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Supporting information for the manuscript

Two-electron Versus One-electron Reduction of Chalcogens by Uranium(III): Synthesis of a Terminal U(V) Persulphide Complex.

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A) Experimental procedures

General Experimental Procedures

All manipulations were carried out at ambient temperature under an inert argon atmosphere using Schlenk techniques and an MBraun glovebox equipped with a purifier unit. The water and oxygen level were always kept at less than 0.1 ppm. Glassware was systematically dried in oven overnight at 130°C followed by 3 vacuum/argon cycles before use. Syntheses were performed using glass-covered stirring bars. Unless otherwise noted, reagents were purchased from commercial suppliers and used without further purification. The solvents were purchased from Aldrich in their anhydrous form, conditioned under argon and vacuum distilled from K/benzophenone (toluene and THF) or sodium dispersion (hexane) and degassed by three freeze-pump-thaw cycles. The deuterated solvents were purchased from Eurisotop and prepared identically. All reagents were dried under high-vacuum (10^{-7} mBar) for 5 days prior to use. Dry dioxygen was prepared upon storing an O_2 atmosphere upon P_4O_{10} for one week prior to use. Depleted uranium turnings were purchased from the "Société Industrielle du Combustible Nucléaire" of Annecy (France). [U{($SiMe_2NPh)_3$-tacn}], **1** was prepared according to the published procedure.[1]

Elemental analyses were performed under argon by Analytische Laboratorien GMBH at Lindlar, Germany.

^{1}H NMR experiments were carried out using NMR tubes adapted with J. Young valves. ^{1}H NMR spectra were recorded on a Bruker 200 MHz spectrometer, at various temperatures. NMR chemical shifts are reported in ppm with solvent as internal reference.

Magnetic susceptibility measurements. Temperature-dependent magnetic susceptibility curves were measured in the temperature range 2 K to 300 K using a Quantum Design SQUID MPMS-XL 5.0 Superconducting Quantum Interference Devices (SQUID). The sample was prepared in the glovebox (37.8 mg), by pressing powder sample into a 5 mm Suprasil-Quartz tube. The tube was sealed, and transferred in the SQUID machine. The contribution to the signal from the empty sample holder was measured independently and subtracted from the total signal. The resulting data were corrected for the diamagnetic contribution using tabulated Pascal's constants[2] (χdia = -4.37×10^{-4} $cm^3 \cdot mol^{-1}$ for **2**).

Caution: *Depleted uranium (primary isotope ^{238}U) is a weak α-emitter (4.197 MeV) with a half-life of 4.47×10^9 years. Manipulations and reactions should be carried out in monitored fume hoods or in an inert atmosphere glovebox in a radiation laboratory equipped with α- and β-counting equipment.*

Syntheses

Synthesis of [{U(($SiMe_2NPh)_3$-tacn)}$_2$(μ-S)] (2)

A 0.5 mL toluene solution of [U{($SiMe_2NPh)_3$-tacn}], **1** (30.0 mg, 0.037 mmol, 1 eq.) was added onto a 0.5 mL toluene solution of S_8 (0.6 mg, 0.018 mmol, 0.0625 eq.). The mixture was stirred for 6 hours affording a yellow suspension. The solid was recovered by centrifugation, washed with 1 mL toluene and dried *in vacuo* to give [{U(($SiMe_2NPh)_3$-tacn)}$_2$(μ-S)], **2** as a yellow solid. Yield: 71 % (21.8 mg, 0.0132 mmol). Yellow crystals of **2** suitable for X-ray diffraction studies were obtained by slow diffusion of pentane to a solution of **2** in THF.

^{1}H NMR (200 MHz, toluene-d_8, 298 K): δ = 42.69 (s, 6H, $SiMe_2$), 28.25 (s, 4H), 20.11 (s, 4H), 13.89 (s, 2H), 9.00 (s, 6H, $SiMe_2$), 6.13 (s, 2H), -5.55 (s, 2H), -8.24 (s, 1H, H_p), -11.63 (s, 2H), -18.60 (s, 6H, $SiMe_2$), -46.19 (s, 2H), -54.00 (s, 2H), -65.47 (s, 2H), -67.45 (s, 2H), -107.50 (s, 2H). Anal. Calcd. for $C_{60}H_{90}N_{12}SSi_6U_2$: C, 43.52; H, 5.48; N, 10.15; S, 1.94. Found: C, 43.24; H, 5.47; N, 10.09; S, 1.83.

Reaction of 1 with PPh_3S

At room temperature, a toluene solution (0.5 mL) of Ph_3P=S (2.3 mg, 0.008 mmol, 0.5 eq.) was slowly added to a solution of compound **1** (12.9 mg, 0.016 mmol, 1.0 eq.) in toluene (1 mL). After 4 h stirring, a yellow suspension is obtained. The ^{1}H NMR spectrum (200 MHz, toluene-d_8, 298 K) recorded for the crude reaction mixture shows the clean formation of **2** from **1**.

Synthesis of [{U(($SiMe_2NPh)_3$-tacn)}$_2$(μ-Se)] (3)

A 2 mL toluene solution of [U{($SiMe_2NPh)_3$-tacn}], **1** (30.0 mg, 0.037 mmol, 1 eq.) was added onto a 4 mL toluene suspension of selenium powder (1.5 mg, 0.018 mmol, 0.5 eq.). The mixture was stirred for 12 hours affording a brown/orange suspension. The solid was recovered by centrifugation, washed with 2 x 0.5 mL toluene and dried in vacuo to give

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[1] B. Monteiro, D. Roitershtein, H. Ferreira, J.R. Ascenso, A. M. Martins, A. Domingos, and N.Marques, *Inorg. Chem.* 2003, **42**, 4223–4231.

[2] G. A. Bain and J. F. Berry, *J. Chem. Ed.*, 2008, **85**, 532-536.

[{U((SiMe$_2$NPh)$_3$-tacn)}$_2$(μ-Se)], **3** as an orange solid. Yield: 56 % (17.2 mg, 0.010 mmol). Recrystallization from toluene produced single crystals of **3** suitable for X-ray diffraction.

^{1}H NMR (200 MHz, toluene-*d$_8$*, 298 K): δ = 44.69 (s, 6H, SiMe$_2$), 30.59 (s, 4H), 20.29 (s, 4H), 13.92 (s, 2H), 9.90 (s, 6H, SiMe$_2$), 6.62 (s, 2H), -5.63 (s, 2H,), -8.39 (s, 1H, H$_p$), -12.98 (s, 2H), -18.91 (s, 6H, SiMe$_2$), -47.72 (s, 2H), -65.64 (s, 2H), -66.75 (s, 2H), -67.77 (s, 2H), -107.23 (s, 2H).

Anal. Calcd. for $C_{60}H_{90}N_{12}SeSi_6U_2$: C, 42.32; H, 5.33; N, 9.87. Found: C, 41.89; H, 5.14; N, 9.62.

Similar results were obtained when using 1 or 2 equivalents of Se *per* uranium complex.

Synthesis of [U{(SiMe$_2$NPh)$_3$-tacn}(η^2-S$_2$)] (4)

A solution of sulfur (7.9 mg, 0.246 mmol, 0.25 (2) eq.) in toluene (4 mL) was added to a solution of [U{(SiMe$_2$NPh)$_3$-tacn}], **1** (100.0 mg, 0.123 mmol, 1 eq.) in toluene (4 mL). The mixture was stirred at room temperature for 3 hours, affording a dark brown suspension that was left standing for 2 days at room temperature before filtration. The resulting microcrystalline black solid was washed with 0.5 mL toluene and dried in vacuo, affording [U{(SiMe$_2$NPh)$_3$-tacn}(η^2-S$_2$)] **4** as a black powder (82.0 mg, 0.091 mmol, 74 % yield).

The ^{1}H NMR (200 MHz, toluene-*d$_8$*) shows broad signals in the temperature range -80°C - +80°C. Anal. Calcd. for **4**.(toluene)$_{0.27}$ $C_{61.89}H_{47.16}N_6S_2Si_3U$: C, 42.51; H, 5.28; N, 9.33; S, 7.12. Found: C, 42.50; H, 5.18; N, 9.07; S, 6.88.

Reaction of 4 with PPh$_3$

A suspension of **4** (30.0 mg, 0.034 mmol, 1 eq.) in toluene (1.5 mL) was reacted with PPh$_3$ (9.0 mg, 0.034 mmol, 1 eq.) and the resulting reaction mixture was heated at 80°C for 5 hours. Upon cooling to room temperature, orange single crystals of [{U((SiMe$_2$NPh)$_3$-tacn)}$_2$(μ-η^2:η^2-S$_2$)], **5** suitable for X-ray diffraction studies formed in the reaction tube. Analysis of the mother liquor by ^{1}H NMR showed that a complex mixture of products was formed, among which the resonances of [{U((SiMe$_2$NPh)$_3$-tacn)}$_2$(μ-S)], **2**, could be identified.

Reaction of 1 with dry O$_2$

1 equivalent of dry dioxygen was condensed onto an NMR tube containing a 0.5 mL frozen deuterated toluene (0.5 mL) solution of [U{(SiMe$_2$NPh)$_3$-tacn}], **1** (33.3 mg, 0,041 mmol). Upon warming to room temperature, the solution turned light brown. The ^{1}H NMR spectrum recorded for the crude mixture showed that a complex mixture of products had formed.

Brown single crystals of {Na[U(η^2-(OSiMe$_2$NPh))((SiMe$_2$NPh)$_2$-tacn)]}$_2$, **6** suitable for X-ray diffraction were isolated from a concentrate toluene reaction mixture obtained reacting a sample of **1** containing traces of NaI. It was impossible to obtain crystals from pure samples of **1**.

The reaction pathway for the formation of **6** could involve the formation of a highly reactive uranium-dioxygen adduct followed by oxygen atom insertion into the N3-Si bond causing the cleavage of one pendant arm of the original ligand. The formation of a strong Si-O bond is probably the driving force of the reaction. As such, the isolation of **6** is quite informative, and demonstrates that the {tacn(SiMe$_2$NPh)} platform, due to the electrophilic character of silicon, is quite sensitive to oxygenated substrates. This is probably at the origin of the multiple reaction products observed in this reaction. Nucleophilic reactions at the Si leading to ligand rearrangements are known and have already been observed with titanium complexes.[3]

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[3] S. Barroso, J. Cui, A. R. Dias, M. T. Duarte, H. Ferreira, R. T. Henriques, M. C. Oliveira, J. R. Ascenso, and A. M. Martins, *Inorg. Chem.*, **2006**, *45*, 3532–3537 ; A. M. Martins, J. R. Ascenso, S. M. B. Costa, A. R. Dias, H. Ferreira and J. A. B. Ferreira, *Inorg. Chem.*, **2005**, *44*, 9017–9022.

B) X-ray Crystallography

Diffraction data were taken using a Agilent-technologies Xcalibur-S kappa geometry diffractometer (Mo-Kα radiation, graphite monochromator, λ = 0.71073 Å). To prevent evaporation of co-crystallised solvent molecules the crystals were coated with light hydrocarbon oil and the data were collected at 150 K. The cell parameters were obtained with intensities detected on three batches of 5 frames. The crystal-detector distance was 4.5 cm. The number of settings and frames has been established taking in consideration the Laue symmetry of the cell by CrysAlisPro Oxford-Diffraction software.[4] 504 (for **2**), 462 (for **4**), 489 (for **6**) and 255 (for **7**) narrow data were collected for 1° increments in ω with a 120 s exposure time for **2**, 60 s for **4**, 40 s for **6** and 50 s for **7**. Unique intensities detected on all frames using the Oxford-Diffraction Red program were used to refine the values of the cell parameters. Space groups were determined from systematic absences, and they were confirmed by the successful solution of the structure. The structures were solved by direct methods using the SHELXTL 6.14 package[5] and for all structures all atoms except hydrogens were found by difference Fourier syntheses. All non-hydrogen atoms were anisotropically refined on F^2. Hydrogen atoms were fixed in ideal position. Experimental details for X-ray data collections of all complexes are given in Table 1.

A single crystal of compound **3** was mounted in thin walled glass capillary in a nitrogen filled glovebox. Data were collected at room temperature on an Enraf-Nonius CAD4-diffractometer, with graphite-monochromated Mo Kα radiation, using the $\omega\text{–}2\theta$ scan technique. The data were corrected for Lorentz and polarization effects for linear decay, and empirically for absorption by psi–scans[6] using the Enraf-Nonius reduction program.[7] The structure was solved by Patterson methods and successive difference Fourier techniques, and refined by full-matrix least squares refinement on *F*2 using SHELXL-97.[5] All the non-hydrogen atoms were refined with anisotropic thermal motion parameters. The contributions of the hydrogen atoms were included at calculated positions. Crystallographic data have been deposited with the Cambridge Crystallographic Data Centre (CCDC numbers for complexes 2-6 are CCDC .These data can be obtained free of charge from CCDC via www.ccdc.cam.ac.uk/data_request/cif.

Table S1. X-ray Crystallographic data

Compound	$[\{U((SiMe_2NPh)_3\text{-}tacn)\}_2(\mu\text{-}S)]$ (toluene) **-2**	$[\{U((SiMe_2NPh)_3\text{-}tacn)\}_2(\mu\text{-}Se)].(toluene)$ **3**	$[U\{(SiMe_2NPh)_3\text{-}tacn\}(\eta^2\text{-}S_2)]_2.(toluene)_{0.75}$ **4**	$[\{U((SiMe_2NPh)_3\text{-}tacn)\}_2(\mu\text{-}\eta^2{:}\eta^2\text{-}S_2)]$ **5**	$\{Na[U(\eta^2\text{-}(OSiMe_2NPh))((SiMe_2NPh)_2\text{-}tacn)]\}_2$ **6**
Formula	$C_{67}H_{98}N_{12}SSi_6U_2$	C67 H98 N12 Se Si6 U2	C35.25 H51 N6 S2 Si3 U	C60 H90 N12 S2 Si6 U2	C30 H45 N6 Na O Si3 U
Crystal size [mm]	0.380 x 0.199 x 0.126	0.20 x 0.08 x 0.04	0.21 x 0.12 x 0.10	0.20 x 0.13 x 0.03	0.18 x 0.11 x 0.07
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	$P\ 2_1/n$	$P\ 2_1/n$	$P\ 2_1/n$	$P\ 2_1/n$	$P\ 2_1/n$
V [Å^3]	7169.4(6)	7216.0(3)	7736.4(18)	3390.8(3)	3368.97(18)
a [Å]	18.1014(9)	18.1375(3)	22.725(4)	14.1895(9)	10.5247(3)
b [Å]	17.6622(9)	17.5716(4)	19.8120(7)	12.4113(5)	18.5060(5)
c [Å]	22.4297(13)	22.6446(5)	30.101(5)	20.2745(10)	17.3041(6)
α [°]	90	90	90	90	90
β [°]	91.229(6)	90.9355(19)	145.19(4)	108.259(6)	91.612(3)
γ [°]	90	90	90	90	90
Z	4	4	8	2	4
Absorption coefficient [mm^{-1}]	4.690	5.135	4.431	4.984	4.971
F (000)	3472	3544	3764	1668	1680
T [K]	150(2)	150(2)	150(2)	150(2)	150(2)
Total no. reflexions	43397	69833	70075	33752	20741
Unique reflexions [R(int)]	21646 [0.0888]	17890 [0.0987]	15789[0.0761]	8390 [0.0942]	10190 [0.0530]
Final R indice [I>2σ(I)]	0.1092	0.0470	0.0728	0.0706	0.0496
Largest diff. peak and hole [eA^{-3}]	7.846 and -4.305	1.075 and -0.913	4.615 and -1.842	5.558 and -1.861	1.706 and -1.287
GOF	1.081	0.990	1.075	1.104	1.016

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[4] Agilent, in *CrysAlis PRO.*, ed. A. technologies, Yarnton, England, 2010.

[5] SHELXTL Version 6.1, G. M. Sheldrick (1997), ed. Brucker AXS Inc, Madison,Wisconsin, USA.

[6] North, A. C. T.; Phillips, D. C.; Mathews, F. S. Acta. Crystallogr. 1968, A24, 351-359.

[7] Enraf–Nonius (1994). CAD-4 Software. Enraf–Nonius, Delft, The Netherlands.

Crystal structure of 3

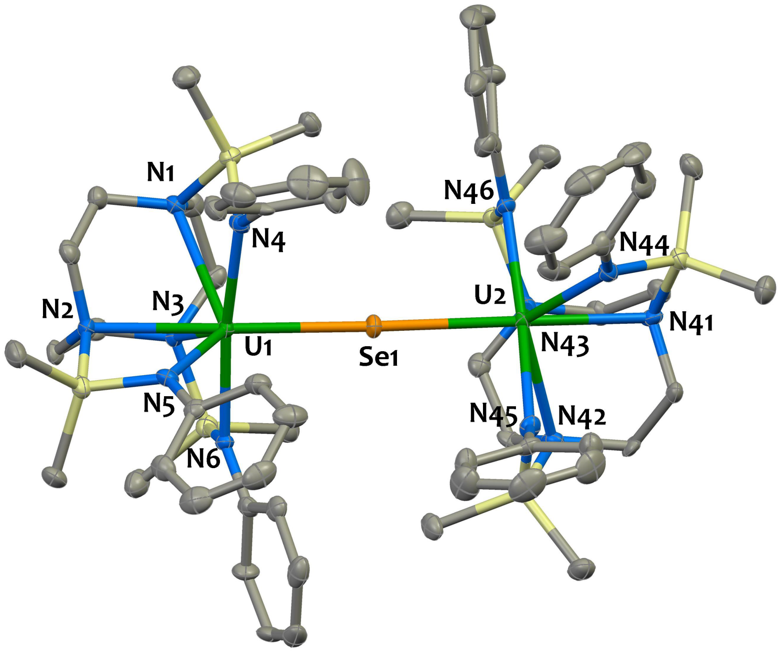


Figure S1. Solid-state molecular structure of $[\{U((SiMe_2NPh)_3\text{-tacn})\}_2(\mu\text{-Se})]$, **3** (50% probability ellipsoids). Hydrogen atoms and solvent molecules are omitted for clarity. Color code: uranium (green), nitrogen (blue), silicon (light yellow), selenium (orange) and carbon (grey). Selected bond distances (Å): U-Namido$_{avg}$ 2.33(2); U-Namino$_{avg}$ 2.68(4); U-Se$_{avg}$ 2.830(5).

Crystal structure of 6

The analysis of the solid-state structure of **6** (Figure S2) reveals that the ligand has undergone strong structural changes, with the cleavage of a $SiMe_2NPh$ arm from the tacn platform as a result of the nucleophilic attack of the oxygen on the silicon atom and formation of a dianionic $\{OSiMe_2NPh\}^{2-}$ bridging ligand. The metrical parameters for this unit (short U1-O1 (2.412(3) Å) and U1-N6 (2.300(5) Å) bond distances) are in agreement with a dianionic silyloxy/silylamido ligand formulation. The analysis of the U-N bond distances of the tacn anchor suggests that the nitrogen atom N3 is acting as an amido donor, the U1-N3 bond distance (2.284(4) Å) being significantly shorter than the uranium-amino bond distances (U1-N1 =2.700(5) Å and U1-N2 = 2.721(4) Å). The complex can thus be formulated as a heteroleptic U(IV) complex where the uranium cation is heptacoordinated by a N_5 trianionic ligand platform and a N_1O_1 dianionic ligand. The overall negative charge of the complex is balanced by the presence of a sodium counter cation that holds two complexes together.

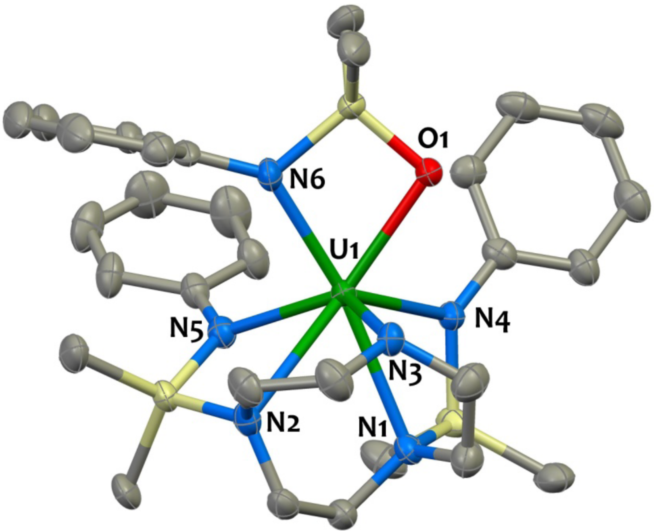


Figure S2. View of the anion $[U(\eta^2\text{-}(OSiMe_2NPh))((SiMe_2NPh)_2\text{-tacn})]$ in the solid-state molecular structure $\{Na[U(\eta^2\text{-}(OSiMe_2NPh))((SiMe_2NPh)_2\text{-tacn})]\}_2$ **6** (50% probability ellipsoids). Hydrogen and sodium atoms are omitted for clarity. Color code: uranium (green), nitrogen (blue), silicon (light yellow), oxygen (red) and carbon (grey). Selected bond distances

(Å): U(1)-N(3) 2.284(4), U(1)-N(6) 2.300(5), U(1)-N(5) 2.344(4), U(1)-O(1) 2.412(3), U(1)-N(4) 2.417(4), U(1)-N(1) 2.700(5), U(1)-N(2) 2.721(4).

C) ^{1}H NMR spectra

Figure S3. ^{1}H NMR spectrum of **2** (toluene-d_8, 200MHz, 298K).

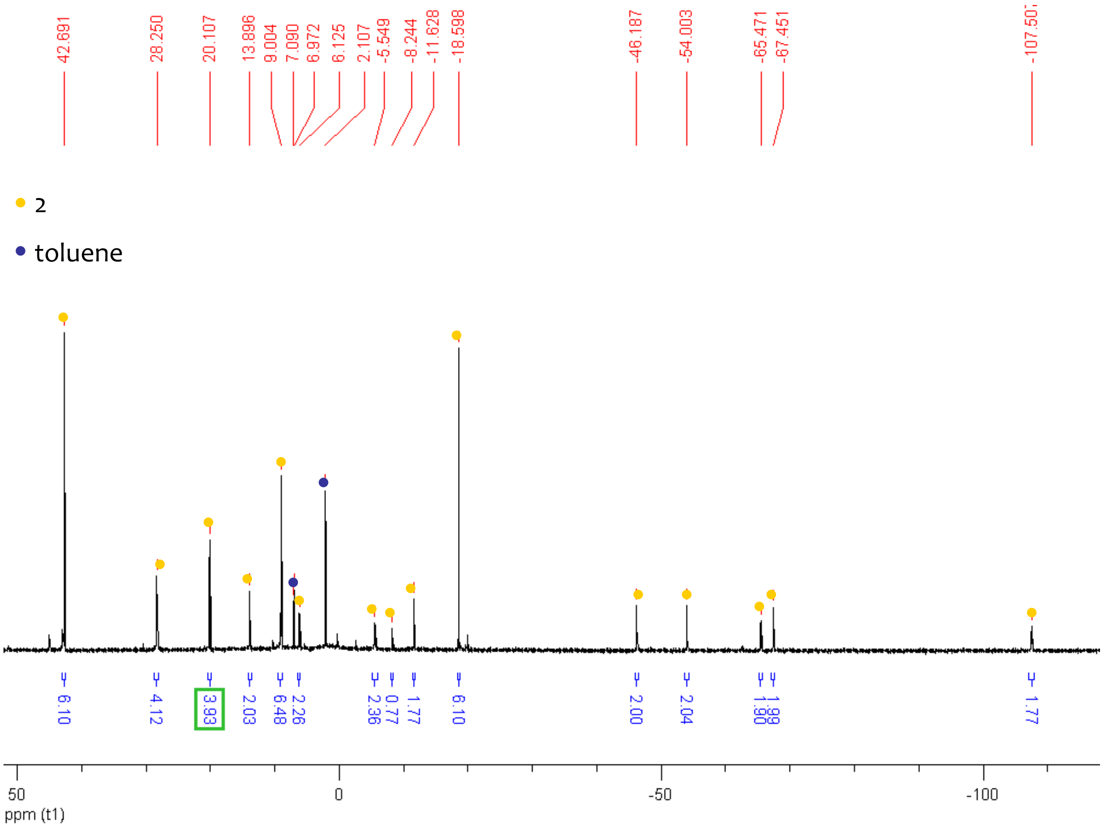


Figure S4. ^{1}H NMR spectrum of the crude reaction mixture of **1** with 0,5 equiv. Ph_3PS, giving **2** (toluene-d_8, 200MHz, 298K).

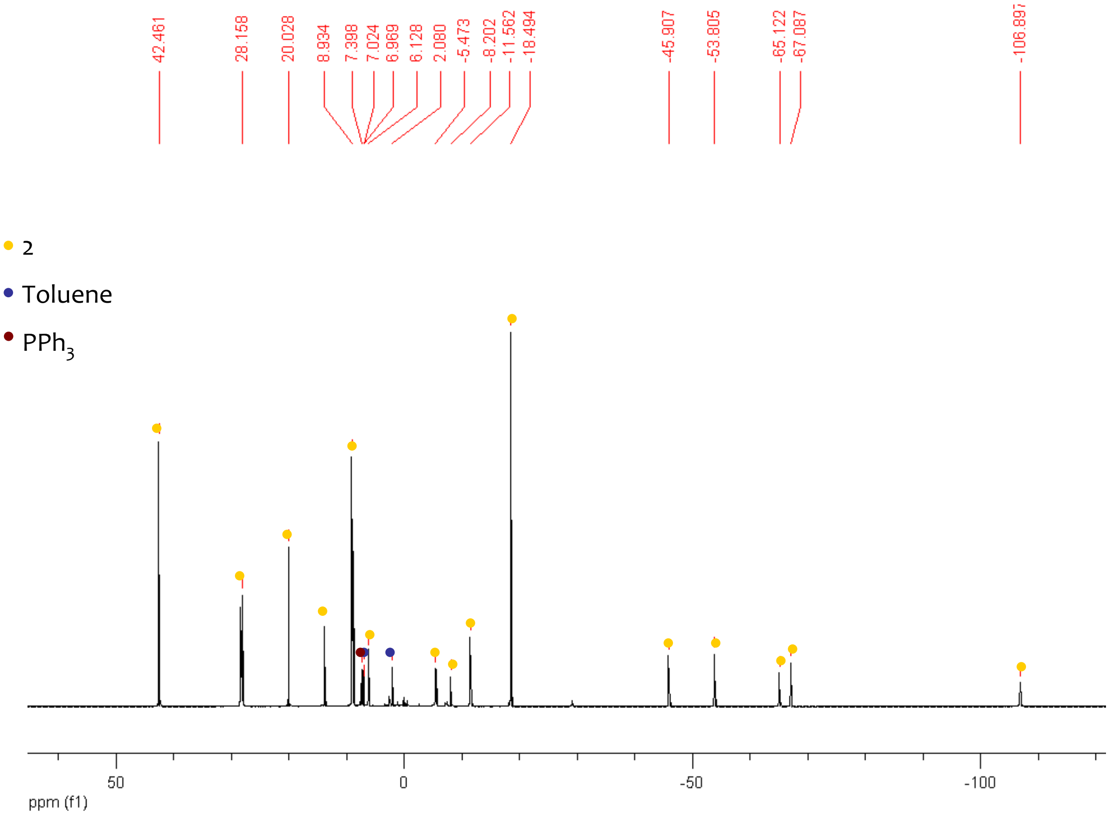


Figure S5. ^{1}H NMR spectrum of **3** (toluene-d_8, 200MHz, 298K).

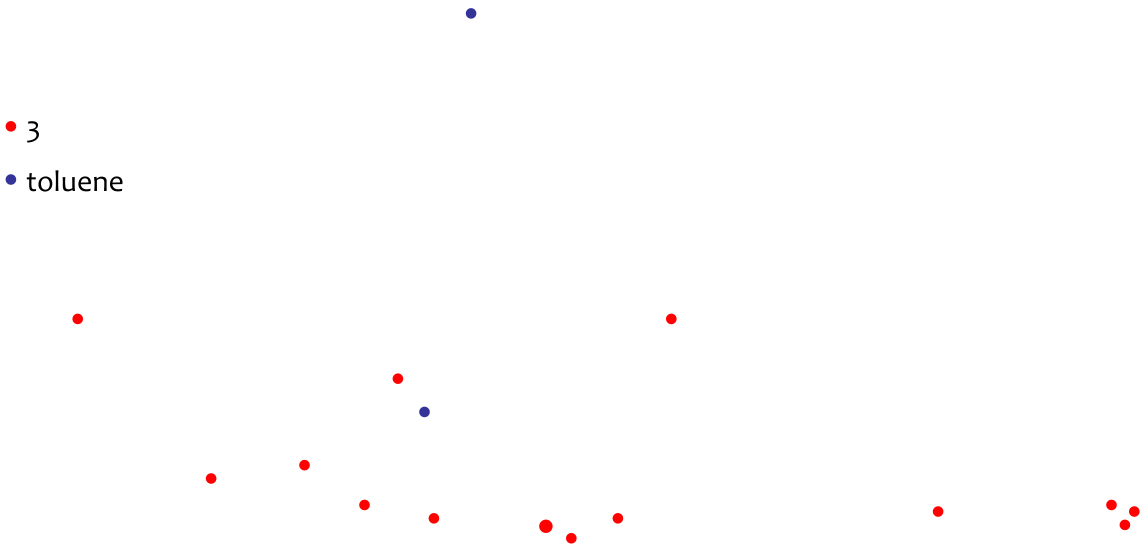


Figure S6. ^{1}H NMR spectrum of **4** (toluene-d_8, 200MHz, 298K).

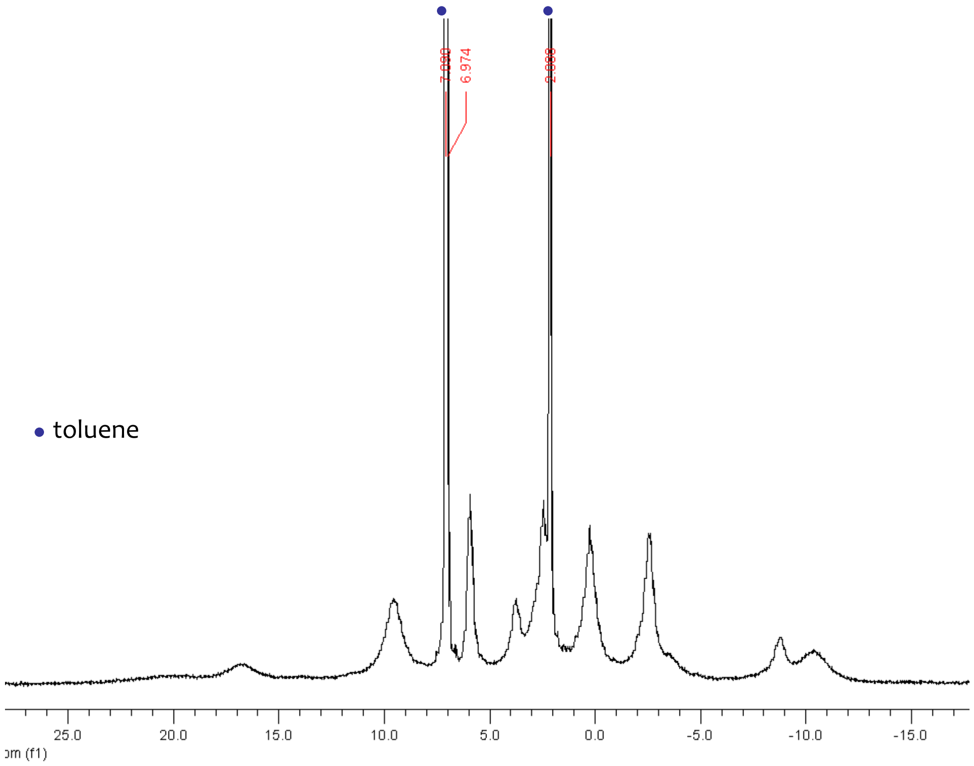
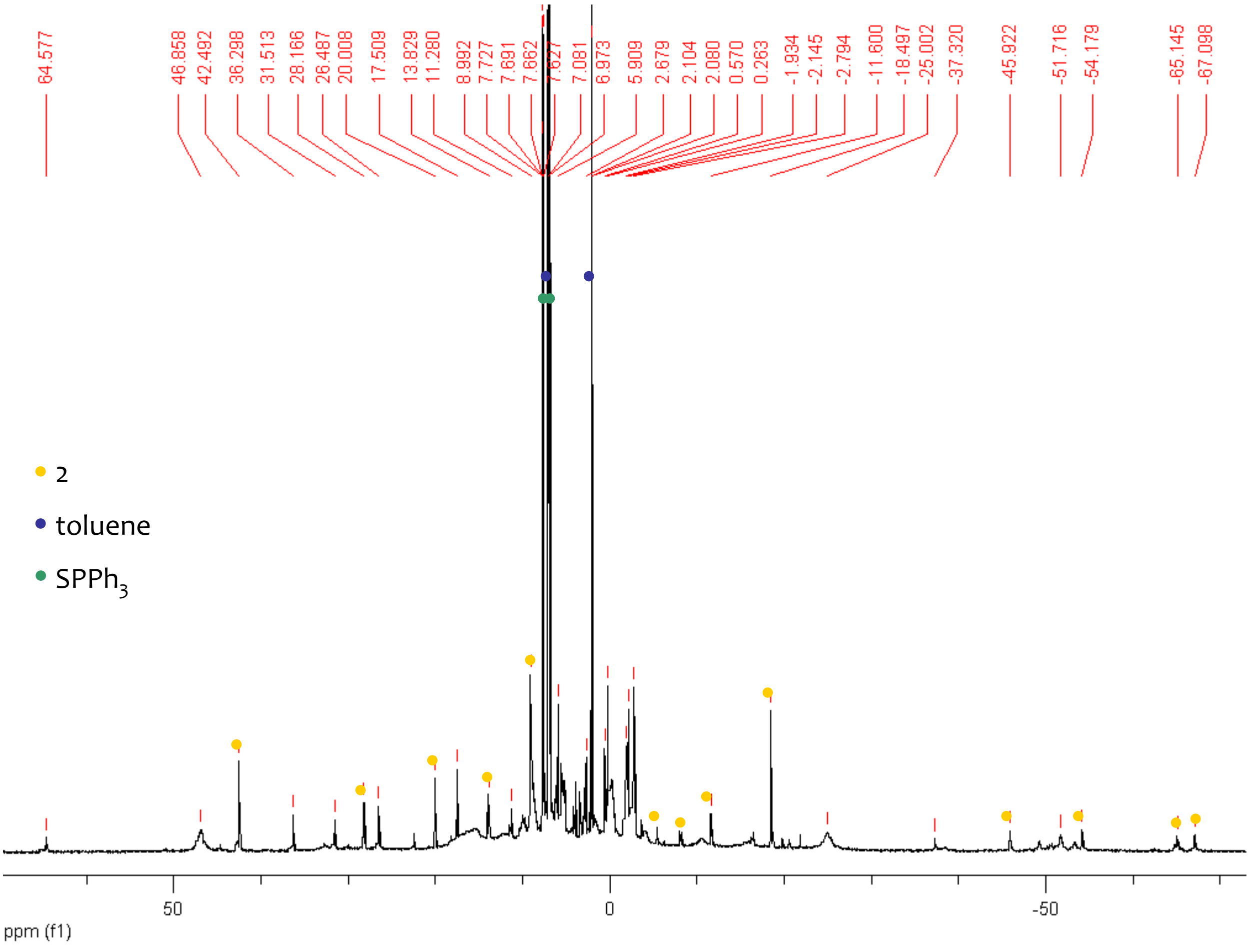


Figure S7. In-situ ^{1}H NMR spectrum (toluene-d_8, 200MHz, 298K).of the equimolar reaction between **4** and PPh_3 showing the formation of $SPPh_3$ and **2** among other species.



D) UV/vis/NIR spectra

Figure S8. UV-visible spectrum of a THF solution of **4**.

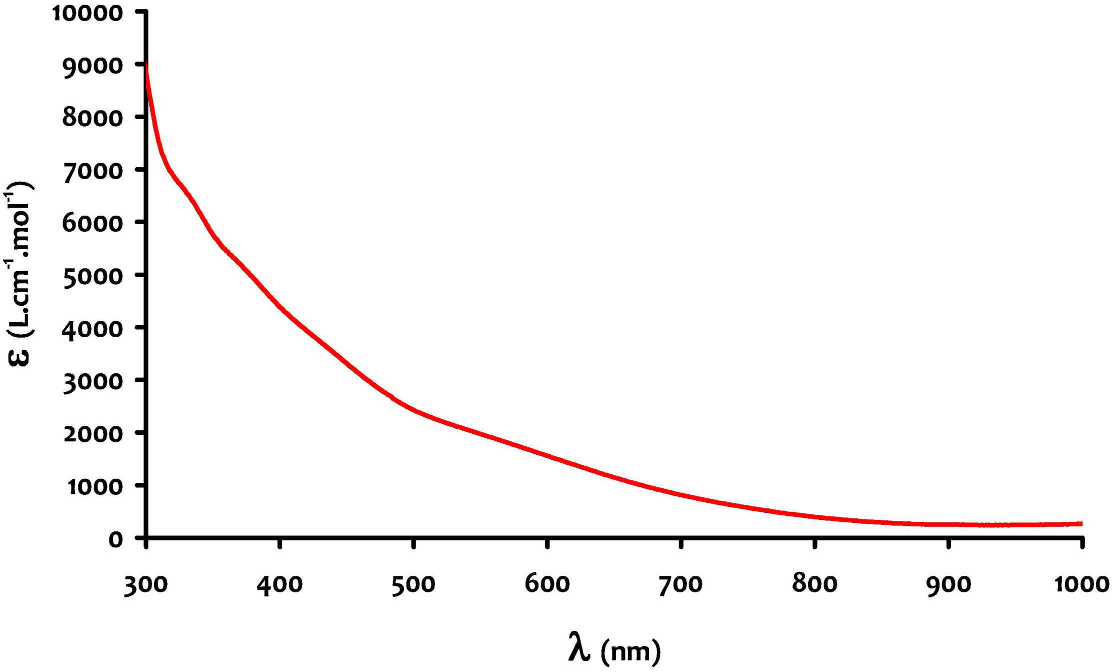
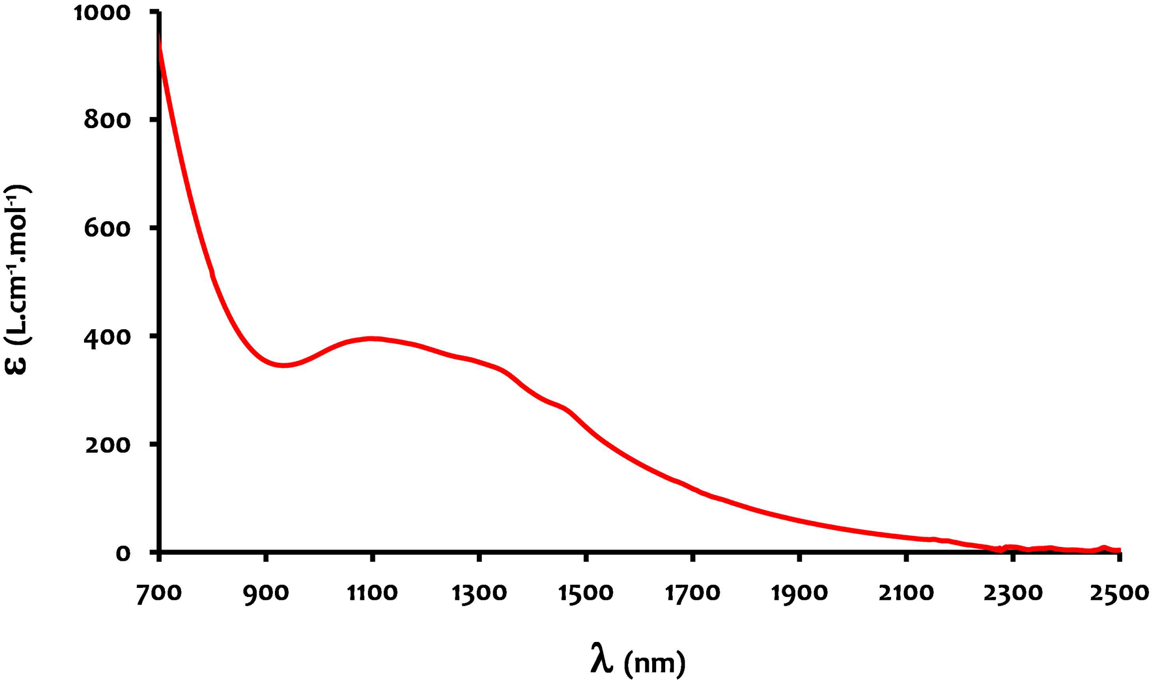


Figure S9. NIR spectrum of a THF solution of **4**.



E) Computational data

Computational Details

Calculations were performed at DFT level of theory using the hybrid PBE0 functional and a double zeta basis set and a relativistic pseudo potential to describe the U atom . This level of theory has been previously applied to describe the electronic and geometrical structure and the spectroscopic properties of metal containing complexes showing a good accuracy and agreement with the experimental data.[1-4] Single point (on X-Ray structure) and structural optimization calculations were performed using Gaussian 09 program package.[5] The PBE0 exchange correlation functional[6] was used throughout together with the 6-31G* / 6-31+G* basis sets[10] for light atoms not linked (C, H, and Si) / linked (N and S) to uranium atom, while the quasi-relativistic effective core potential, called as ECP60MWB, of the Stuttgart group along with its valence basis set has been used for uranium.[7,8]

Figure S10. Optimized molecular structure of complex X. H atoms are omitted for clarity

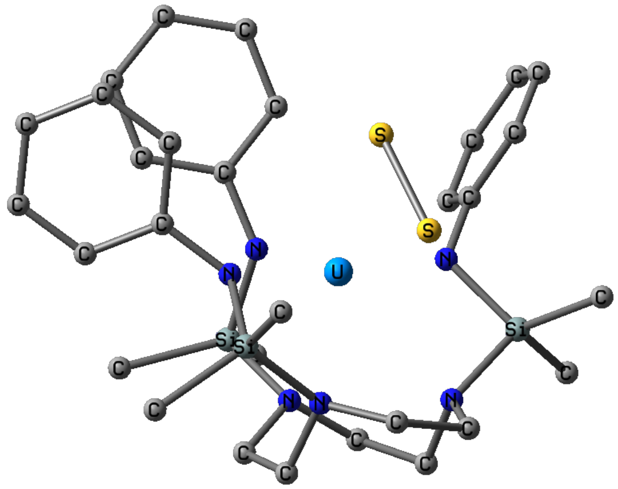


Table S2. Cartesian coordinates of complex **4** optimized in gas phase.

H	-1.44732000	-1.73503100	3.74784000
H	-0.76370500	0.77896000	4.94786900
H	-0.35908700	2.36118400	4.27079800
C	2.68740000	4.18886000	0.57959000
H	3.68477900	4.51675400	0.86108400
C	1.92574700	4.94842700	-0.30821700
H	2.31771800	5.87737300	-0.71303400
C	-4.01974600	3.20349300	-1.72823800
H	-4.33100500	3.52394500	-2.71947800
C	-4.26333400	4.01719400	-0.62324300
H	-4.76543500	4.97307000	-0.74462600
C	-3.84946200	3.59415800	0.63763400
H	-4.02662500	4.22032300	1.50858100
Si	-3.29798300	-1.12873600	-0.17270300
N	-2.05902100	-2.29647100	0.41353900
H	-0.06480700	-3.94100400	1.74070600
H	0.86574200	-2.51927800	3.46961100
C	-1.44847800	-1.41796000	2.69035700
H	-2.05837900	-0.51289500	2.62779500
C	-2.13643100	-2.50660100	1.87078500
H	-3.18022100	-2.54882600	2.21597600
H	-1.72594800	-3.48686100	2.11525200
C	-1.78526600	-3.52573500	-0.33699500
H	-2.31493200	-3.48453200	-1.29265900
H	-2.20386000	-4.38567100	0.20565400
C	-0.72872500	1.35943400	4.01756800
H	-1.75015700	1.47851100	3.64580300
C	-4.07112300	-1.64439400	-1.80154500
H	-4.79531500	-0.87280400	-2.09211800

H	-4.62558500	-2.58614300	-1.70086000
H	-3.33779000	-1.73523200	-2.60729400
C	-4.73587100	-0.96554500	1.03970400
H	-4.44867100	-0.61388500	2.03618400
H	-5.28974600	-1.90671100	1.14791200
H	-5.43345900	-0.22363800	0.63166800
U	-0.14144700	-0.28278700	-0.26747000
Si	2.21914800	-2.44160300	-0.68996800
Si	0.45601900	0.60109800	2.77018600
S	-0.19014500	0.77078000	-2.65827500
S	-0.61040200	-1.25209500	-2.68166000
N	0.64273200	-2.90816800	0.06441500
N	-0.09224600	-1.06127800	2.25090700
N	2.05225200	-0.72592300	-0.49163300
N	0.40908800	1.31128300	1.21089700
N	-2.31298000	0.29548600	-0.14349800
C	0.78092800	-3.30777900	1.47512700
H	1.66630200	-3.94268200	1.62860400
C	0.90064800	-2.12804900	2.43797700
H	1.88922800	-1.68218600	2.30045300
C	-0.27609100	-3.78829800	-0.65562500
H	-0.04550400	-4.84582200	-0.44748400
H	-0.11351900	-3.63897600	-1.72573700
C	2.43359300	-3.09337500	-2.43356000
H	1.68962100	-2.68961800	-3.12499400
H	2.39483800	-4.18974800	-2.45821400
H	3.42729200	-2.79381700	-2.79032700
C	3.66713700	-3.17388900	0.27990700
H	4.59865100	-2.80770500	-0.16833100
H	3.67338000	-4.26776600	0.18734500
H	3.70108000	-2.92084200	1.34451600
C	3.16984400	0.12521100	-0.64480600
C	4.19919300	0.13862000	0.31261300
H	4.12287400	-0.51829000	1.17490400
C	5.30710900	0.96708000	0.16561300
H	6.08949100	0.95495600	0.92101000
C	5.41473700	1.80689800	-0.94038200
H	6.27793600	2.45689300	-1.05521100
C	4.40364600	1.79903600	-1.89819200
H	4.47360300	2.44676100	-2.76843500
C	3.29660500	0.96794100	-1.75891700
H	2.50489900	0.96237700	-2.50208900
C	2.12568000	0.50588600	3.63340600
H	2.94484200	0.23220200	2.96246400
H	2.10343800	-0.20410100	4.46976500
H	2.36023300	1.49198300	4.05269000
C	0.91343800	2.53430200	0.74158900
C	2.19587100	2.99627400	1.09252100
H	2.81921700	2.39142000	1.74301800
C	0.15099700	3.31398800	-0.14513900
H	-0.85740200	3.00152000	-0.39685900
C	-2.95001100	1.54401900	-0.31284400
C	-3.36943200	1.98214800	-1.57958200
H	-3.14759000	1.36217300	-2.44332400
C	-3.20346500	2.37140500	0.79167600
H	-2.86862300	2.04418400	1.77156400
C	0.65921700	4.50073600	-0.66822100
H	0.04589900	5.08090400	-1.35278200

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