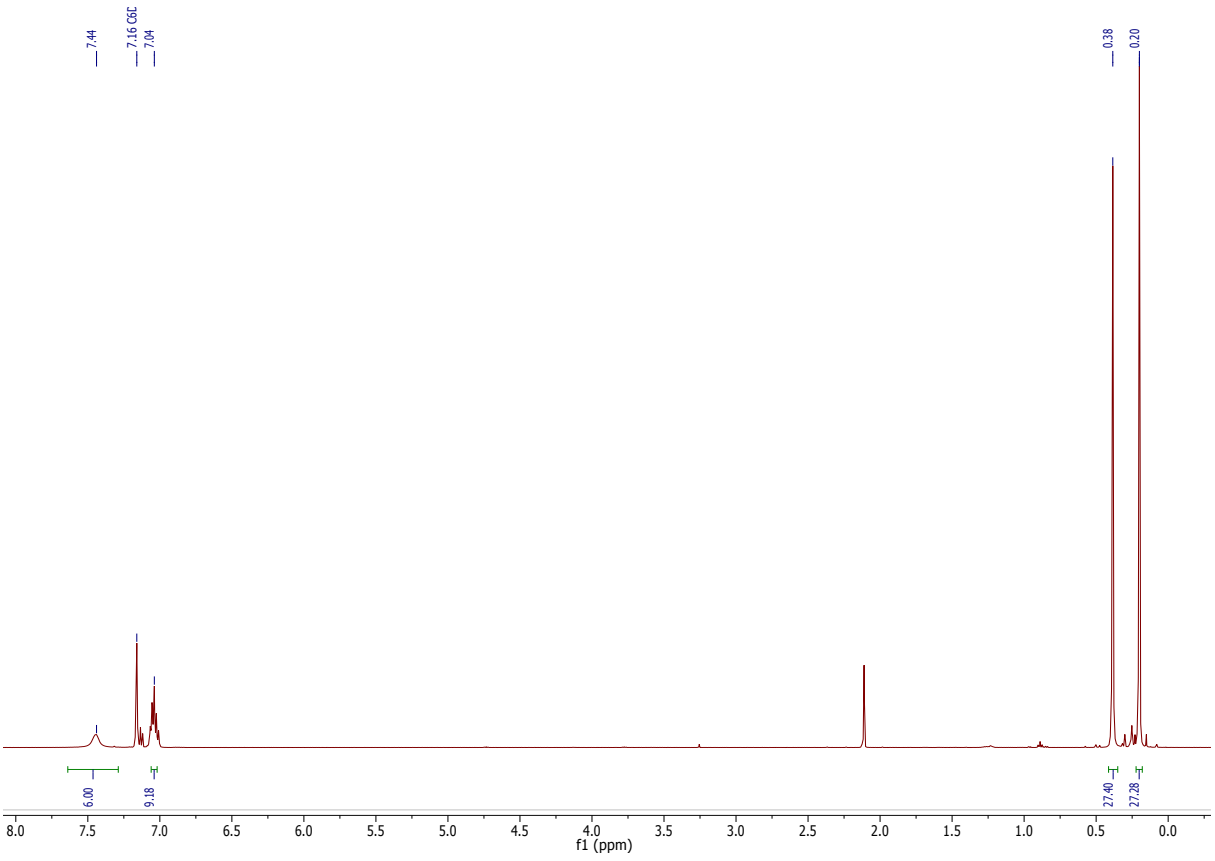


Figure S3. ^{1}H NMR spectrum for U(OCP)L_3 **3** (C_6D_6, 293K, 400MHz).

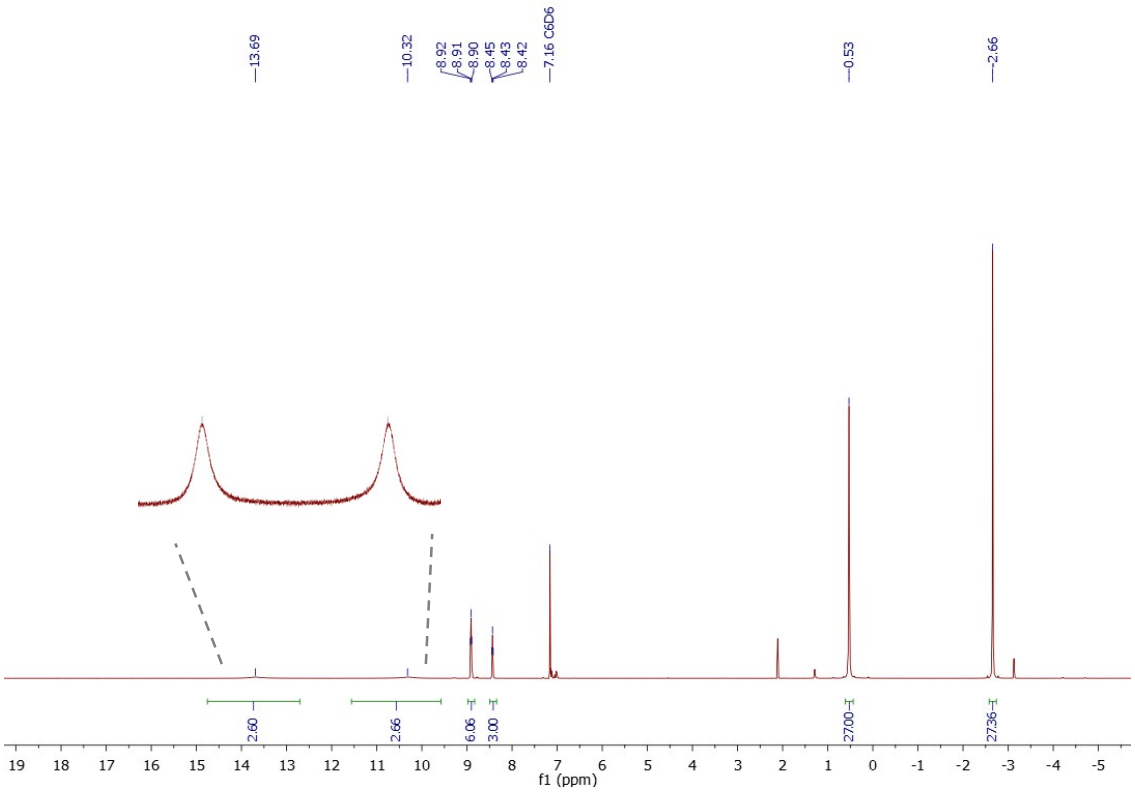


Figure S4. ^{1}H NMR spectrum for Th(OCP)L_3 **4** (C_6D_6, 293K, 400MHz).

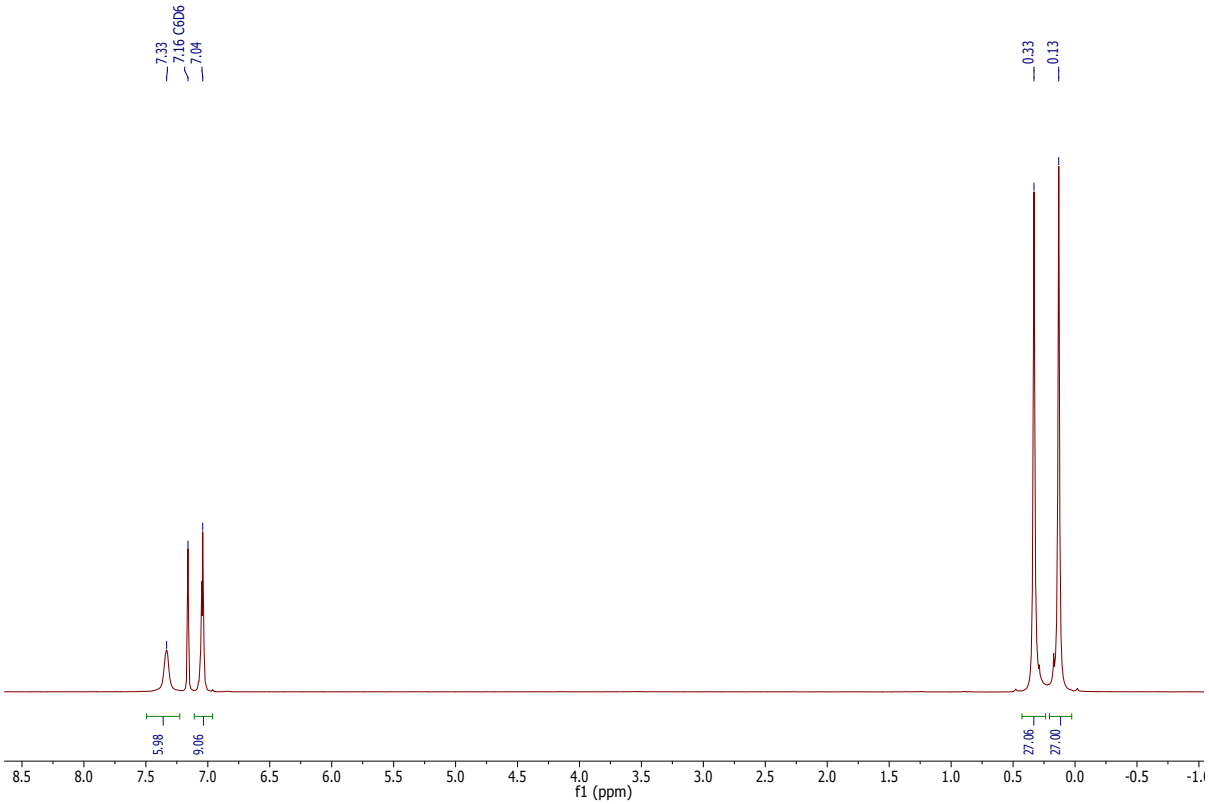


Figure S5. ^{31}P NMR spectrum for U(OCP)L_3 **3** (C_6D_6, 293K, 243MHz).

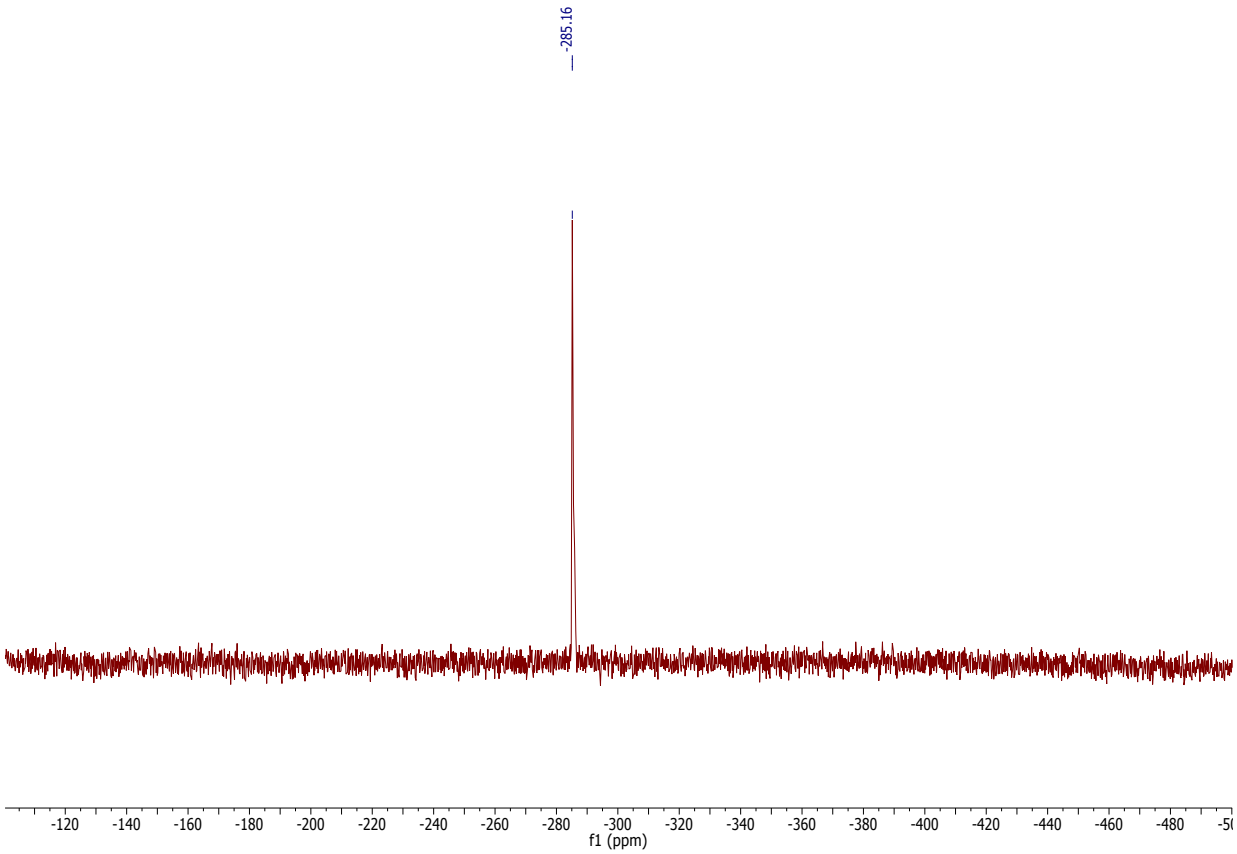


Figure S6. ^{31}P NMR spectrum for Th(OCP)L_3 **4** (C_6D_6, 293K, 243MHz).

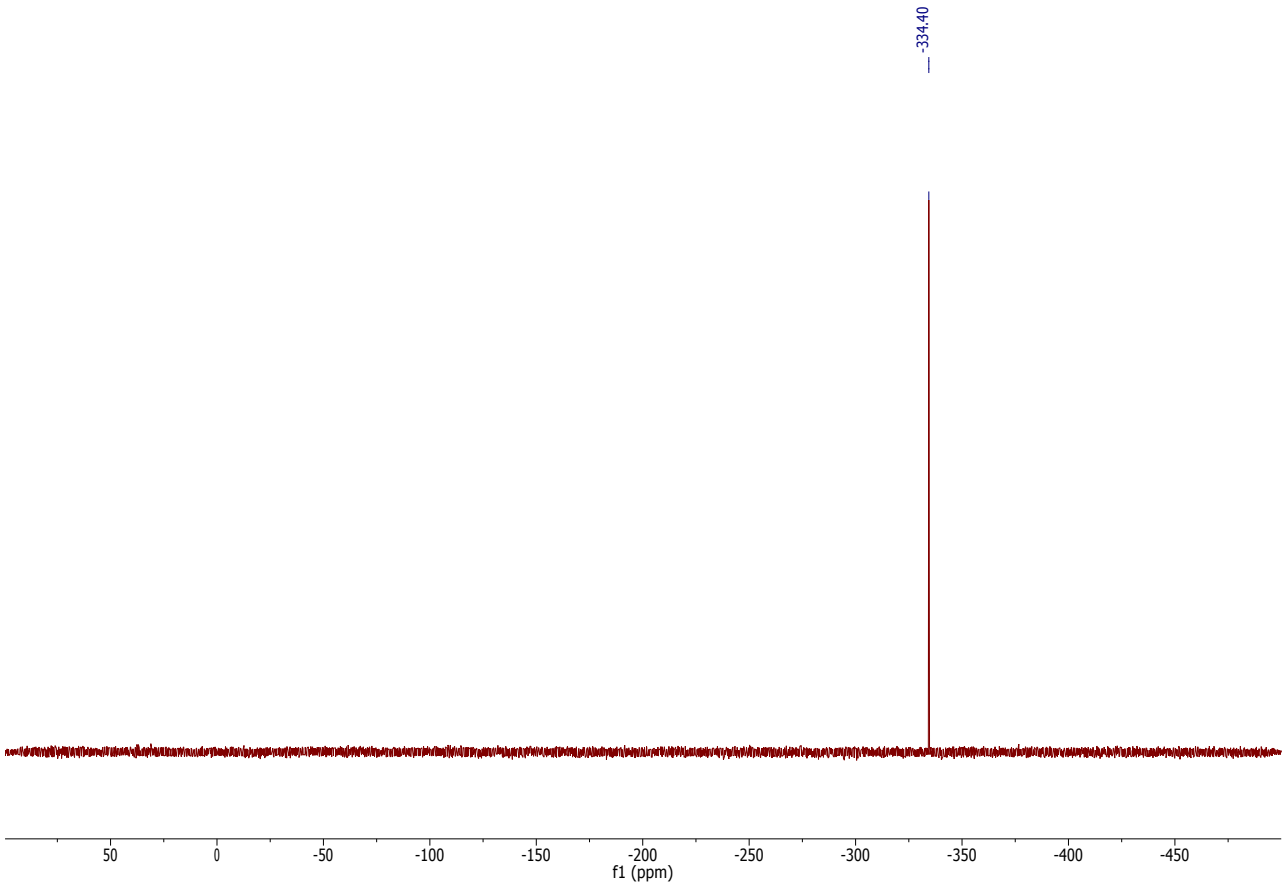


Figure S7. ^{1}H NMR spectrum for U(NCO)L_3 **5** (C_6D_6, 293K, 400MHz).

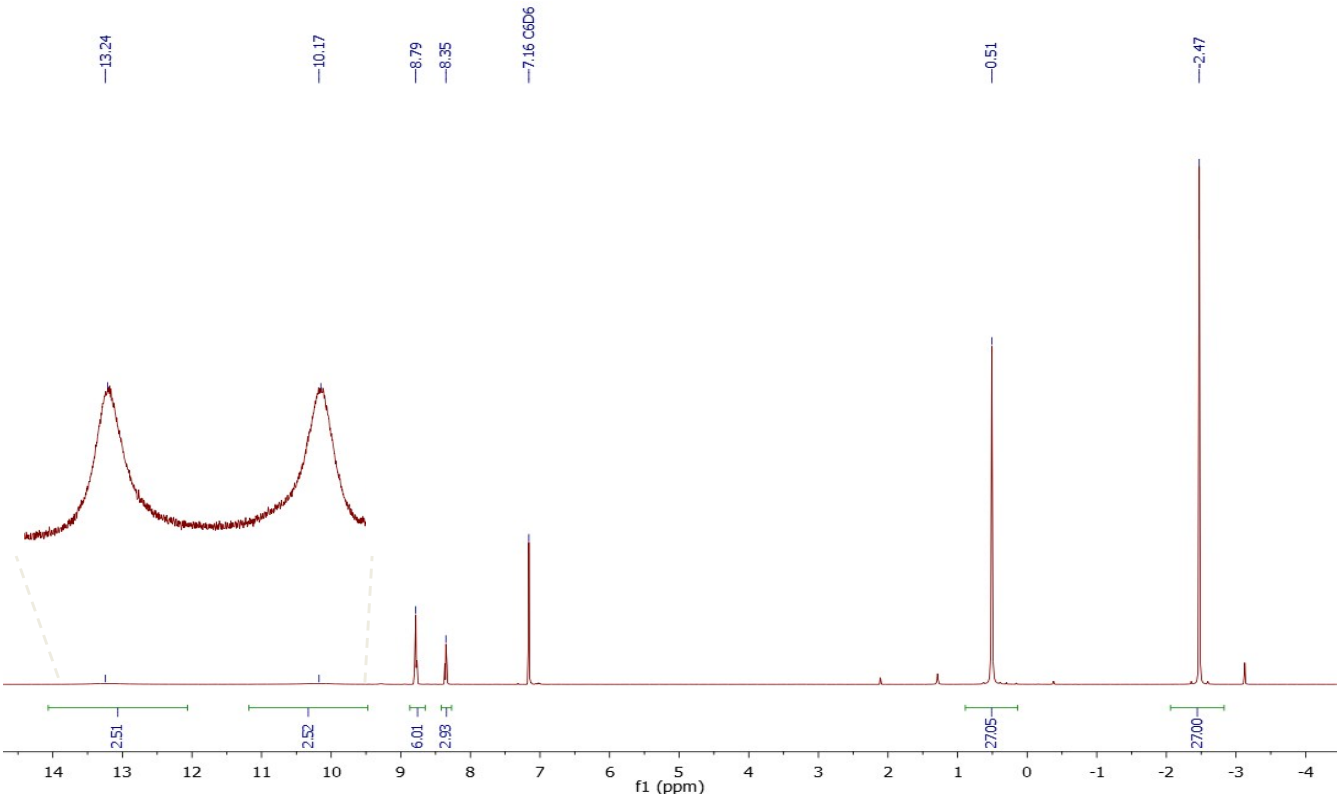


Figure S8. ^{1}H NMR spectrum for Th(NCO)L_3 **6** (C_6D_6, 293K, 400MHz).

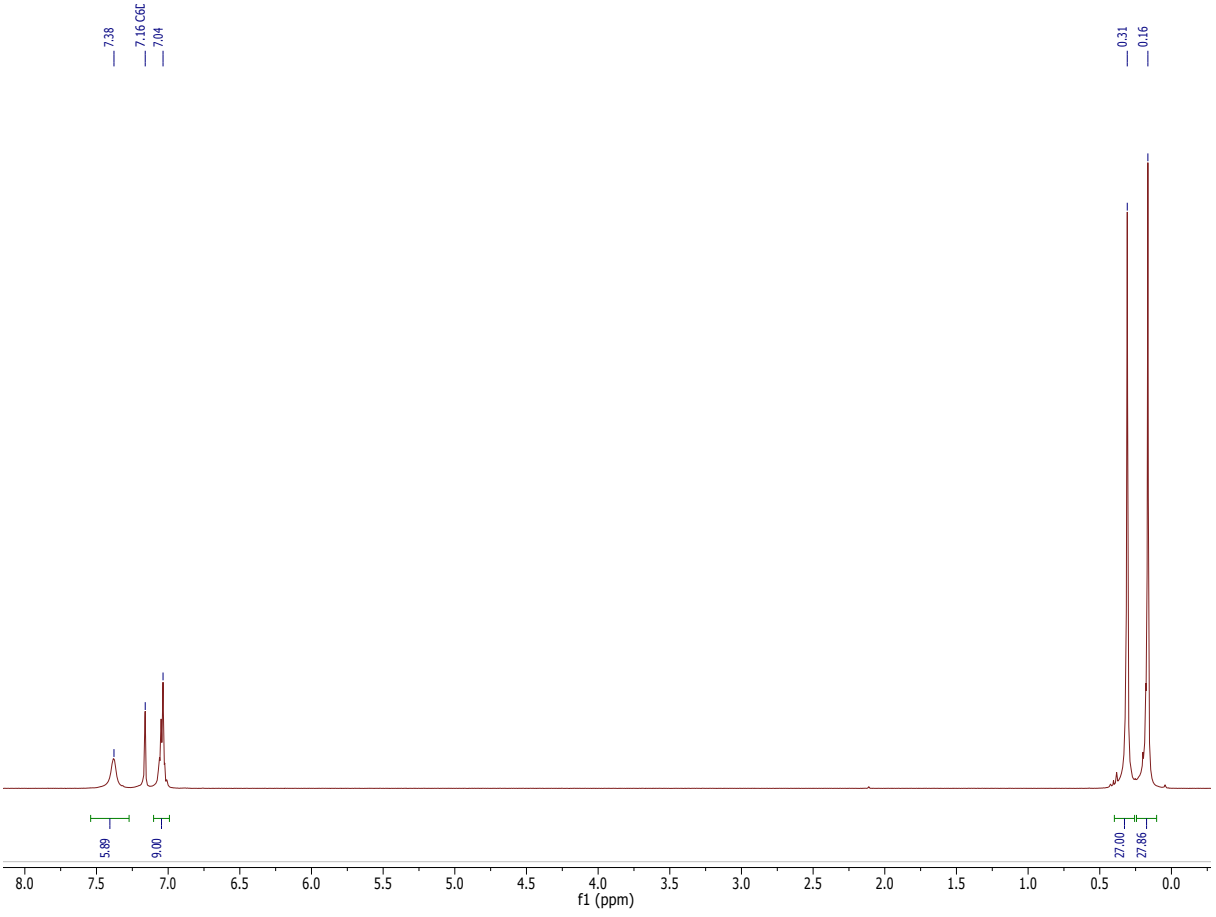


Figure S9. ^{1}H NMR spectrum for U(NCS)L_3 **7** (C_6D_6, 293K, 400MHz).

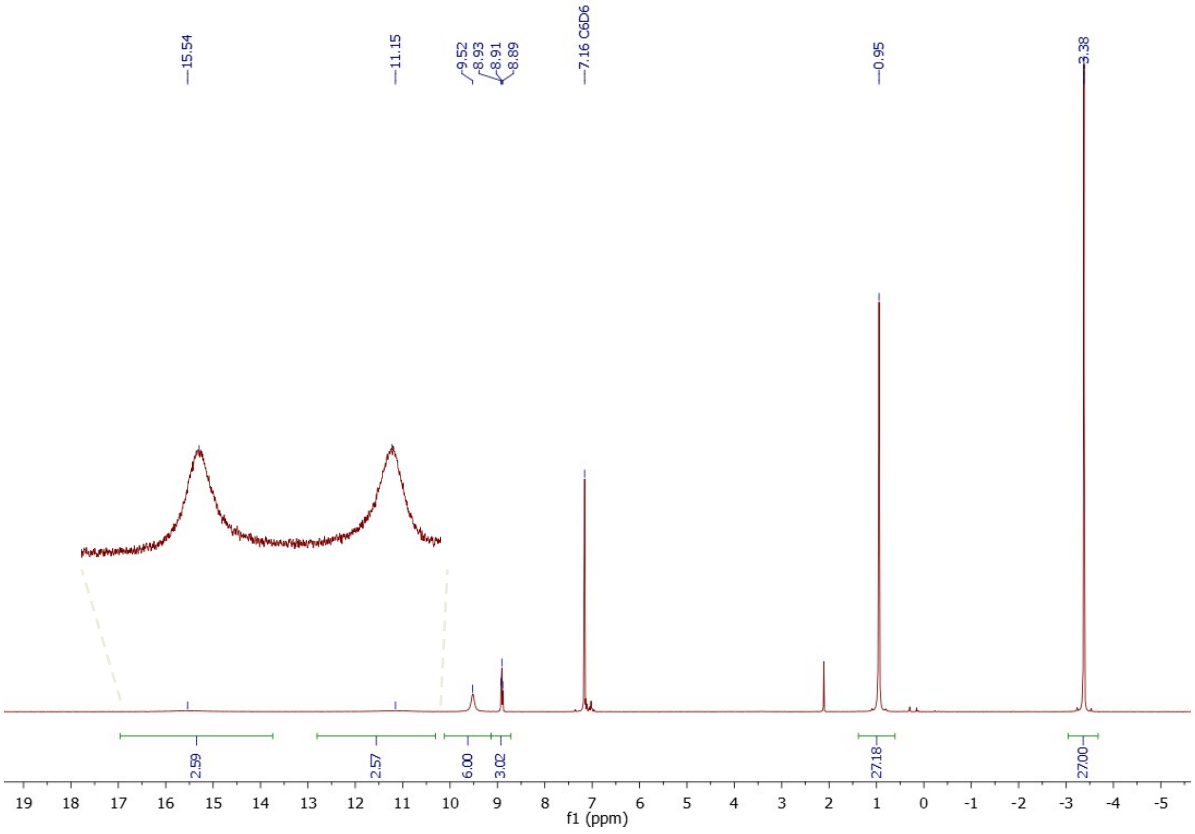


Figure S10. ^{1}H NMR spectrum for Th(NCS)L_3 **8** (C_6D_6, 293K, 400MHz).

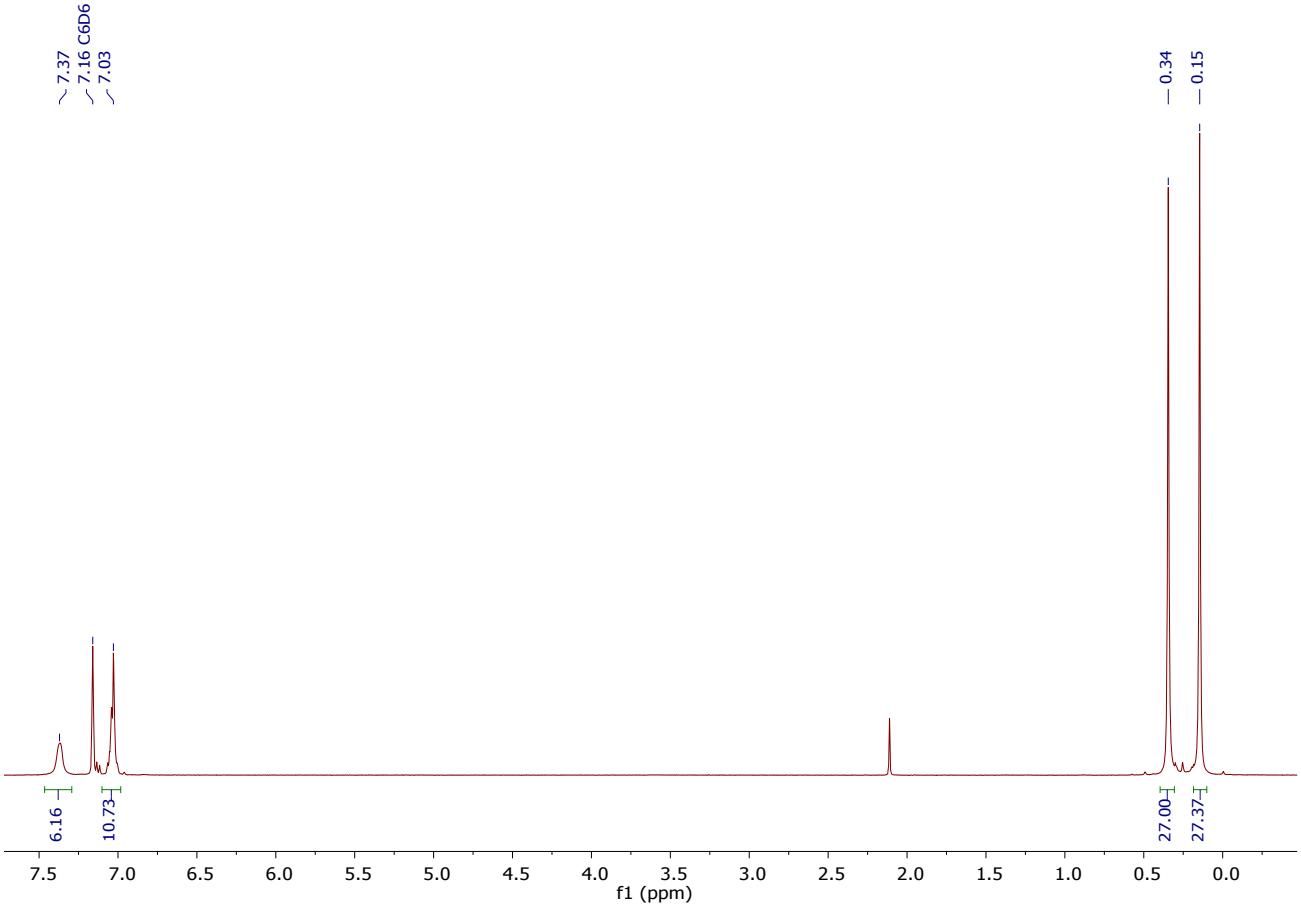


Figure S11. FT-IR spectra (nujol mull) for $UClL_3$ **1** (red), $U(OCP)L_3$ **3** (green), $U(NCO)L_3$ **5** (blue) and $U(NCS)L_3$ **7** (orange) ; L = amid.

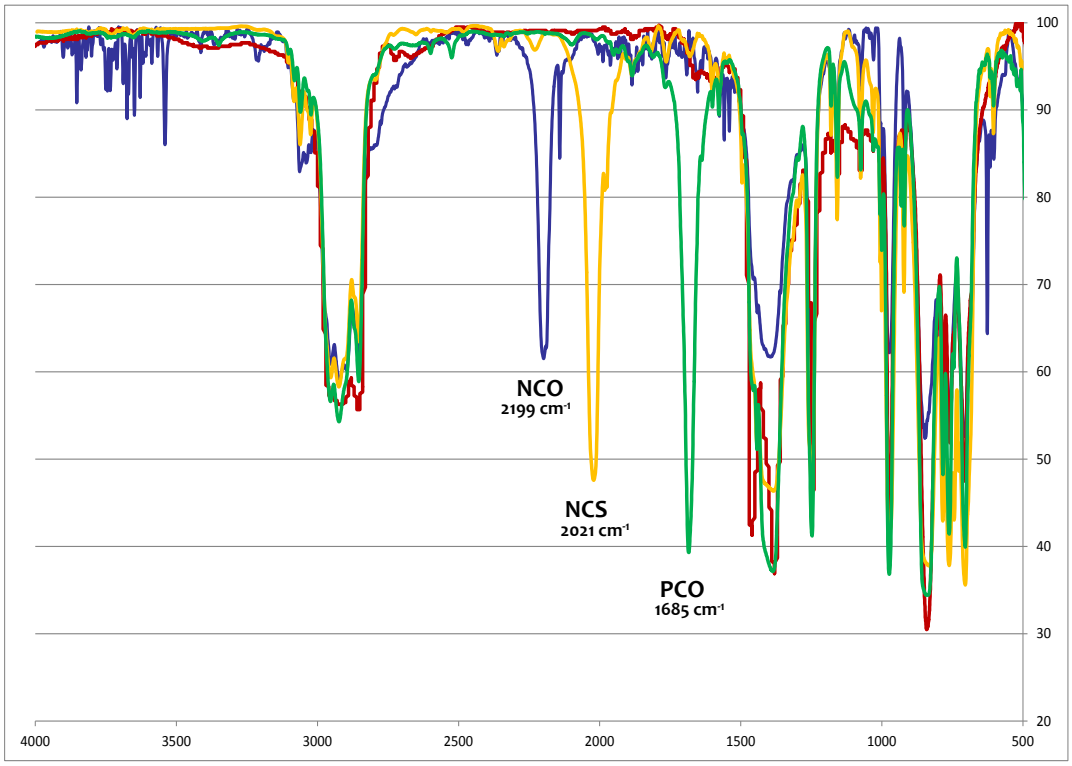


Figure S12. FT-IR spectra (nujol mull) for $ThClL_3$ **2** (red), $Th(OCP)L_3$ **4** (green), $Th(NCO)L_3$ **6** (blue) and $Th(NCS)L_3$ **8** (orange) ; L = amid.

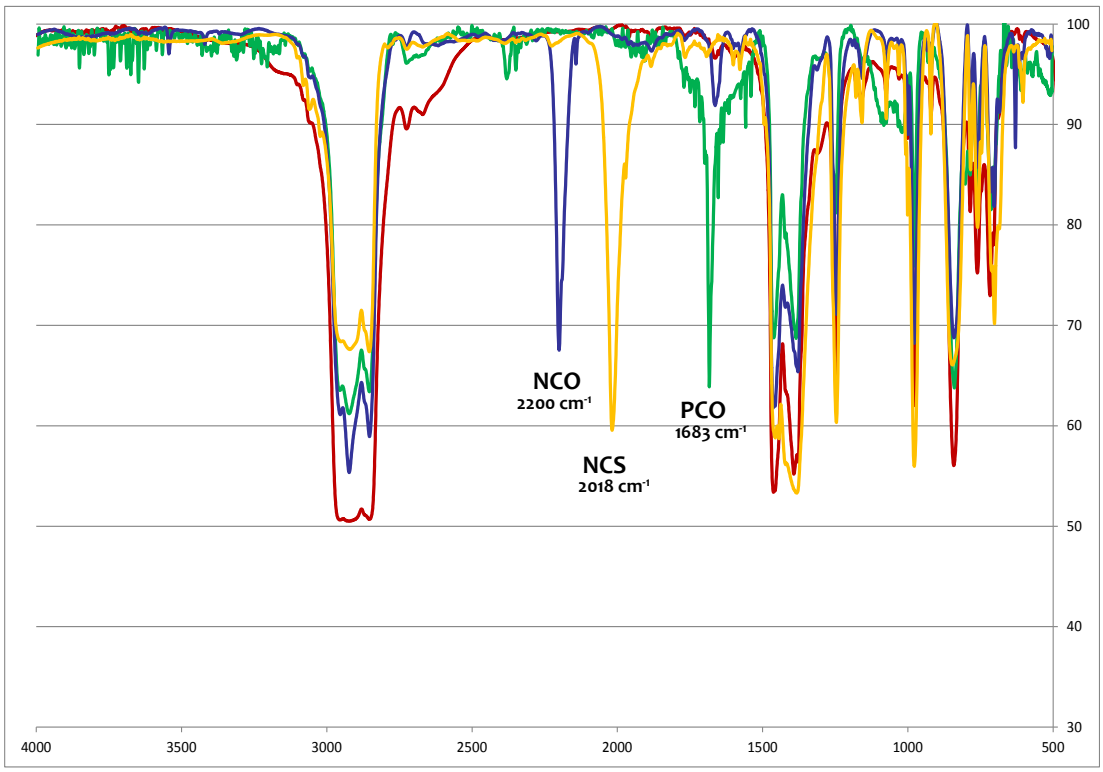


Table S.1 Infrared stretches for the anisotropic vibration of the heteroallene moiety in compounds **3**-**8**.

Compd	**3**	**4**	**5**	**6**	**7**	**8**
IR stretch (cm^{-1})	**1685**	**1683**	**2199**	**2200**	**2021**	**2018**

Figure S13. In-situ ^{1}H NMR spectrum for the reaction between **4** and $Ni(COD)_2$, recorded after 24h at r.t. (C_6D_6, 293K, 600MHz). The spectrum features the resonances for **9**, **4**, Ni(COD)2 and free COD. The relative ratio **9**:**4** does not evolve further when the reaction is kept at r.t.

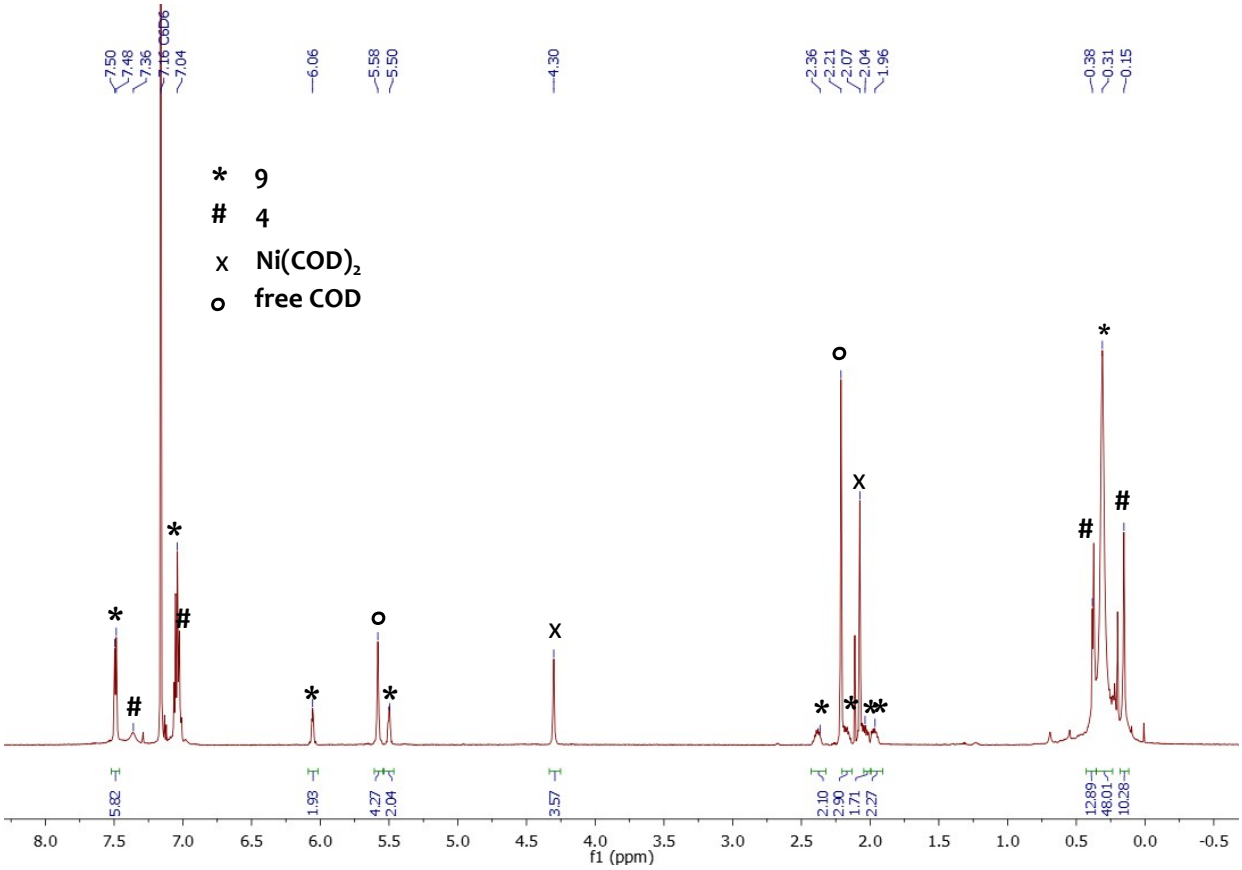


Figure S14. In-situ ^{31}P NMR spectrum for the reaction between **4** and $Ni(COD)_2$, recorded after 24h at r.t. (C_6D_6, 293K, 243MHz).

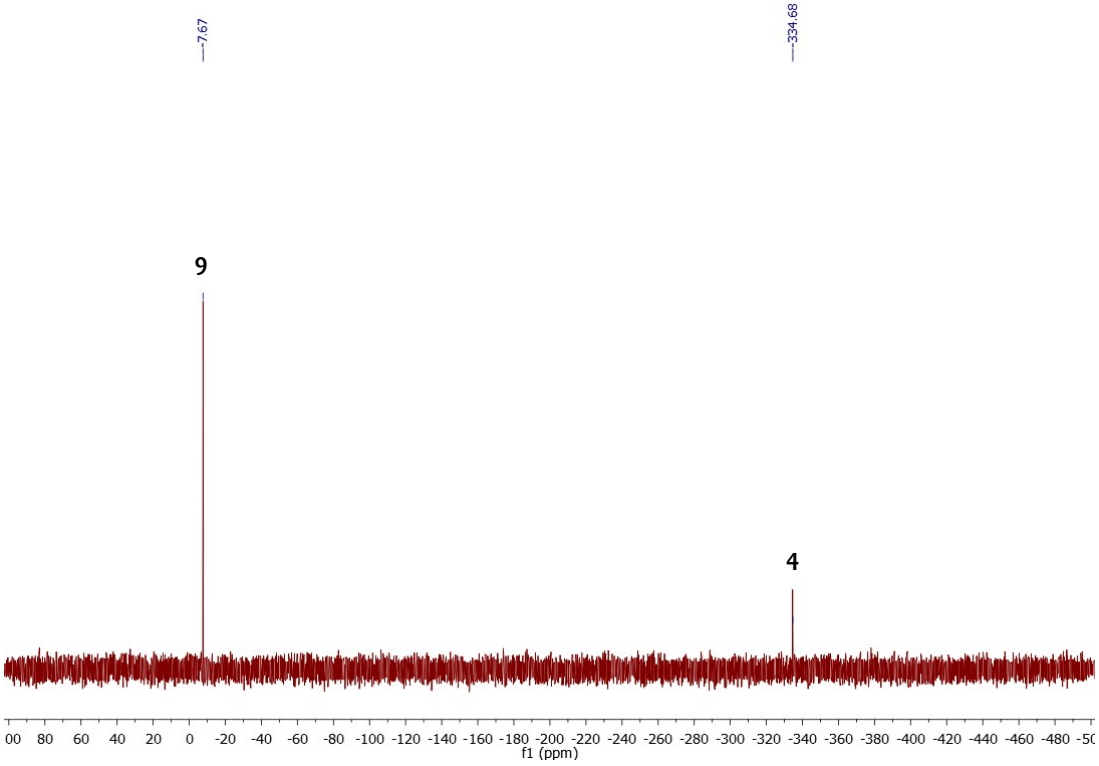


Figure S15. ^{1}H NMR spectrum for **9** (C_6D_6, 293K, 600MHz).

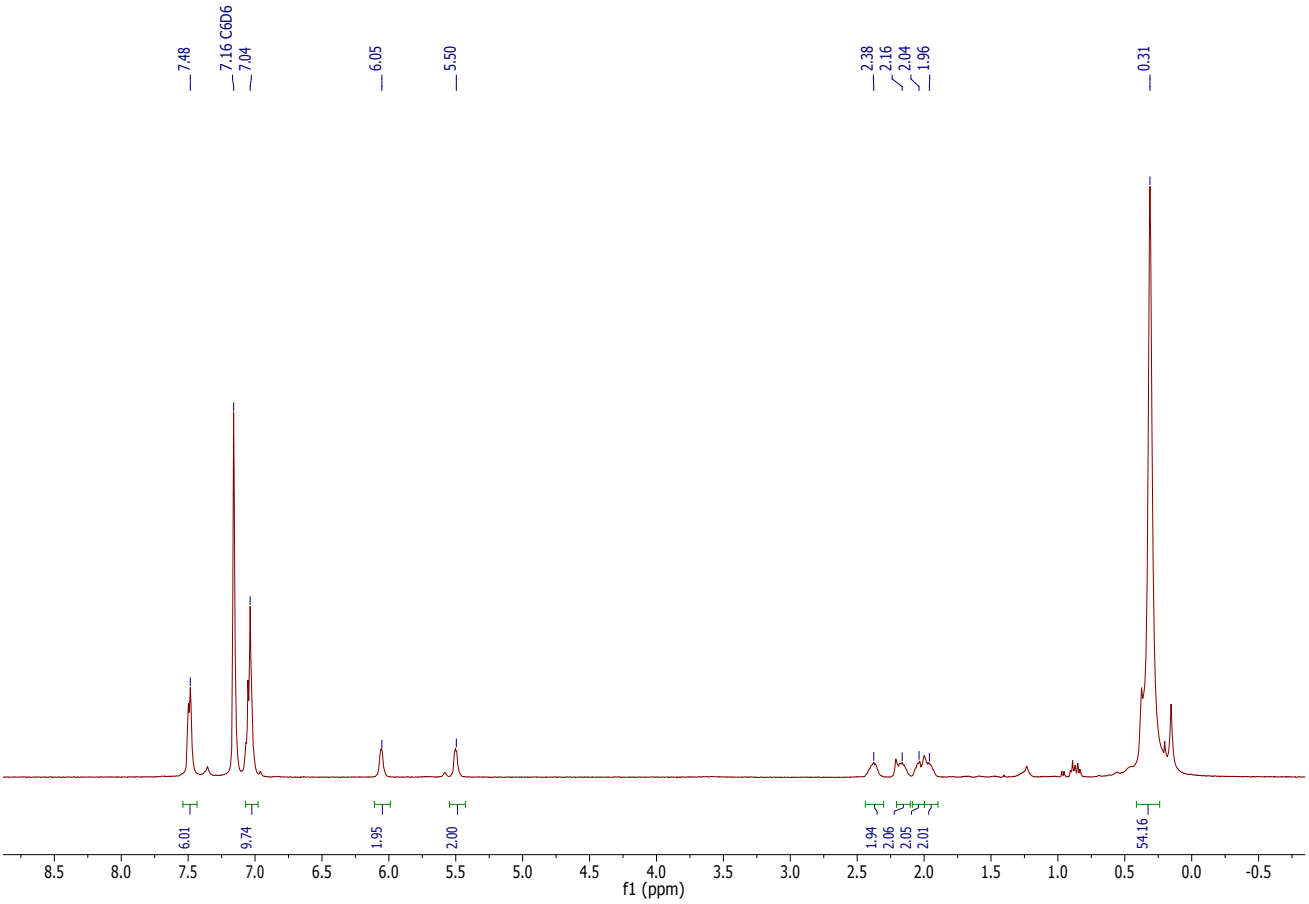


Figure S16. ^{1}H-^{1}H COSY NMR spectrum for **9** (C_6D_6, 293K, 600MHz).

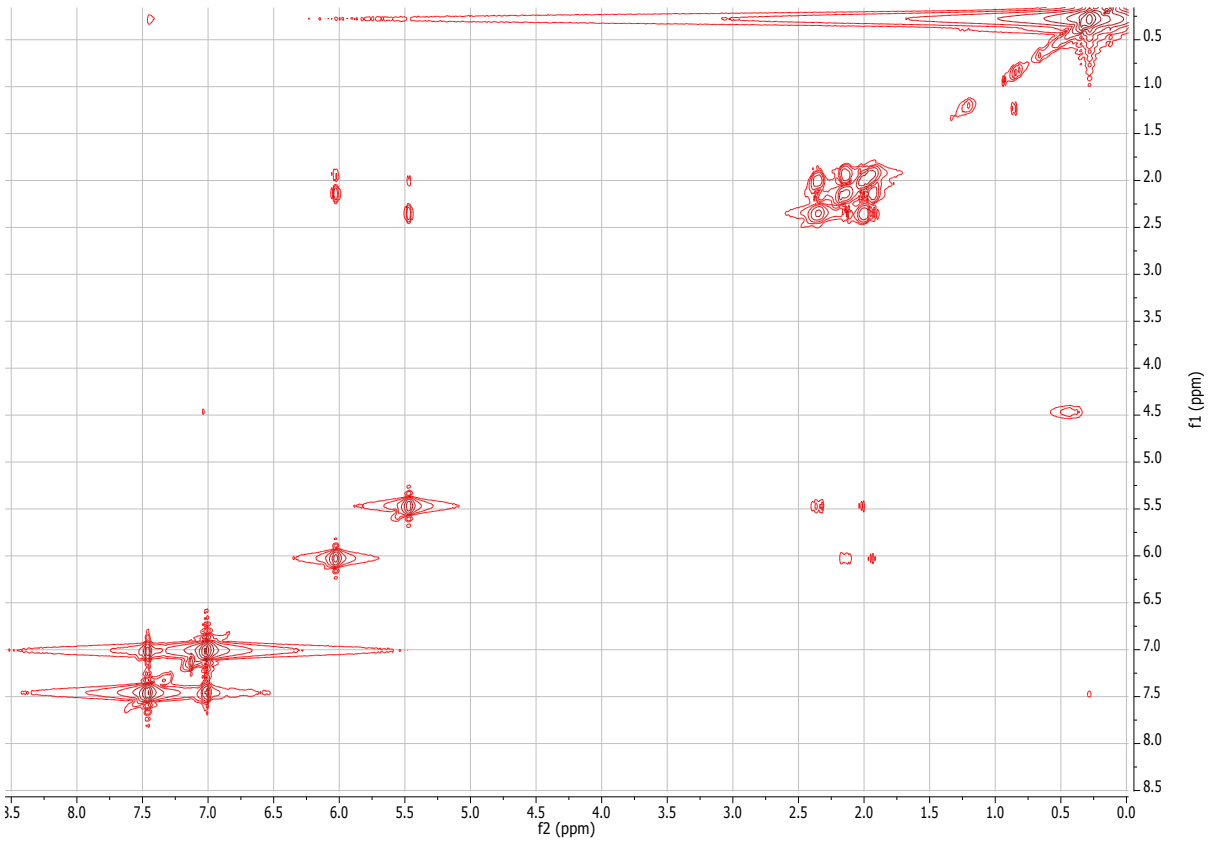


Figure S17. Evolution of the ^{31}P NMR spectrum for **9** (C_6D_6, 293 K, 600 MHz) over time showing that **9** is converted into **4**, releasing COD and $Ni(COD)_2$.

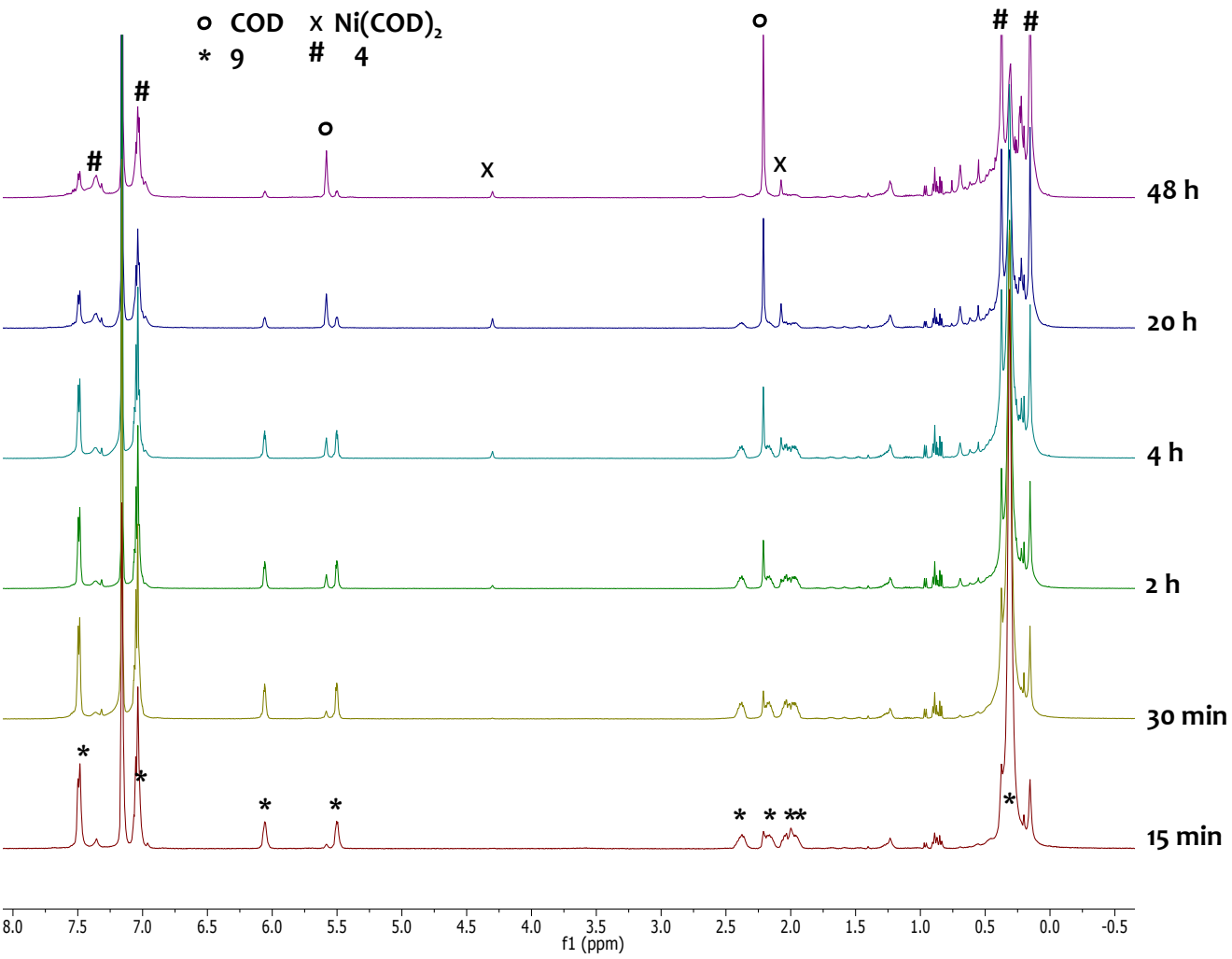
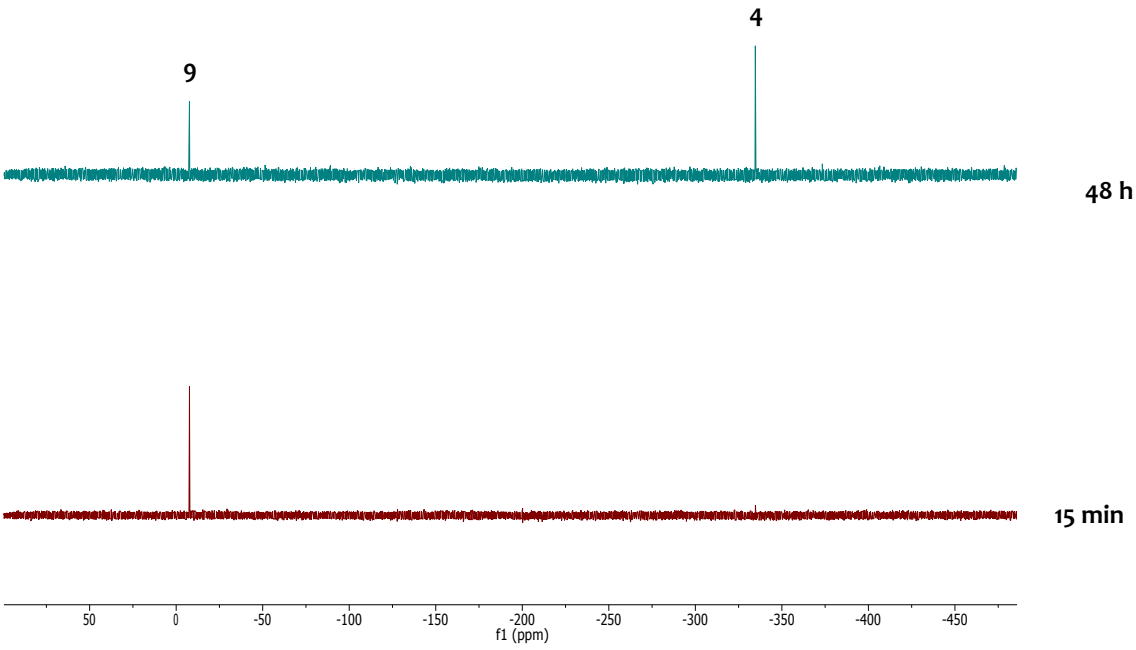


Figure S18. Evolution of the ^{31}P NMR spectrum for **9** (C_6D_6, 293 K, 243 MHz) over time.



C. X-ray crystallography

X-ray structural determinations were performed on a Bruker SMART QUAZAR diffractometer which is a 3-circle diffractometer that couple a CCD detector with a sealed-tube source of monochromated Mo Ka radiation (λ = 0.71073 Å). A crystal of appropriate size was coated in Paratone-N oil and mounted on a Kapton® loop. The loop was transferred to the diffractometer, centered in the beam, and cooled by a nitrogen flow low-temperature apparatus that had been previously calibrated by a thermocouple placed at the same position as the crystal. Preliminary orientation matrices and cell constants were determined by collection of 60 10 s frames, followed by spot integration and least-squares refinement. The reported cell dimensions were calculated from all reflections with $I > 10\ \sigma$. The data were corrected for Lorentz and polarization effects; no correction for crystal decay was applied. An empirical absorption correction based on comparison of redundant and equivalent reflections was applied using SADABS.[6] All software used for diffraction data processing and crystal-structure solution and refinement are contained in the APEX2 program suite (Bruker AXS, Madison, WI).[7] Thermal parameters for all non-hydrogen atoms were refined anisotropically. For all structures, $R_1 = \Sigma(||F_o| - |F_c||)/\Sigma(|F_o|)$; $wR_2 = [\Sigma\{w(F_o^2 - F_c^2)^2\}/\Sigma\{w(F_o^2)^2\}]^{1/2}$. Thermal ellipsoid plots were created using Mercury supplied with Cambridge Structural Database (CCDC: Cambridge, U.K., 2004-2009). In the case of **5** and **6**, both O- and N- coordination to the metal were proposed and refined. Improved ellipsoid e.s.d's values were found at the O and N positions for the An-N=C=O coordination mode compared to the An-O=C=N one, the latter featuring additional residual electron intensity located at close proximity of the misattributed N-atom. This is in agreement with N-coordination to the actinide metal in both cases. No evidence of any sort of disorder involving the An-NCO unit was found.

Table S.2 Experimental metrical parameters for complexes **3**-**9** determined by single-crystal X-ray diffraction.

Compound	**3**	**4**	**5**	**6**	**7**	**8**	**9**
An-X	2.297(3)	2.3118(2)	2.340(3)	2.410(2)	2.385(4)	2.428(4)	2.279(3)
X-C1	1.219(6)	1.246(4)	1.128(5)	1.146(3)	1.165(7)	1.169(6)	1.287(5)
C1-Y	1.576(5)	1.561(4)	1.211(5)	1.206(3)	1.609(5)	1.608(5)	1.660(4)
$An\text{-}N_{amidavg}$	2.44(3)	2.49(3)	2.44(2)	2.50(5)	2.43(3)	2.49(4)	2.51(5)
Ni1-C1	/	/	/	/	/	/	1.895(4)
Ni1-P1	/	/	/	/	/	/	2.1705(13)
An-X-C1	170.9(3)	176.4(3)	171.6(3)	177.1(2)	171.3(4)	169.6(4)	157.5(3)
X-C1-Y	179.1(4)	179.7(4)	179.2(5)	179.5(3)	179.3(5)	178.7(5)	148.1(3)

*Distances are in [Å] and angles in [°]. Complexes **4, 6** and **9** crystallized as two independent molecules in the asymmetric unit, therefore the discussion of metrical parameters for these compounds is performed on the Th1 molecule only.*

Table S.3 Calculated metrical parameters for complexes **3**-**8** determined by DFT.

Compound	**3**	**4**	**5**	**6**	**7**	**8**
An-X	2.30	2.32	2.32	2.34	2.38	2.41
X-C1	1.24	1.24	1.20	1.27	1.19	1.19
C1-Y	1.60	1.60	1.18	1.18	1.63	1.63
An-X-C1	177.55	179.21	179.09	178.12	179.62	179.01
X-C1-Y	179.44	179.85	179.82	179.97	179.91	179.90

Distances are in [Å] and angles in [°].

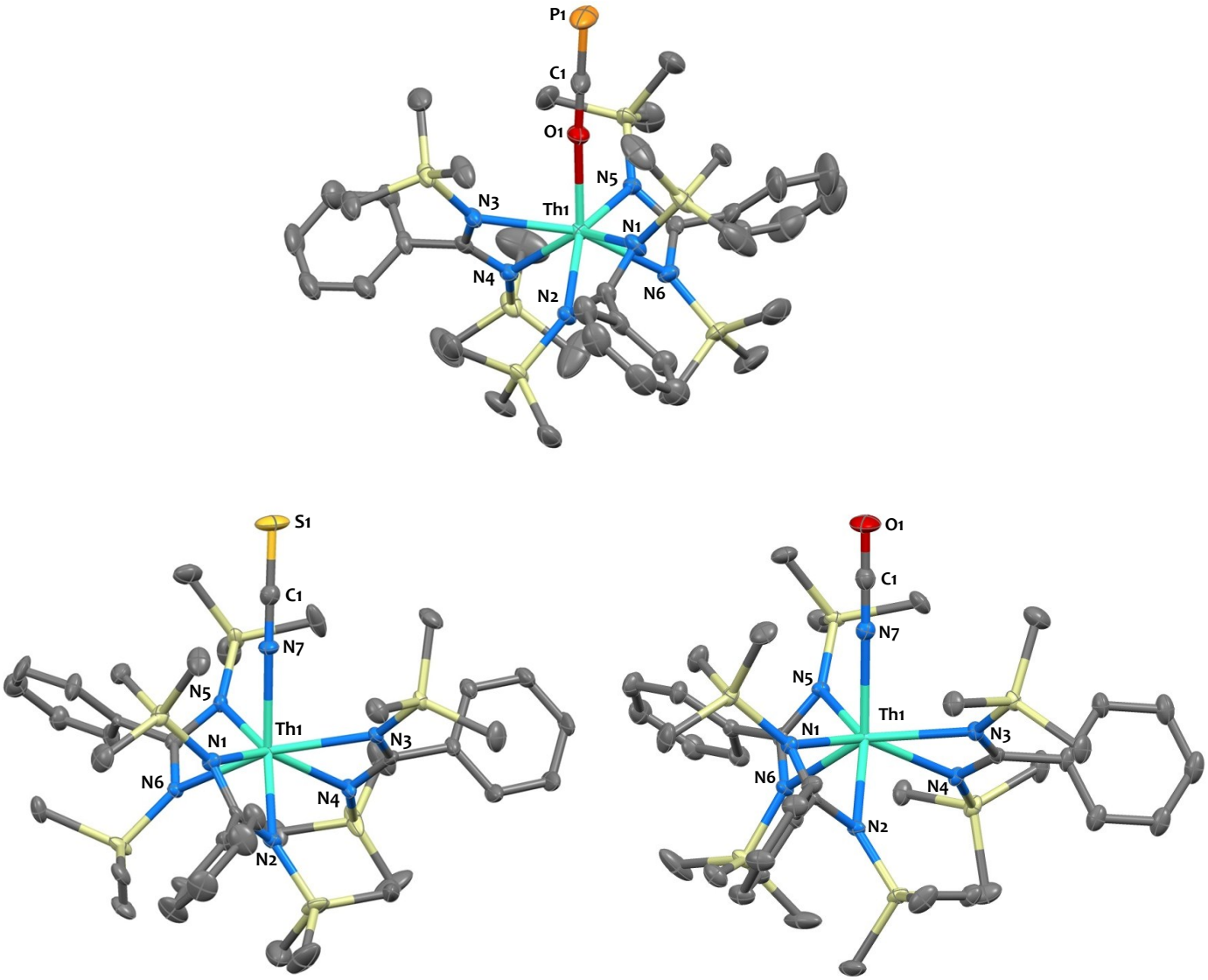


Figure S19. Solid-state molecular structures of compounds **4** (top), **6** (bottom-left) and **8** (bottom-right) determined by single-crystal X-ray diffraction. Ellipsoids are represented with 50% probability.

Table S.4 Crystallographic parameters for complexes **3** to **6**.

Compound	**3.(toluene)$_{0.5}$**	**4**	**5**	**6.(toluene)$_{0.5}$**
Formula	$C_{43.5}H_{73}N_6OPSi_6U$	$C_{40}H_{69}N_6OPSi_6Th$	$C_{43.5}H_{73}N_6OPSi_6U$	$C_{43.5}H_{73}N_6OPSi_6Th$
cryst syst	Triclinic	Triclinic	Monoclinic	Triclinic
space group	P-1	P-1	C2/c	P-1
volume (Å^3)	2750.1(5)	5882.7(8)	10388.9(8)	5419.7(16)
a (Å)	11.5703(12)	11.4301(9)	15.5201(7)	11.2966(19)
b (Å)	11.7055(13)	21.3302(16)	17.9868(8)	23.057(4)
c (Å)	21.152(2)	24.614(2)	37.3806(17)	23.270(4)
α (deg)	86.747(5)	99.881(4)	90	66.405(6)
β (deg)	83.810(5)	90.073(4)	97.783(2)	87.390(6)
γ (deg)	75.030(5)	95.606(4)	90	77.614(6)
Z	2	4	4	4
formula weight (g/mol)	1133.61	1081.56	2141.18	1110.66
density (g cm^{-3})	1.369	1.221	1.376	1.361
absorption coefficient (mm^{-1})	3.146	2.715	3.314	2.921
F(000)	1150	2192	4336	2260
temp (K)	100(2)	100(2)	100(2)	100(2)
total no. reflections	67609	89182	90811	86355
unique reflections [R(int)]	10048 [0.033]	21550 [0.036]	9521 [0.034]	19891 [0.033]
Final R indices [I > 2σ(I)]	R1 = 0.0279, wR2 = 0.0702	R1 = 0.0282, wR2 = 0.0683	R1 = 0.0285, wR2 = 0.0545	R1 = 0.0195, wR2 = 0.0482
Largest diff. peak and hole (e.A^{-3})	0.865 and -2.201	3.278 and -0.874	1.204 and -1.664	2.311 and -0.454
GoF	1.371	0.975	1.319	1.019

Table S.5 Crystallographic parameters for complexes **7** to **9**.

Compound	**7.(toluene)$_{0.5}$**	**8.(toluene)$_{0.5}$**	**9.(hexane)$_{0.75}$**
Formula	$C_{43.5}H_{73}N_7SSi_6U$	$C_{43.5}H_{73}N_7SSi_6Th$	$C_{52.5}H_{91.5}N_6NiOPSi_6Th$
cryst syst	Triclinic	Triclinic	Triclinic
space group	P-1	P-1	P-1
volume (Å^3)	2733.3(3)	2759.5(2)	6587.8 (8)
a (Å)	11.5810(7)	11.6047(6)	14.8598(10)
b (Å)	11.6278(7)	11.6602(6)	19.6824(13)
c (Å)	21.1150(13)	21.2040(11)	24.2681(17)
α (deg)	86.775(2)	86.479(2)	105.8698(27)
β (deg)	83.982(2)	83.836(2)	101.3208(26)
γ (deg)	75.259(3)	75.464(2)	96.5472(27)
Z	2	2	4
formula weight (g/mol)	1132.71	1126.72	1313.07
density (g cm^{-3})	1.376	1.356	1.324
absorption coefficient (mm^{-1})	3.174	2.905	2.711
F(000)	1150	1146	2694
temp (K)	100(2)	100(2)	100(2)
total no. reflections	45826	50449	171492
unique reflections [R(int)]	9978 [0.024]	10054 [0.028]	23909 [0.031]
Final R indices [I > 2σ(I)]	R1 = 0.0294, wR2 = 0.0796	R1 = 0.0278, wR2 = 0.0781	R1 = 0.0333, wR2 = 0.0857
Largest diff. peak and hole (e.A^{-3})	1.005 and -2.243	1.059 and -2.196	3.024 and -3.064
GoF	1.383	1.417	1.034

D. DFT calculations

Computational details

Calculations were carried out at the DFT level using the hybrid functional B3PW91[8,9] with the Gaussian 03[10] suite of programs. Polarized all-electron triple-ζ 6-31G(d,p)[11] basis sets were used for C, H and N. Thorium, Uranium, Phosphorus and silicon atoms were treated with an effective core potential from the Stuttgart-Dresden-Köln group in association with its adapted basis set.[12] Geometry optimizations were carried out without any symmetry restriction. The nature of the extrema (minimum) was verified with analytical frequency calculations. NBO analysis[13] was also carried out in order to analyze the bonding.

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NBO Analysis of the O-bound Th(OCP)(amid)$_3$ complex **4** vs the P-bound isomer:

O – bound Th(OCP)(amid)$_3$

162. CR (1) O 25	/193. LP*(3)Th 1	12.11	19.23	0.455
227. LP (1) O 25	/193. LP*(3)Th 1	57.28	1.04	0.223
227. LP (1) O 25	/194. LP*(4)Th 1	18.51	0.91	0.118
227. LP (1) O 25	/194. LP*(4)Th 1	18.51	0.91	0.118

P – bound Th(OCP)(amid)$_3$

230. LP (1) P 27	/193. LP*(3)Th 1	0.18	0.71	0.011
230. LP (1) P 27	/194. LP*(4)Th 1	0.43	0.58	0.015
230. LP (1) P 27	/197. LP*(7)Th 1	0.09	0.61	0.007

230. LP (1) P 27 /200. LP*(10)Th 1 0.89 0.65 0.022

230. LP (1) P 27 /203. LP*(13)Th 1 3.63 0.60 0.042

E. References

[1] J. L. Kiplinger, D. E. Morris, B. L. Scott, C. J. Burns, *Organometallics* **2002**, *21*, 5978–5982.

[2] T. Cantat, B. L. Scott, J. L. Kiplinger, *Chem. Commun.* **2010**, *46*, 919–921.

[3] V. Volkis, E. Nelkenbaum, A. Lisovskii, G. Hasson, R. Semiat, M. Kapon, M. Botoshansky, Y. Eishen, M. S. Eisen, *J. Am. Chem. Soc.* **2003**, *125*, 2179–94.

[4] F. F. Puschmann, D. Stein, D. Heift, C. Hendriksen, Z. a Gal, H.-F. Grützmacher, H. Grützmacher, *Angew. Chem. Int. Ed. Engl.* **2011**, *50*, 8420–8423.

[5] M. Wedler, F. Knösel, M. Noltemeyer, F. T. Edelmann, U. Behrens, *J. Organomet. Chem.* **1990**, *388*, 21–45.

[6] SADABS: Bruker-Nonius Area Detector Scaling and Absorption, **2003**.

[7] G. M. Sheldrick, *Acta Crystallogr. Sect. A* **2008**, *64*, 112–122.

[8] Becke, A. D. Density-functional thermochemistry. III. The role of exact exchange. *J. Chem. Phys.* **1993**, *98*, 5648-5652.

[9] Perdew, J. P. & Wang, Y. Erratum: Pair-distribution function and its coupling-constant average for the spin-polarized electron gas [*Phys. Rev. B* **1992**, *46*, 12 947]. *Phys. Rev. B* **1997**, *56*, 7018-7018.

[10] Gaussian 03 (Pittsburgh PA **2006**).

[11] Hehre, W. J.; Ditchfield, R.; Pople, J. A. *J. Chem. Phys.* **1972**, *56*, 2257.

[12] (a) Kuechle, W.; Dolg, M.; Stoll, H.; Preuss,H. *J. Chem. Phys.* **1994**, *100*, 7535. (b) Cao, X.; Dolg, M.; Stoll, H. *J. Chem. Phys.* **2003**, *118*, 487. (c) Cao, X.; Dolg, M. *J. Molec. Struct.* (Theochem) **2004**, *673*, 203. (d) Bergner, A.; Dolg, M.; Kuechle, W.; Stoll, H.; Preuss, H. *Mol. Phys.* **1993**, 80, 1431.

[13] Reed, A. E., Curtiss, L. A. & Weinhold, F. Intermolecular interactions from a natural bond orbital, donor-acceptor viewpoint. *Chem. Rev.* **1988**, *88*, 899-926.