Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information for:

Elemental Chalcogen Reactions of a Tetravalent Uranium Imidophosphorane Complex: Cleavage of Dioxygen

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General Considerations

Unless otherwise stated, all reagents were obtained from commercial suppliers, and the syntheses and manipulations were conducted under argon with exclusion of dioxygen (O_2) and H_2O using Schlenk techniques or in an inert atmosphere box (Vigor) under a dinitrogen (<0.1 ppm O_2/H_2O) atmosphere. All glassware was stored in an oven over-night (>8 h) at a temperature of ca. 160˚C prior to use. Celite and molecular sieves were dried under vacuum at a temperature >250 °C for a minimum of 24 h. C_6D_6 was vacuum transferred off sodium benzophenone and stored over 3 Å molecular sieves prior to use. Diethyl ether, *n*-pentane, *n*-hexane, and tetrahydrofuran (THF) were purged with UHP-grade argon (Airgas) and passed through columns containing Q-5 and molecular sieves in a solvent purification system (JC Meyer Solvent Systems). All solvents in the glovebox were stored in bottles over 3 Å molecular sieves. The elemental sulphur (S_8) powder and selenium (Se^0) metal powder were purchased from Sigma Aldrich. UHP-grade O_2 was purchased from Airgas and adapted to a Schlenk line, which was purged prior to use. The reagents $UI_4(dioxane)_3$, $K[NP(pip)_3]$, and $[U(NP(pip)_3)_4]$ (**1-U**) were prepared following published procedures.[1-3] The structure and spectroscopic data of $[UO(NP(pip)_3)_4]$ (**2-U**) has been previously reported. NMR spectra were obtained on a Bruker Avance III 400 MHz spectrometer at 295 K, unless otherwise noted. ^1H, $^{13}C\{^1H\}$, and $^{31}P\{^1H\}$ NMR chemical shifts are reported in δ, parts per million. All NMR samples were prepared in C_6D_6 (unless otherwise noted) and ^1H NMR are references to the residual ^1H resonances of C_6D_6.[4] The peak position is listed, followed by the peak multiplicity, integration value, and proton assignment, where applicable. The multiplicity and shape are indicated by one or more of the following abbreviations: s (singlet); d (doublet); t (triplet); q (quartet); m (multiplet); br (broad). Elemental analyses were determined at Robertson Microlit Laboratories (Ledgewood, NJ) and University of California, Berkeley, Microanalytical Facility (Berkeley, CA. Infrared (IR) samples were taken on a Bruker ALPHA FTIR spectrometer from 400 to 4000 cm^{-1}. IR samples were prepared as Nujol mulls sandwiched between two KBr plates. The peaks are listed in wavenumber [cm^{-1}] and intensity by using the following abbreviations: vw (very weak); w (weak); m (medium); s (strong); vs (very strong); br (broad). UV/visible/NIR spectroscopy was performed in Teflon-valve sealed quartz cuvettes with a 1 cm path length on a Hitachi UH4150 UV-vis-NIR scanning spectrophotometer between 2400-240 nm.

Depleted uranium (primary isotope ^{238}U) is a weak α-emitter (4.197 MeV, $t_{1/2}$ = $4.47x10^9$ years). Manipulations and reactions should be carried out in a ventilated fume hood or in an inert atmosphere glovebox in a radiation laboratory that is equipped with α- and β-counting equipment. Caution should be exercised when handling ^{238}U.

Synthetic Procedures

Synthesis of [UO(NP(pip)$_3$)$_4$] (2-U) by reaction of [U(NP(pip)$_3$)$_4$] with O_2

Inside a glovebox, 30 mL of THF was added to a 100-mL Schlenk pear flask charged with [U(NP(pip)$_3$)$_4$] (0.115 g, 0.081 mmol), a stir bar, and was adapted with a gas addition glass bulb. The reaction vessel was connected to a Schlenk line that was fitted with an O_2 cylinder. The gas addition bulb was evacuated, filled with O_2 gas, sealed from the line, and then opened to the reaction flask. The reaction mixture immediately adopted a red/brown color, and was allowed to stir for 10 minutes to ensure that the reaction was complete. The mixture was reduced *in vacuo* to a residue and triturated three times with 4-6 mL of pentane. The mixture extracted into approximately 10 mL of THF and the mixture was filtered through a pipet packed with glass filter paper and Celite. The filtrate was reduced *in vacuo* to a residue and triturated three times with 4-6 mL of pentane. The residue was then dissolved in THF and concentrated *in vacuo* until saturated and placed in the freezer at −35 °C for 24 hours, during which time, red crystals formed. Decantation and removal of volatiles yielded the title compound in 74% yield (0.086 g, 0.060 mmol). ^{1}H NMR (400.13 MHz, C_6D_6, 295 K): δ 3.69, 3.49 (br, m, 48H, piperidinyl methylene C-*H*), 1.61 (br, m, 72H, piperidinyl methylene C-*H*). ^{31}P{^{1}H} NMR (161.98 MHz, C_6D_6, 295 K): δ 6.26 (consistent with previously reported data of the title compound).[3]

Synthesis of [U(κ^2-S$_3$)(NP(pip)$_3$)$_4$] (3-U)

Inside a glovebox, 12 mL of THF was added to a 20-mL scintillation vial charged with [U(NP(pip)$_3$)$_4$] (0.150 g, 0.105 mmol) and a stir bar. In a separate 20-mL scintillation vial, elemental sulfur powder, S_8, (0.010 g, 0.040 mmol) was suspended in 3 mL of THF and transferred as a suspension to the vial containing [U(NP(pip)$_3$)$_4$]. The reaction mixture was stirred for 24 hours. The mixture was then passed through a pipette packed with glass filter paper. The filtrate was reduced *in vacuo* to a residue and triturated three times with 2-3 mL of pentane. Removal of volatiles yielded the title compound as a brown microcrystalline solid in 57% yield (0.091 g). X-ray quality crystals were obtained by crystallization inside a 20-mL scintillation from a concentrated THF solution. Crystals formed at -35 °C within 24 hours. ^{1}H NMR (400.13 MHz, C_6D_6, 295 K): δ 3.61, 3.46 (br, m, 48H, piperidinyl methylene C-*H*), 1.64, 1.61, 1.59 (br, m, 72H, piperidinyl methylene C-*H*). ^{31}P{^{1}H NMR (161.98 MHz, C_6D_6, 295 K): δ 4.54, -7.98. ^{13}C{^{1}H} NMR (100.61 MHz, C_6D_6, 295 K δ 47.71 (br, m, piperidinyl methylene C-*H*), 46.64 (br, s, piperidinyl methylene C-*H*), 46.32 (br, s, piperidinyl methylene C-*H*), 28.18 (br, s, piperidinyl methylene C-*H*), 27.68 (br, m, piperidinyl methylene C-*H*), 25.97 (br, m, piperidinyl methylene C-*H*). IR (cm^{-1}): ν 1461 (vs), 1337 (s), 1260 (vw), 1214 (w), 1183 (w), 1159 (w), 1105 (m), 1059(m), 1017 (m), 949 (m), 854 (vw), 799 (vw), 721 (m). Elem. Anal. Found (calculated) for $C_{60}H_{120}UN_{16}P_4S_3$: C 47.43 (47.29), H 8.23 (7.94), N 14.61 (14.71).

Synthesis of [U(κ^2-Se$_3$)(NP(pip)$_3$)$_4$] (4-U)

Inside a glovebox, 12 mL of THF was added to a 20-mL scintillation vial charged with [U(NP(pip)$_3$)$_4$] (0.154 g, 0.108 mmol) and a stir bar. In a separate 20-mL scintillation vial, elemental selenium powder (0.025 g, 0.324 mmol) was suspended in 3 mL of THF and transferred as a suspension to the vial containing [U(NP(pip)$_3$)$_4$]. The reaction mixture was stirred for 24 hours. The reaction mixture was then passed through a pipette packed with

glass filter paper. The filtrate was reduced *in vacuo* to a residue and triturated three times with 2-3 mL of pentane. Removal of volatiles yielded the title compound as a brown microcrystalline solid in 69% yield (0.125 g). X-ray quality crystals were obtained by crystallization inside a 20-mL scintillation from a concentrated THF solution. Crystals formed at -35 °C within 24 hours. ^{1}H NMR (400.13 MHz, C_6D_6, 295 K): δ 3.69, 3.43 (br, m, 48H, piperidinyl methylene C-*H*), 1.65, 1.60 (br, m, 72H, piperidinyl methylene C-*H*). ^{31}P{^{1}H} NMR (161.98 MHz, C_6D_6, 295 K): δ 7.99, -11.17. ^{13}C{^{1}H} NMR (100.61 MHz, C_6D_6, 295 K δ 47.88 (br, s, piperidinyl methylene C-*H*), 47.42 (br, m, piperidinyl methylene C-*H*), 46.71 (br, s, piperidinyl methylene C-*H*), 28.02 (br, m, piperidinyl methylene C-*H*), 27.73 (br, m, piperidinyl methylene C-*H*), 27.46 (br, m, piperidinyl methylene C-*H*). IR (cm^{-1}): ν 1461 (vs), 1377 (s), 1261 (vw), 1215 (w), 1158 (w), 1109 (w), 1060 (m), 1019 (m), 949 (m), 799 (vw), 721 (m). Elem. Anal. Found (calculated) for $C_{60}H_{120}UN_{16}P_4S_3$: C 43.56 (43.29), H 7.29 (7.27), N 13.23 (13.46).

NMR Spectra of Reported Compounds

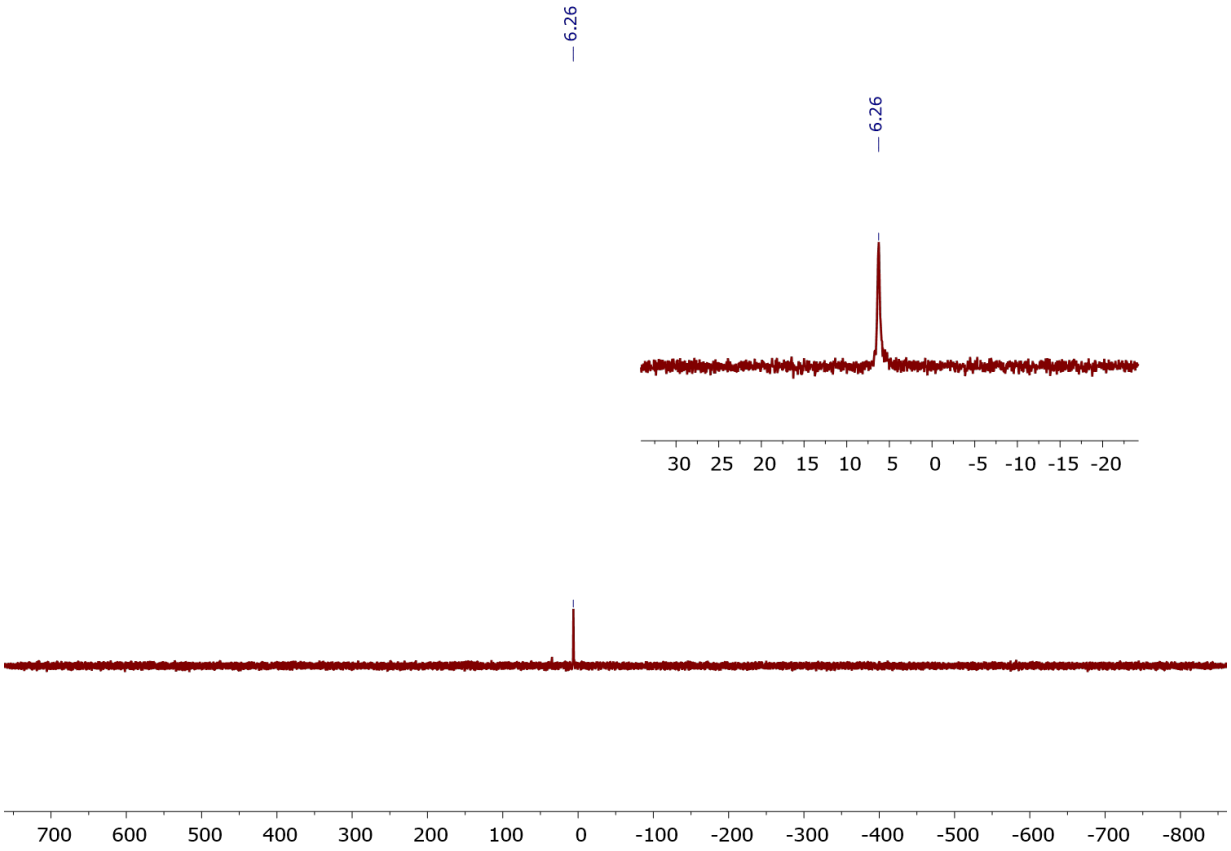

Figure S1. $^{31}P\{^{1}H\}$ NMR of **2-U** synthesized by the reaction between $[U(NP(pip)_3)_4]$ and O_2 (161.98 MHz, C_6D_6, 295 K).

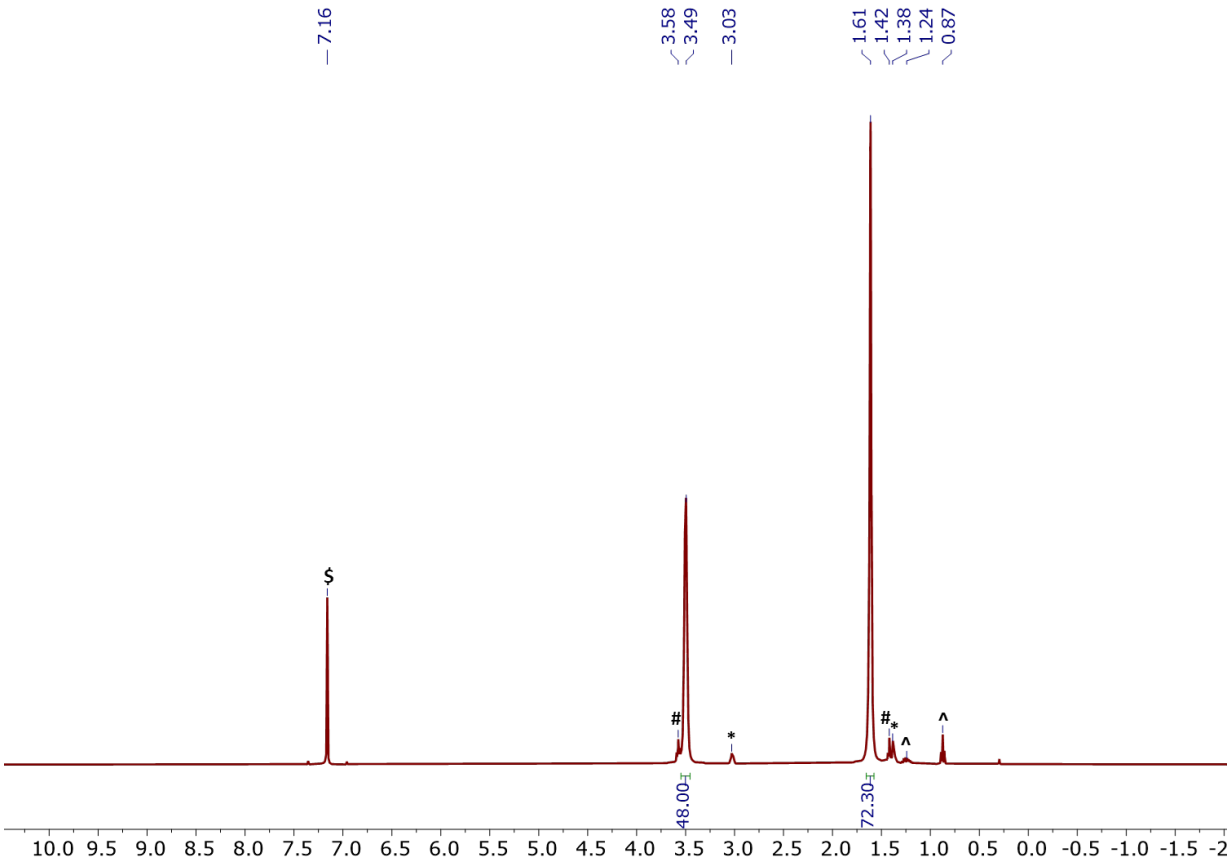

Figure S2. ^{1}H NMR of **2-U** synthesized by the reaction between [U(NP(pip)$_3$)$_4$] and O_2 (400.13 MHz, C_6D_6, 295 K). C_6D_5H noted as $. Residual *n*-pentane noted as ^. Residual THF noted as #. * is trace HNP(pip)$_3$.

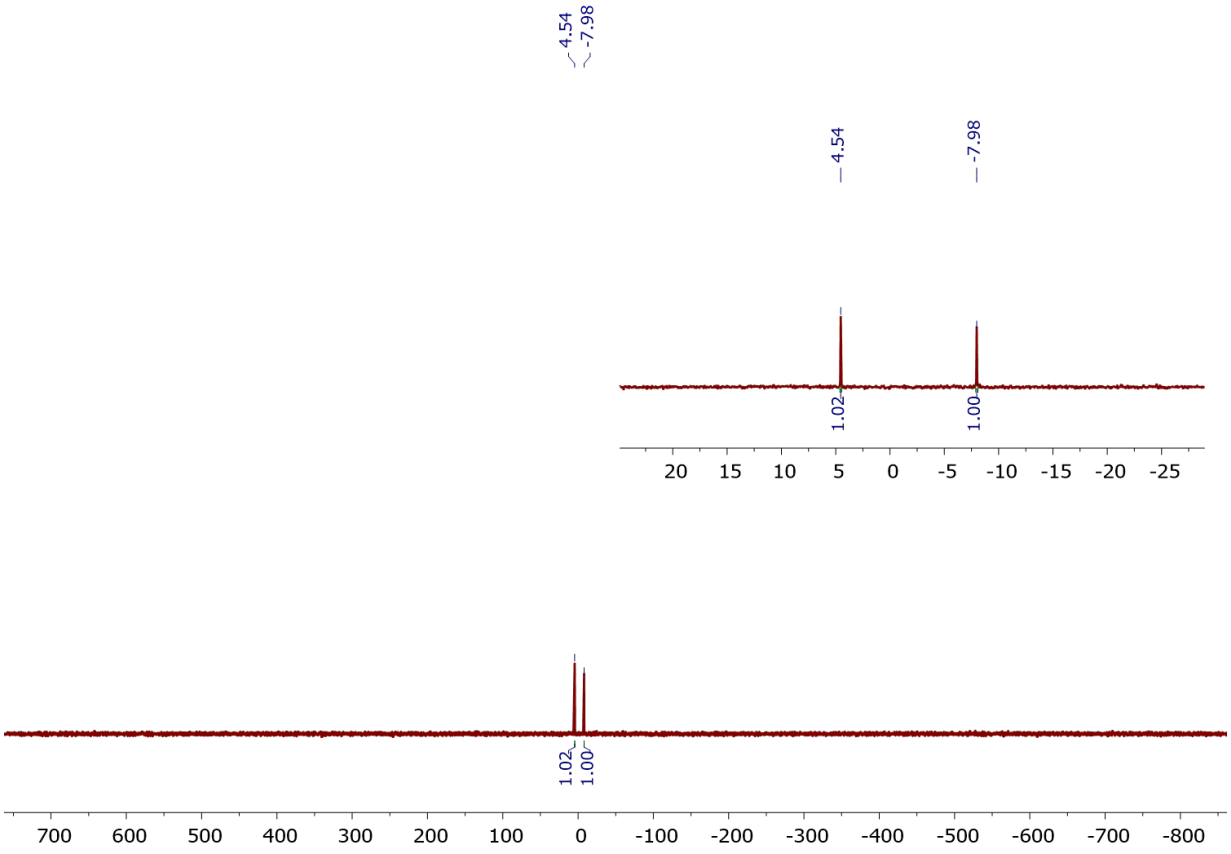

Figure S3. $^{31}P\{^{1}H\}$ NMR of **3-U** (161.98 MHz, C_6D_6, 295 K).

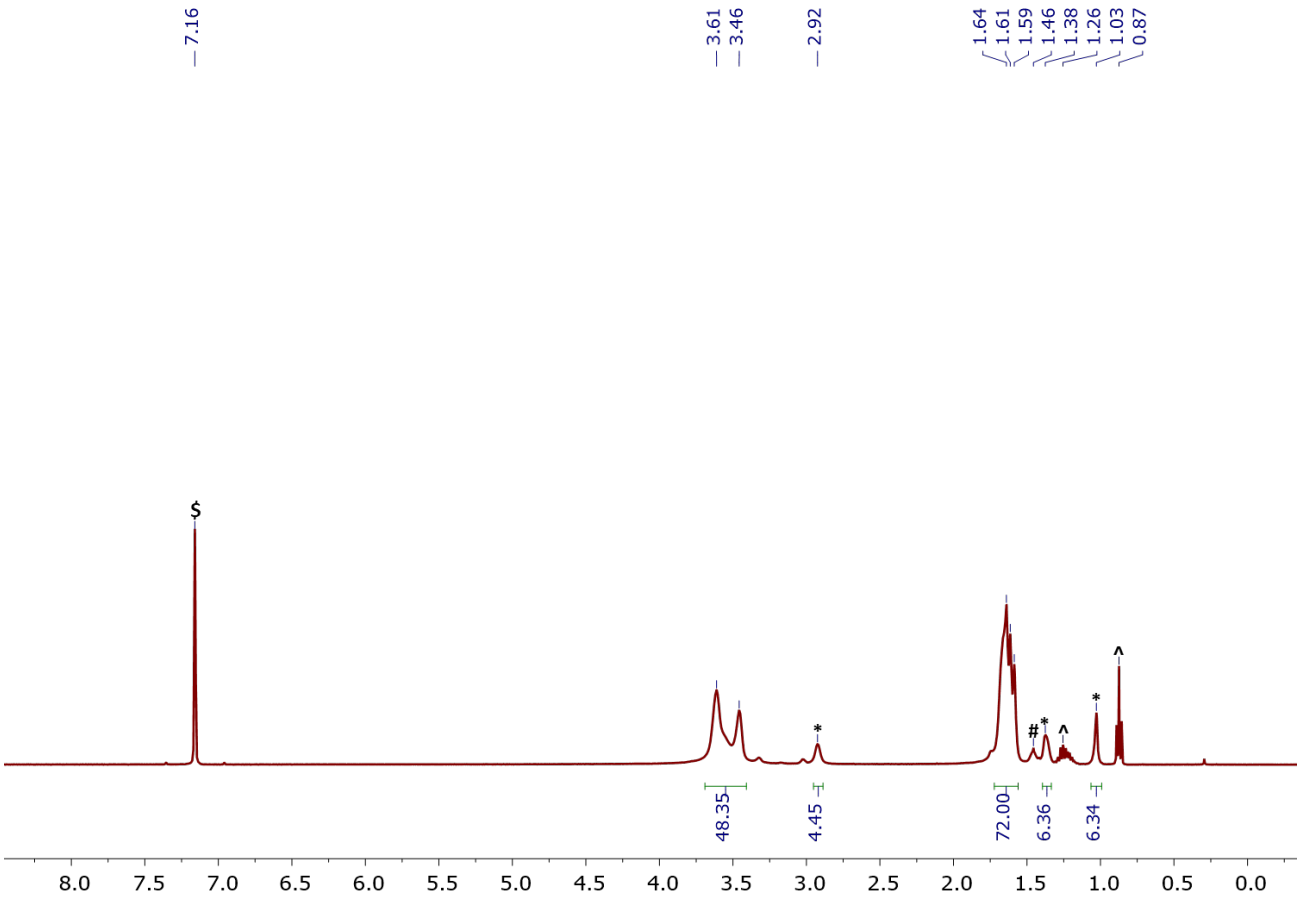

Figure S4. ^{1}H NMR of **3-U** (400.13 MHz, C_6D_6, 295 K). C_6D_5H noted as $. Residual *n*-pentane noted as ^. Residual THF noted as #. * is unknown.

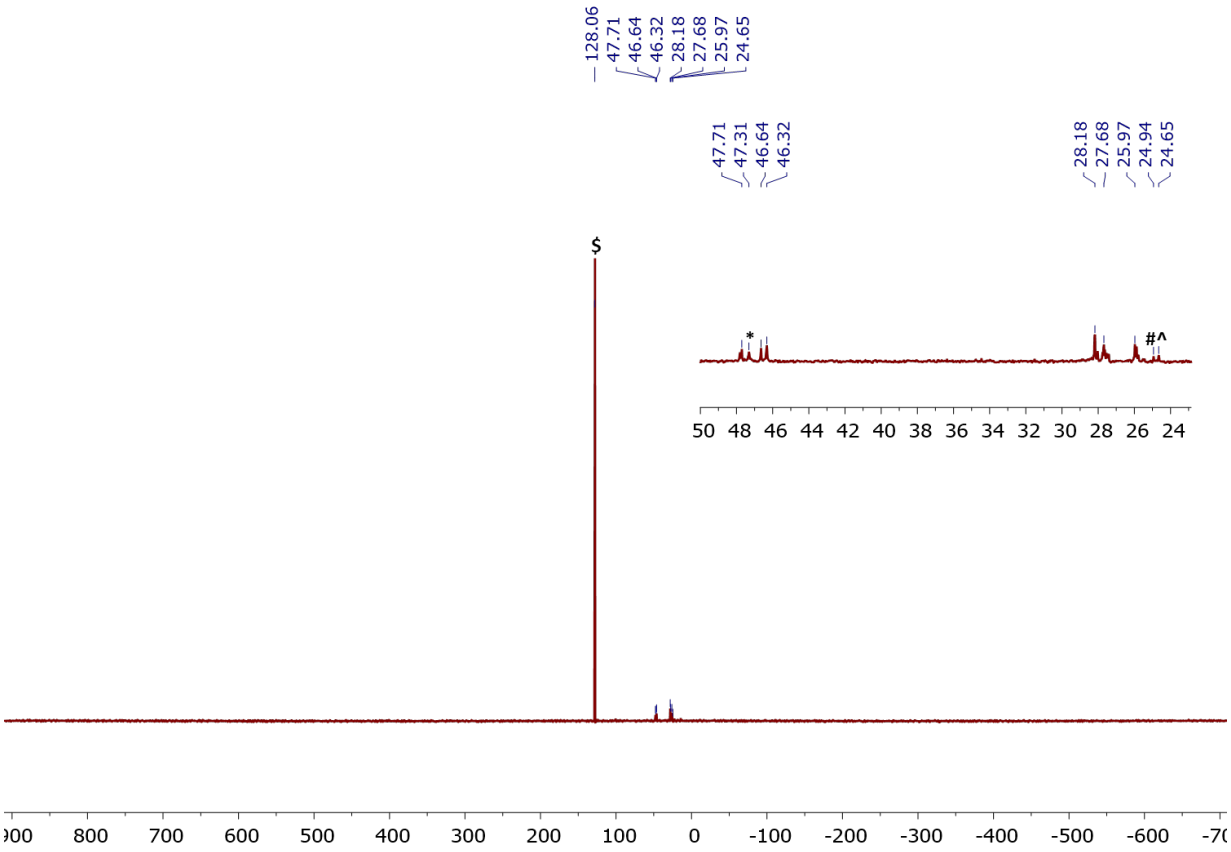

Figure S5. $^{13}C\{^{1}H\}$ NMR of **3-U** (100.61 MHz, C_6D_6, 295 K). C_6D_5H noted as $. Residual *n*-pentane noted as ^. Residual THF noted as #. * is unknown.

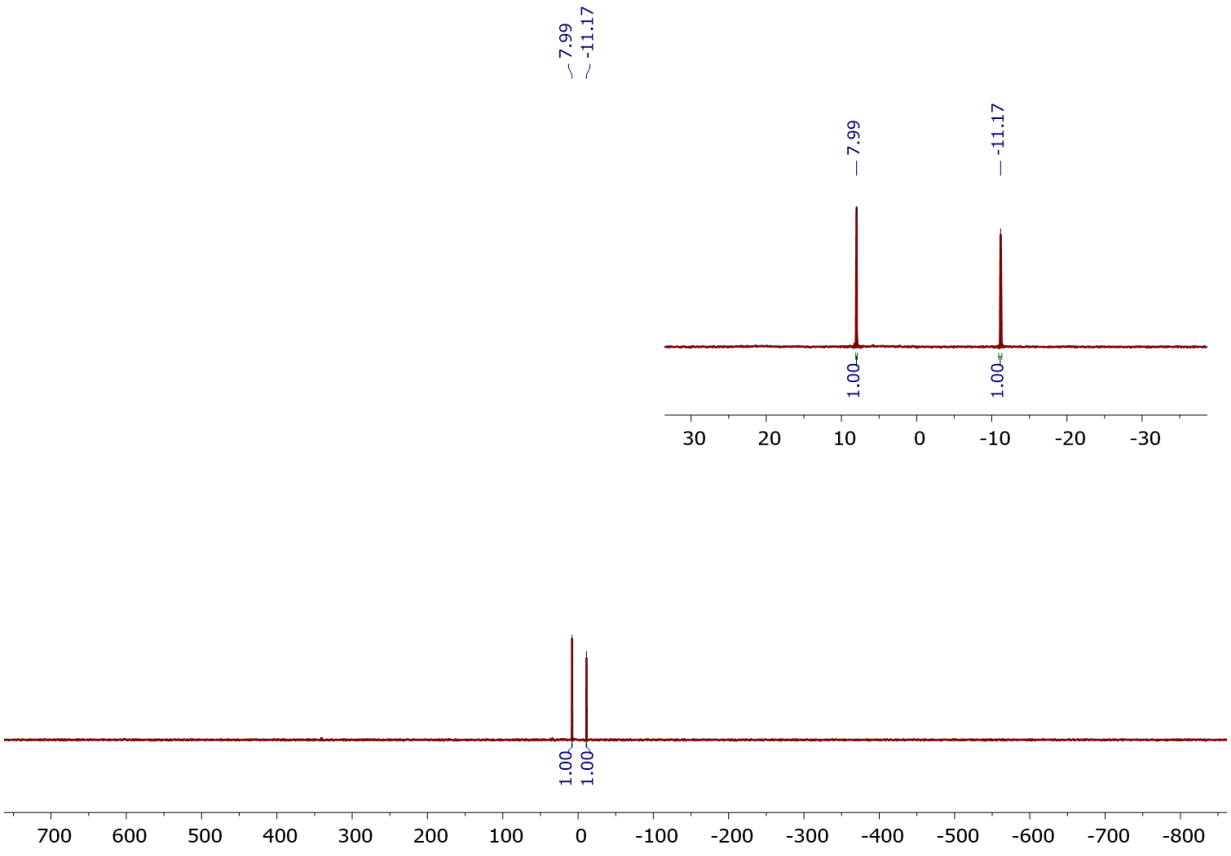

Figure S6. $^{31}P\{^{1}H\}$ NMR of **4-U** (161.98 MHz, C_6D_6, 295 K).

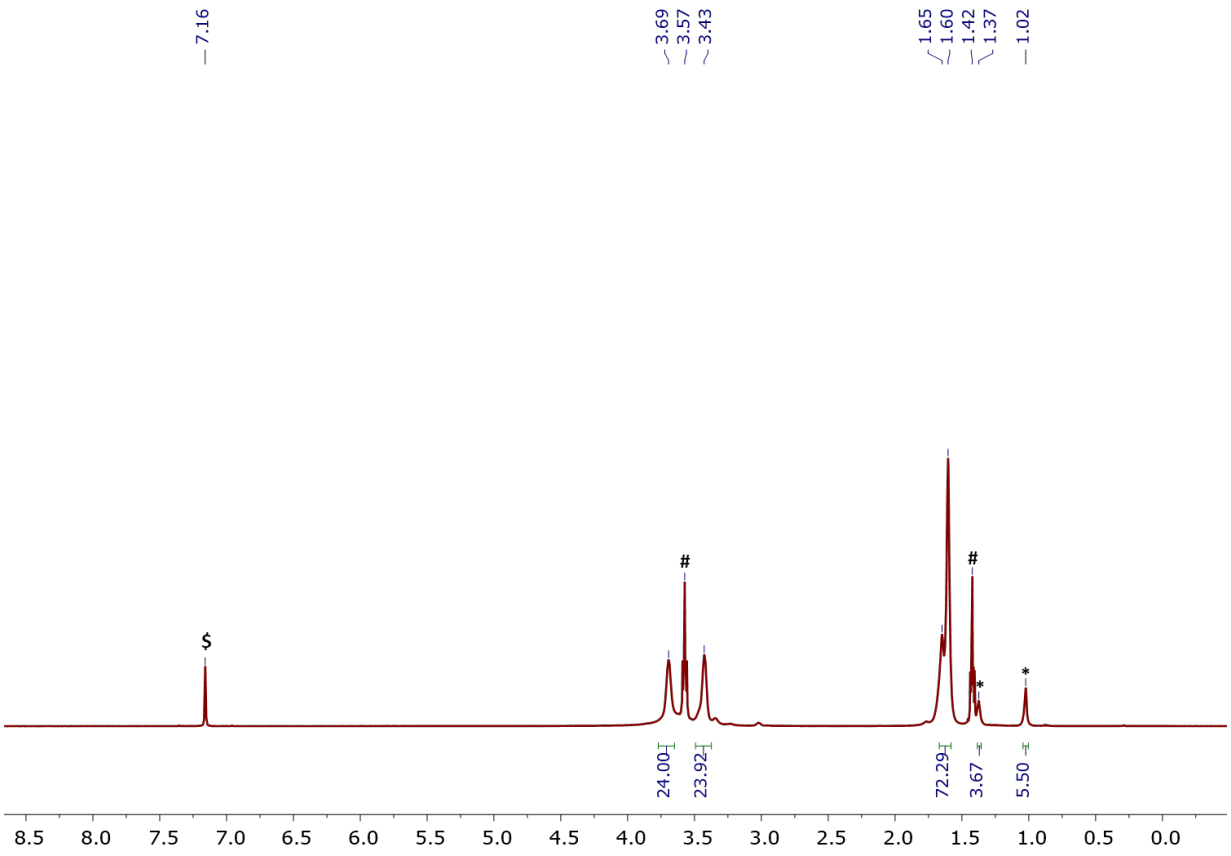

Figure S7. ^{1}H NMR of **4-U** (400.13 MHz, C_6D_6, 295 K). C_6D_5H noted as $. Residual THF noted as #. * is unknown.

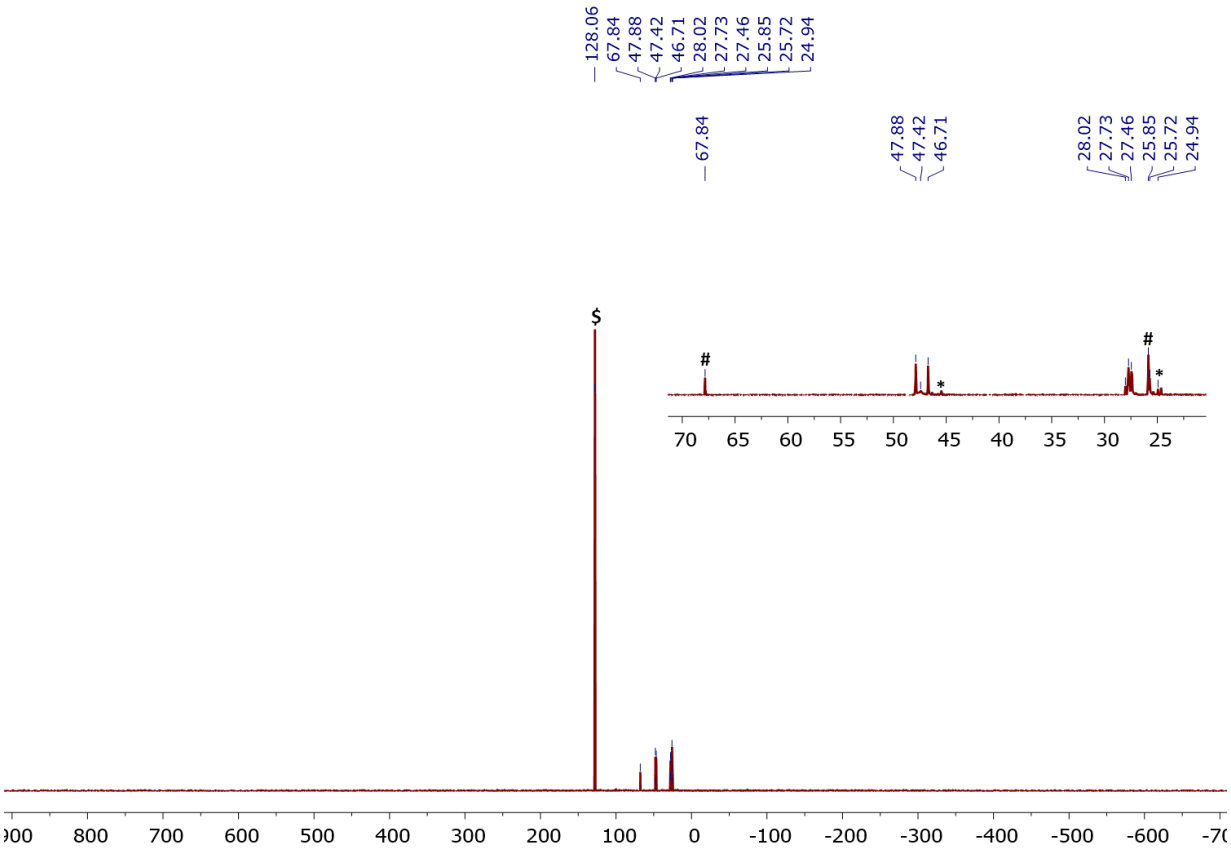

Figure S8. $^{13}C\{^{1}H\}$ NMR of **4-U** (100.61 MHz, C_6D_6, 295 K). C_6D_5H noted as $. Residual THF noted as #. * is unknown.

UV-Vis-NIR Spectroscopy

The broad and intense signal between 610-620 nm that is diagnostic of the $[S3]^{\cdot-}$ radical monoanion is absent in the UV-Vis spectra of both **3-U** and **4-U**.[5-8] This, in conjunction with the rest of the spectroscopic and structural data, confirms two the oxidation state of both **3-U** and **4-U** is as 6+, and that the tri-chalcogenide ligands are best described as the dianions, $[S_3]^{2-}$ and $[Se_3]^{2-}$, respectively.

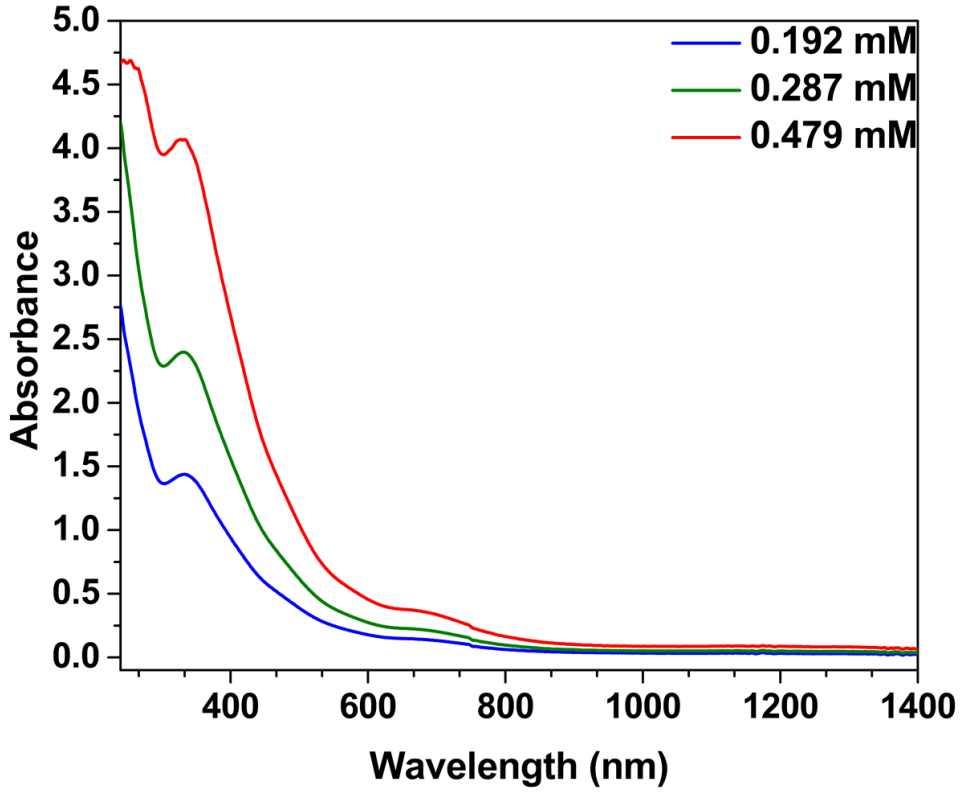

Figure S9. UV-Vis-NIR spectra of **3-U** in THF that depicts an absorbance maximum at 331 nm (where ε = 9021 $cm^{-1}M^{-1}$) and 702 nm (where ε = 700 $cm^{-1}M^{-1}$).

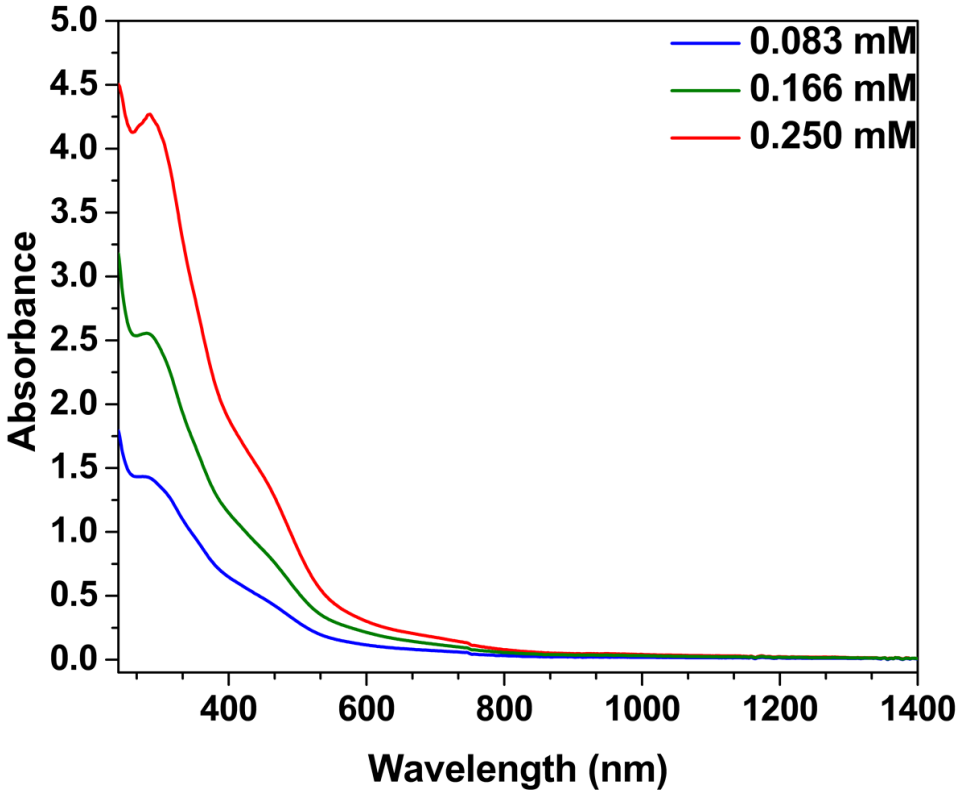

Figure S10. UV-Vis-NIR spectra of **4-U** in THF that depicts an absorbance maximum at 295 nm (where ε = 16821 $cm^{-1}M^{-1}$) and 510 nm (where ε = 2965 $cm^{-1}M^{-1}$).

Calculated Energy Profile

The optimization of different spin states for uranium complexes was carried out by employing DFT hybrid functional (B3PW91) along with small core pseudopotential Stuggart basis set for uranium, phosphorus with additional polarization functions for phosphorus atoms.[9-12] Pople basis sets (6-31G** for carbon, nitrogen, oxygen, hydrogen atoms) were employed for the rest of the atoms.[13, 14] Frequency calculations were performed to locate minima for the optimized structures. All the calculations were performed using Gaussian 09 suite of programs.[15]

Atom Label	Natural charges	
	s=0	s=1
U4	1.33376	1.11700
N1	-1.31751	-1.20820
N2	-1.30832	-1.19763
N103	-1.31081	-1.19605
N153	-1.32710	-1.22080
O3	-0.17866	-0.33785
O203	-0.20402	-0.32090

Table S1. DFT Computed Natural charges for $[UO_2(NP(pip)_3)_4]$.

Atom Label	Wiberg bond index	
	s=0	s=1
U4	0.0000	0.0000
N1	1.1801	1.3098
N2	1.1757	1.3141
N103	1.1733	1.3065
N153	1.1682	1.3019
O3	0.4902	1.0441
O203	0.5409	1.0505

Table S2. Computed Wiberg bond index for $[UO_2(NP(pip)_3)_4]$.

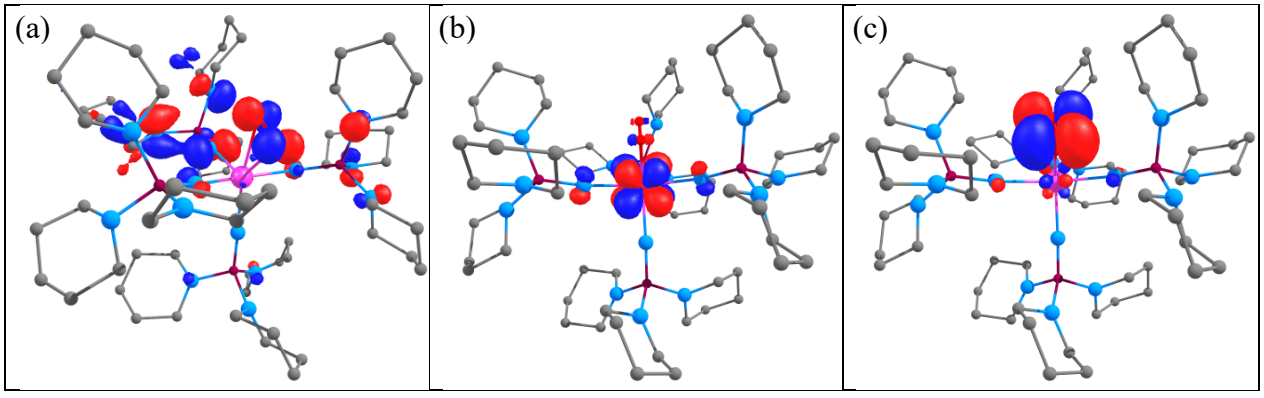

Figure S11. DFT computed MOs of $[UO_2(NP(pip)_3)_4]$ (s=1) (a) AMO-SOMO-1 (b) AMO-SOMO (c) BMO-LUMO (AMO=Alpha Molecular Orbital, BMO=Beta Molecular Orbital.

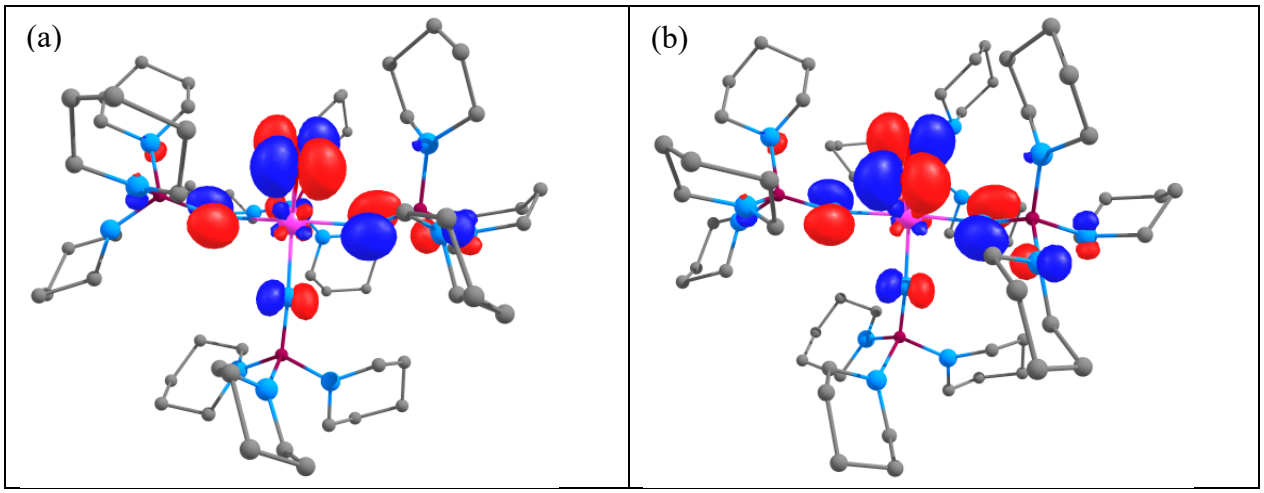

Figure S12. DFT computed MOs of $[UO_2(NP(pip)_3)_4]$ (s=0) (a) AMO-HOMO (b) BMO-HOMO (AMO=Alpha Molecular Orbital, BMO=Beta Molecular Orbital).

Natural Bond Analysis for $UO_2[NP(pip)_3]_4$ (s=0)

(0.97352) BD (1) N 1 - U 4
(85.17%) 0.9229* N 1 s(62.11%)p 0.61(37.88%)d 0.00(0.00%)
(14.83%) 0.3851* U 4 s(11.41%)p 1.89(21.57%)d 3.70(42.18%) f 2.17(24.76%)g 0.01(0.07%)

(0.90446) BD (2) N 1 - U 4
(87.20%) 0.9338* N 1 s(0.01%)p99.99(99.98%)d 0.42(0.01%)
(12.80%) 0.3578* U 4 s(0.42%)p45.83(19.46%)d65.40(27.78%) f99.99(52.29%)g 0.12(0.05%)

(0.89161) BD (3) N 1 - U 4
(89.27%) 0.9448* N 1 s(0.00%)p 1.00(99.99%)d 0.00(0.01%)
(10.73%) 0.3276* U 4 s(0.01%)p99.99(24.10%)d99.99(18.40%) f99.99(57.38%)g 7.11(0.11%)

(0.97384) BD (1) N 2 - U 4
(85.29%) 0.9235* N 2 s(62.23%)p 0.61(37.76%)d 0.00(0.01%)
(14.71%) 0.3835* U 4 s(14.09%)p 1.61(22.66%)d 2.65(37.34%) f 1.83(25.83%)g 0.01(0.09%)

(0.90709) BD (2) N 2 - U 4
(87.20%) 0.9338* N 2 s(0.00%)p 1.00(99.99%)d 0.00(0.01%)
(12.80%) 0.3578* U 4 s(0.55%)p22.25(12.29%)d61.45(33.94%) f96.28(53.18%)g 0.07(0.04%)

(0.89522) BD (3) N 2 - U 4
(88.53%) 0.9409* N 2 s(0.00%)p 1.00(99.98%)d 0.00(0.01%)
(11.47%) 0.3386* U 4 s(0.35%)p31.30(11.10%)d99.99(42.01%) f99.99(46.49%)g 0.15(0.05%)

(0.98346) BD (1) O 3 - U 4
(90.38%) 0.9507* O 3 s(30.94%)p 2.23(69.02%)d 0.00(0.04%)

(9.62%) 0.3102* U 4 s(8.25%)p 2.64(21.76%)d 4.09(33.79%) f 4.38(36.16%)g 0.00(0.04%)
(0.97309) BD (1) U 4 - N 103
(14.70%) 0.3834* U 4 s(14.33%)p 1.59(22.80%)d 2.57(36.81%) f 1.81(25.97%)g 0.01(0.09%)
(85.30%) 0.9236* N 103 s(62.22%)p 0.61(37.77%)d 0.00(0.01%)
(0.90522) BD (2) U 4 - N 103
(11.63%) 0.3410* U 4 s(0.34%)p34.04(11.58%)d99.99(41.08%) f99.99(46.94%)g 0.19(0.06%)
(88.37%) 0.9400* N 103 s(0.11%)p99.99(99.87%)d 0.17(0.02%)
(0.89705) BD (3) U 4 - N 103
(12.24%) 0.3498* U 4 s(0.06%)p99.99(12.56%)d99.99(35.90%) f99.99(51.43%)g 0.60(0.04%)
(87.76%) 0.9368* N 103 s(0.01%)p99.99(99.97%)d 1.60(0.02%)
(0.97093) BD (1) U 4 - N 153
(14.34%) 0.3787* U 4 s(18.50%)p 1.23(22.72%)d 2.33(43.05%) f 0.85(15.64%)g 0.01(0.10%)
(85.66%) 0.9255* N 153 s(62.74%)p 0.59(37.25%)d 0.00(0.01%)
(0.90397) BD (2) U 4 - N 153
(12.01%) 0.3466* U 4 s(0.09%)p99.99(20.51%)d99.99(31.90%) f99.99(47.44%)g 0.63(0.06%)
(87.99%) 0.9380* N 153 s(0.00%)p 1.00(99.99%)d 0.00(0.01%)
(0.89492) BD (3) U 4 - N 153
(11.67%) 0.3416* U 4 s(0.23%)p96.77(22.47%)d99.99(28.45%) f99.99(48.78%)g 0.29(0.07%)
(88.33%) 0.9398* N 153 s(0.04%)p99.99(99.95%)d 0.21(0.01%)
(0.98413) BD (1) U 4 - O 203
(10.54%) 0.3247* U 4 s(14.43%)p 1.35(19.48%)d 2.04(29.43%) f 2.54(36.63%)g 0.00(0.02%)
(89.46%) 0.9458* O 203 s(31.09%)p 2.22(68.87%)d 0.00(0.04%)

Natural Bond Analysis for $UO_2[NP(pip)_3]_4$ (s=1)
(0.97083) BD (1) N 1 - U 4
(82.83%) 0.9101* N 1 s(62.12%)p 0.61(37.88%)d 0.00(0.00%)
(17.17%) 0.4143* U 4 s(11.41%)p 1.85(21.05%)d 3.63(41.44%) f 2.28(26.03%)g 0.01(0.06%)
(0.90621) BD (2) N 1 - U 4
(85.70%) 0.9257* N 1 s(0.01%)p99.99(99.98%)d 0.57(0.01%)
(14.30%) 0.3782* U 4 s(0.28%)p73.76(20.62%)d83.49(23.34%) f99.99(55.70%)g 0.20(0.06%)
(0.97268) BD (1) N 2 - U 4
(82.38%) 0.9077* N 2 s(61.93%)p 0.61(38.06%)d 0.00(0.01%)
(17.62%) 0.4197* U 4 s(15.14%)p 1.41(21.36%)d 2.26(34.29%) f 1.93(29.15%)g 0.00(0.07%)
(0.89967) BD (2) N 2 - U 4
(86.64%) 0.9308* N 2 s(0.00%)p 1.00(99.99%)d 0.00(0.01%)

(13.36%) 0.3655* U 4 s(0.34%)p30.03(10.36%)d99.99(34.77%) f99.99(54.46%)g 0.21(0.07%)
(0.89158) BD (3) N 2 - U 4
(87.53%) 0.9356* N 2 s(0.21%)p99.99(99.77%)d 0.08(0.02%)
(12.47%) 0.3531* U 4 s(0.64%)p28.29(18.02%)d58.63(37.36%) f68.91(43.91%)g 0.11(0.07%)
(0.96637) BD (1) O 3 - U 4
(85.58%) 0.9251* O 3 s(34.07%)p 1.93(65.87%)d 0.00(0.06%)
(14.42%) 0.3798* U 4 s(10.56%)p 1.73(18.26%)d 3.70(39.05%) f 3.03(32.03%)g 0.01(0.10%)
(0.98438) BD (2) O 3 - U 4
(89.05%) 0.9437* O 3 s(0.36%)p99.99(99.59%)d 0.16(0.06%)
(10.95%) 0.3309* U 4 s(0.10%)p99.99(10.55%)d99.99(13.61%) f99.99(75.66%)g 0.83(0.08%)
(0.97142) BD (1) U 4 - N 103
(17.37%) 0.4168* U 4 s(15.24%)p 1.46(22.20%)d 2.22(33.76%) f 1.89(28.74%)g 0.00(0.06%)
(82.63%) 0.9090* N 103 s(62.10%)p 0.61(37.89%)d 0.00(0.01%)
(0.89962) BD (2) U 4 - N 103
(12.22%) 0.3495* U 4 s(0.25%)p53.34(13.58%)d99.99(37.52%) f99.99(48.56%)g 0.30(0.08%)
(87.78%) 0.9369* N 103 s(0.47%)p99.99(99.49%)d 0.07(0.03%)
(0.89179) BD (3) U 4 - N 103
(13.54%) 0.3680* U 4 s(0.42%)p34.05(14.32%)d85.45(35.94%) f99.99(49.26%)g 0.16(0.07%)
(86.46%) 0.9298* N 103 s(0.04%)p99.99(99.93%)d 0.60(0.03%)
(0.97076) BD (1) U 4 - N 153
(16.10%) 0.4013* U 4 s(18.37%)p 1.24(22.79%)d 2.34(42.94%) f 0.86(15.81%)g 0.00(0.09%)
(83.90%) 0.9160* N 153 s(63.92%)p 0.56(36.08%)d 0.00(0.01%)
(0.90406) BD (2) U 4 - N 153
(13.57%) 0.3683* U 4 s(0.17%)p90.70(15.65%)d99.99(31.91%) f99.99(52.22%)g 0.28(0.05%)
(86.43%) 0.9297* N 153 s(0.02%)p99.99(99.97%)d 0.36(0.01%)
(0.89432) BD (3) U 4 - N 153
(13.14%) 0.3625* U 4 s(0.24%)p61.43(14.89%)d99.99(27.91%) f99.99(56.90%)g 0.22(0.05%)
(86.86%) 0.9320* N 153 s(0.10%)p99.99(99.89%)d 0.10(0.01%)
(0.96612) BD (1) U 4 - O 203
(15.24%) 0.3904* U 4 s(16.80%)p 0.97(16.21%)d 1.71(28.73%) f 2.27(38.19%)g 0.00(0.07%)
(84.76%) 0.9207* O 203 s(32.24%)p 2.10(67.71%)d 0.00(0.05%)
(0.97779) BD (2) U 4 - O 203
(10.27%) 0.3204* U 4 s(0.15%)p99.99(19.85%)d99.99(17.51%) f99.99(62.37%)g 0.74(0.11%
(89.73%) 0.9473* O 203 s(0.32%)p99.99(99.62%)d 0.18(0.06%)

Optimized coordinates

[U(P(pip)$_3$)$_4$] (s=1)

U	0.020927000	-0.011305000	2.301813000
N	-0.010562000	2.016459000	3.105603000
N	-0.018812000	0.038619000	0.128459000
P	-0.024012000	0.048662000	1.448523000
P	-0.568014000	3.385639000	3.649832000
N	0.205714000	4.738502000	2.914182000
C	1.302025000	4.545205000	1.979124000
H	0.972827000	4.820984000	0.959906000
H	1.552087000	3.482053000	1.967314000
C	2.507098000	5.407561000	2.359617000
H	3.298871000	5.286651000	1.609509000
H	2.908361000	5.050260000	3.316982000
C	2.107549000	6.880330000	2.484116000
H	2.956641000	7.487713000	2.819482000
H	1.823784000	7.260436000	1.491529000
C	0.920599000	7.040979000	3.437569000
H	1.232308000	6.787735000	4.459259000
H	0.573326000	8.081874000	3.451787000
C	-0.232401000	6.120829000	3.026661000
H	-1.062365000	6.185796000	3.732213000
H	-0.622244000	6.465749000	2.050204000
N	-0.458412000	3.508075000	5.375659000
C	0.739944000	2.917644000	5.969829000
H	1.593689000	3.619498000	5.907881000
H	0.998194000	2.028341000	5.389789000
C	0.494200000	2.568052000	7.436997000
H	1.415847000	2.162118000	7.871739000
H	-0.265598000	1.778138000	7.488726000
C	0.020760000	3.792657000	8.222534000
H	-0.216544000	3.524795000	9.259020000
H	0.835460000	4.530298000	8.266764000
C	-1.189766000	4.425260000	7.536119000
H	-1.482373000	5.354667000	8.040238000
H	-2.046303000	3.741083000	7.594236000
C	-0.891237000	4.720605000	6.064929000
H	-1.785312000	5.106547000	5.568572000
H	-0.113878000	5.505882000	6.013467000
N	-2.242181000	3.802086000	3.450073000
C	-2.662492000	4.005481000	2.061240000
H	-2.759848000	3.036910000	1.539655000
H	-1.892152000	4.575855000	1.536185000
C	-4.002508000	4.739151000	2.022753000
H	-4.312605000	4.880654000	0.980134000

H	-3.871910000	5.736790000	2.461924000	C	-0.247116000	-1.960430000	-3.409677000
C	-5.066764000	3.964308000	2.802355000	H	0.527652000	-1.934900000	-4.200208000
H	-6.006544000	4.527892000	2.842603000	H	-1.050458000	-1.291564000	-3.726974000
H	-5.285144000	3.025737000	2.273533000	N	1.151478000	1.101473000	-2.128126000
C	-4.568984000	3.638365000	4.212154000	C	1.321699000	2.431191000	-1.557482000
H	-4.485361000	4.564105000	4.796957000	H	0.827360000	2.444985000	-0.582801000
H	-5.283592000	2.990123000	4.733953000	H	0.832429000	3.190538000	-2.196276000
C	-3.202361000	2.955050000	4.168522000	C	2.803487000	2.779983000	-1.414535000
H	-2.820624000	2.776823000	5.176042000	H	3.244426000	2.120578000	-0.656552000
H	-3.291152000	1.970733000	3.676583000	H	2.902828000	3.810019000	-1.050858000
N	0.289933000	-1.489484000	-2.144426000	C	3.541376000	2.603525000	-2.742845000
C	1.350164000	-2.316805000	-1.584627000	H	3.166590000	3.341846000	-3.467363000
H	1.634776000	-1.894329000	-0.617514000	H	4.612904000	2.801683000	-2.621328000
H	2.241466000	-2.292223000	-2.239090000	C	3.312821000	1.196209000	-3.296849000
C	0.884450000	-3.764518000	-1.423084000	H	3.778930000	1.085297000	-4.283944000
H	0.103424000	-3.793134000	-0.653037000	H	3.775063000	0.457616000	-2.629790000
H	1.719275000	-4.380113000	-1.066445000	C	1.816366000	0.892621000	-3.403160000
C	0.330700000	-4.316315000	-2.738350000	H	1.381848000	1.541788000	-4.187789000
H	1.145612000	-4.385906000	-3.474285000	H	1.661143000	-0.140705000	-3.719775000
H	-0.053562000	-5.334072000	-2.601236000	N	-1.518741000	0.531531000	-2.143199000
C	-0.762140000	-3.396720000	-3.286688000	C	-2.748687000	-0.070586000	-1.647929000
H	-1.109126000	-3.746045000	-4.267300000	H	-2.517734000	-0.609338000	-0.725371000
H	-1.626520000	-3.404849000	-2.610558000	H	-3.135900000	-0.805119000	-2.378842000

C	-3.818358000	0.991578000	- 1.391799000	H	-7.140278000	-2.097296000	1.372872000
H	-3.491981000	1.617426000	- 0.551778000	C	-6.542037000	-2.757172000	3.337508000
H	-4.754126000	0.503656000	- 1.092768000	H	-6.496713000	-2.351121000	4.356466000
C	-4.036800000	1.862190000	- 2.630770000	H	-7.275979000	-3.572970000	3.345008000
H	-4.470419000	1.247749000	- 3.433945000	C	-5.164919000	-3.310570000	2.959684000
H	-4.760626000	2.659049000	- 2.422506000	H	-4.824171000	-4.053289000	3.683037000
C	-2.709597000	2.451898000	- 3.112025000	H	-5.254755000	-3.834310000	1.989220000
H	-2.849428000	3.015388000	- 4.043096000	N	-2.840598000	-2.158414000	5.343109000
H	-2.321422000	3.150551000	- 2.359961000	C	-2.938194000	-0.807776000	5.894694000
C	-1.673741000	1.347205000	- 3.334482000	H	-3.969500000	-0.418147000	5.793138000
H	-1.996860000	0.729150000	- 4.194586000	H	-2.279707000	-0.158398000	5.313461000
H	-0.706889000	1.780667000	- 3.597129000	C	-2.552664000	-0.803766000	7.372870000
N	-1.709169000	-1.090684000	3.071132000	H	-2.665016000	0.210843000	7.774117000
P	-2.636284000	-2.238673000	3.622757000	H	-1.492847000	-1.073888000	7.461689000
N	-4.175458000	-2.250149000	2.849119000	C	-3.406546000	-1.795000000	8.164788000
C	-4.532837000	-1.209404000	1.898465000	H	-3.086017000	-1.838259000	9.212546000
H	-4.595190000	-1.641903000	0.882505000	H	-4.450835000	-1.449503000	8.169395000
H	-3.730970000	-0.467829000	1.890357000	C	-3.340604000	-3.180607000	7.522066000
C	-5.882543000	-0.582099000	2.252228000	H	-4.018452000	-3.878792000	8.028621000
H	-6.154477000	0.161607000	1.492685000	H	-2.324659000	-3.584354000	7.621627000
H	-5.785101000	-0.050942000	3.208210000	C	-3.701630000	-3.112781000	6.036434000
C	-6.968944000	-1.654455000	2.365151000	H	-3.582687000	-4.095492000	5.572200000
H	-7.922461000	-1.212831000	2.678390000	H	-4.766165000	-2.826611000	5.943704000

N	-2.170266000	-3.904183000	3.473979000
C	-2.091196000	-4.398245000	2.096378000
H	-1.178131000	-4.021577000	1.602217000
H	-2.943702000	-4.013249000	1.531220000
C	-2.079110000	-5.926405000	2.088863000
H	-2.010267000	-6.286362000	1.054977000
H	-3.031059000	-6.289612000	2.497451000
C	-0.916996000	-6.463986000	2.926235000
H	-0.954205000	-7.558333000	2.984850000
H	0.030131000	-6.207331000	2.431048000
C	-0.931938000	-5.844840000	4.325067000
H	-1.806180000	-6.208698000	4.881126000
H	-0.041137000	-6.144966000	4.890405000
C	-0.993133000	-4.319141000	4.247661000
H	-1.059162000	-3.877914000	5.244386000
H	-0.069487000	-3.934466000	3.781731000
N	1.828416000	-1.014031000	2.996794000
P	3.285150000	-1.217515000	3.560235000
N	4.067230000	-2.578358000	2.851609000
C	3.355292000	-3.440570000	1.921964000
H	3.770497000	-3.312406000	0.904761000
H	2.311767000	-3.118564000	1.893577000
C	3.484374000	-4.909822000	2.328302000
H	2.988270000	-5.544096000	1.582806000
H	2.962439000	-5.058858000	3.282697000
C	4.955093000	-5.308582000	2.477800000
H	5.044890000	-6.343691000	2.828256000
H	5.439510000	-5.269256000	1.490793000
C	5.681755000	-4.352899000	3.427787000
H	5.290858000	-4.477569000	4.446126000
H	6.754669000	-4.580928000	3.460737000
C	5.479009000	-2.899595000	2.990755000
H	5.944598000	-2.205298000	3.692680000
H	5.988723000	-2.754433000	2.019480000
N	3.314588000	-1.353122000	5.288646000
C	2.201655000	-2.103057000	5.869538000
H	2.396207000	-3.191594000	5.817598000
H	1.309501000	-1.897181000	5.273552000
C	1.990218000	-1.704626000	7.328798000
H	1.175814000	-2.304016000	7.753706000
H	1.674043000	-0.654559000	7.363409000
C	3.273799000	-1.884970000	8.140857000
H	3.138036000	-1.533599000	9.170664000
H	3.514643000	-2.956391000	8.203509000
C	4.433283000	-1.149964000	7.467386000
H	5.377125000	-1.347376000	7.990696000

H 4.258378000 -0.067069000 7.511134000
C 4.569952000 -1.569663000 6.002108000
H 5.356446000 -0.988550000 5.513671000
H 4.868754000 -2.634251000 5.966514000
N 4.491549000 0.014142000 3.358095000
C 4.900257000 0.253044000 1.970648000
H 4.119094000 0.812261000 1.425906000
H 5.018415000 -0.707710000 1.463392000
C 6.205468000 1.047539000 1.939461000
H 6.499293000 1.226999000 0.897959000
H 6.997688000 0.444886000 2.402364000
C 6.052617000 2.369529000 2.693463000
H 7.008200000 2.905686000 2.735933000
H 5.352776000 3.015658000 2.144894000
C 5.505131000 2.123062000 4.100575000
H 6.257669000 1.596223000 4.702187000
H 5.294805000 3.073641000 4.605718000
C 4.230302000 1.281563000 4.053366000
H 3.870377000 1.056168000 5.059566000
H 3.429496000 1.843408000 3.542217000

$[UO_2(P(pip)_3)_4]$ (s=0)

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N -2.141058000 11.536425000 7.469040000
O -0.296552000 9.645597000 8.666359000
U -0.013399000 11.435640000 7.542985000
P -3.657211000 11.283162000 7.863435000
P -0.012492000 11.648163000 3.844455000
N -4.081780000 11.915604000 9.414933000
C -3.152567000 11.595934000 10.502093000
H -2.141047000 11.510136000 10.100089000
H -3.410660000 10.616491000 10.946152000
C -3.220843000 12.665891000 11.590236000
H -2.857054000 13.612373000 11.171793000
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H -4.708599000 13.665253000 12.828323000
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H -5.404855000 14.049884000 10.478813000
C -5.466003000 11.982674000 9.881966000
H -5.776478000 11.020685000 10.329944000
H -6.123845000 12.175912000 9.031703000
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C -5.093626000 11.518784000 5.561565000
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C	-6.462699000	11.946336000	H	-6.494379000	7.764821000
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H	-6.594829000	11.564813000	H	-5.212863000	8.685633000
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H	-7.241290000	11.485829000	C	-5.451186000	9.147816000
5.652898000			7.996075000		
C	-6.611950000	13.469149000	H	-5.832694000	8.638916000
5.060639000			7.091981000		
H	-7.622634000	13.766095000	H	-6.114894000	9.995349000
4.756305000			8.178332000		
H	-5.921262000	13.911764000	N	-1.030410000	12.894854000
4.328710000			3.236102000		
C	-6.281423000	14.014755000	C	-1.783830000	12.814050000
6.451584000			1.993433000		
H	-6.278093000	15.111642000	H	-1.948404000	11.763226000
6.446369000			1.745244000		
H	-7.053251000	13.697767000	H	-1.221683000	13.261781000
7.165328000			1.150850000		
C	-4.922212000	13.504633000	C	-3.118951000	13.550910000
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H	-4.128411000	13.908424000	H	-3.748982000	13.027454000
6.278121000			2.840958000		
H	-4.709532000	13.847726000	H	-3.636958000	13.517247000
7.943574000			1.145122000		
N	-4.104930000	9.634146000	C	-2.901296000	14.995449000
7.728998000			2.563532000		
C	-3.138838000	8.578069000	H	-3.861393000	15.509599000
7.468686000			2.690260000		
H	-2.159245000	9.033401000	H	-2.354787000	15.541673000
7.326293000			1.780380000		
H	-3.422366000	8.059088000	C	-2.094870000	15.026160000
6.535486000			3.862124000		
C	-3.088661000	7.566280000	H	-1.873530000	16.059194000
8.613990000			4.157164000		
H	-2.667932000	8.065430000	H	-2.678777000	14.571980000
9.494538000			4.670985000		
H	-2.402678000	6.752084000	C	-0.787362000	14.249436000
8.349970000			3.719676000		
C	-4.482916000	7.015608000	H	-0.116881000	14.793685000
8.923604000			3.028059000		
H	-4.452993000	6.345702000	H	-0.283178000	14.175799000
9.791186000			4.686639000		
H	-4.830723000	6.409333000	N	-0.604869000	10.202006000
8.073552000			3.139415000		

C	-0.166678000	9.662164000	1.862741000
H	0.786315000	10.120528000	1.593720000
H	-0.886000000	9.908912000	1.058381000
C	-0.018885000	8.140984000	1.934353000
H	0.802766000	7.899399000	2.620228000
H	0.255496000	7.755476000	0.944567000
C	-1.310854000	7.491594000	2.432284000
H	-1.185580000	6.406631000	2.527471000
H	-2.105970000	7.651056000	1.688791000
C	-1.735629000	8.106587000	3.767063000
H	-2.699809000	7.697458000	4.091735000
H	-0.999246000	7.856734000	4.541009000
C	-1.839563000	9.628441000	3.664001000
H	-2.691266000	9.885782000	3.006739000
H	-2.032556000	10.072081000	4.645151000
N	1.518485000	11.967897000	3.142812000
C	1.707476000	12.552041000	1.823307000
H	0.775717000	13.021828000	1.504109000
H	1.948581000	11.773462000	1.075144000
C	2.845020000	13.573986000	1.827620000
H	2.560079000	14.421038000	2.464676000
H	2.988548000	13.961261000	0.811202000
C	4.129357000	12.937006000	2.357010000
H	4.939206000	13.674854000	2.401462000
H	4.457621000	12.153596000	1.657636000
C	3.883668000	12.320312000	3.734041000
H	4.778403000	11.794382000	4.085528000
H	3.668919000	13.114142000	4.460302000
C	2.705766000	11.345149000	3.720047000
H	2.987092000	10.446496000	3.140714000
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C	2.799065000	10.232455000	10.572790000
H	2.263415000	11.073452000	10.129838000
H	3.789596000	10.588287000	10.917247000
C	2.015769000	9.683033000	11.764883000
H	0.994870000	9.478850000	11.426366000
H	1.956752000	10.455532000	12.541308000
C	2.661430000	8.412754000	12.318601000
H	2.054360000	7.989500000	13.127886000
H	3.641327000	8.657378000	12.755996000
C	2.856762000	7.389625000	11.199603000
H	3.394007000	6.505417000	11.565666000
H	1.878808000	7.052433000	10.833788000

C 3.636859000 8.006645000 10.037648000
H 4.655375000 8.248310000 10.394294000
H 3.736867000 7.294394000 9.216001000
N 2.910206000 8.205236000 7.116320000
C 3.306489000 8.123540000 5.710585000
H 4.186632000 8.751022000 5.553406000
H 2.503993000 8.512956000 5.060198000
C 3.596613000 6.669060000 5.337515000
H 3.881923000 6.613127000 4.279581000
H 4.455579000 6.318307000 5.924334000
C 2.382217000 5.780714000 5.616738000
H 2.618355000 4.727824000 5.421390000
H 1.572565000 6.054205000 4.924845000
C 1.893712000 5.971544000 7.054063000
H 0.957890000 5.424260000 7.220552000
H 2.634359000 5.562127000 7.753788000
C 1.675124000 7.452070000 7.364892000
H 0.860082000 7.839628000 6.728744000
H 1.361394000 7.609325000 8.398037000
N 4.665849000 10.169628000 7.486733000
C 5.008212000 11.557764000 7.219718000
H 4.073704000 12.105619000 7.079352000
H 5.575645000 11.605175000 6.274634000
C 5.862437000 12.167962000 8.333126000
H 5.258586000 12.237979000 9.247313000
H 6.151719000 13.189885000 8.057133000
C 7.104279000 11.312163000 8.593698000
H 7.689857000 11.717297000 9.427502000
H 7.756716000 11.344999000 7.708323000
C 6.708364000 9.860300000 8.871759000
H 7.598764000 9.226588000 8.971752000
H 6.165124000 9.806782000 9.823839000
C 5.815259000 9.315117000 7.752821000
H 6.415984000 9.240158000 6.829077000
H 5.467846000 8.304583000 7.980728000
N 0.264717000 13.436331000 8.209427000
P 0.733792000 14.902243000 8.584120000
N 1.412613000 14.957917000 10.172025000
C 0.816598000 14.052775000 11.156721000
H 0.540652000 13.127119000 10.648160000
H -0.106910000 14.491890000 11.578143000
C 1.801083000 13.783417000 12.293343000
H 2.666223000 13.243157000 11.889037000
H 1.325776000 13.129353000 13.033884000
C 2.264033000 15.088616000 12.942201000
H 3.017746000 14.895997000 13.714871000

H	1.410526000	15.564513000	13.447035000
C	2.812386000	16.041373000	11.879568000
H	3.061719000	17.015382000	12.318484000
H	3.738265000	15.629163000	11.457727000
C	1.799738000	16.242360000	10.750493000
H	0.918954000	16.774525000	11.154621000
H	2.231172000	16.867456000	9.964176000
N	1.992809000	15.693504000	7.702641000
C	1.703078000	15.992483000	6.297968000
H	0.656366000	16.292606000	6.205125000
H	1.839752000	15.089818000	5.678334000
C	2.631461000	17.099169000	5.796958000
H	2.419630000	17.302777000	4.740070000
H	2.417434000	18.020679000	6.353796000
C	4.098325000	16.706672000	5.986638000
H	4.760782000	17.533484000	5.704234000
H	4.334667000	15.870495000	5.313216000
C	4.357811000	16.270321000	7.430234000
H	5.379840000	15.887639000	7.539959000
H	4.262353000	17.134204000	8.101214000
C	3.361659000	15.193858000	7.861902000
H	3.508684000	14.289100000	7.249543000
H	3.512667000	14.906776000	8.904034000
N	-0.540307000	16.039979000	8.411545000
C	-1.906809000	15.592821000	8.172096000
H	-1.930405000	14.501362000	8.213523000
H	-2.211923000	15.888350000	7.152039000
C	-2.873098000	16.222546000	9.177156000
H	-2.641025000	15.840707000	10.179749000
H	-3.898796000	15.913335000	8.943369000
C	-2.758930000	17.748216000	9.169479000
H	-3.414242000	18.193111000	9.927723000
H	-3.101110000	18.130557000	8.196281000
C	-1.307673000	18.176720000	9.394390000
H	-1.202859000	19.264875000	9.298907000
H	-1.000400000	17.908799000	10.413521000
C	-0.377729000	17.486667000	8.393271000
H	-0.614084000	17.867713000	7.382044000
H	0.666957000	17.737281000	8.585828000
O	-0.149609000	10.767507000	9.547251000

$[UO_2(P(pip)_3)_4]$ (s=1)

N	0.001523000	11.619991000	5.407219000
N	-2.167339000	11.497074000	7.678040000
O	-0.355069000	9.738319000	9.098050000
U	-0.015763000	11.555848000	7.543134000
P	-3.700381000	11.250523000	7.983570000

P -0.033033000 11.691760000 3.832844000
N -4.198548000 11.916425000 9.501203000
C -3.266727000 11.731611000 10.614889000
H -2.248905000 11.748333000 10.223655000
H -3.420659000 10.743850000 11.087383000
C -3.464310000 12.823490000 11.664453000
H -3.190307000 13.788955000 11.221489000
H -2.780778000 12.644291000 12.503020000
C -4.914087000 12.871601000 12.148206000
H -5.066341000 13.701947000 12.848129000
H -5.141774000 11.948665000 12.701545000
C -5.865514000 12.987579000 10.956546000
H -6.911132000 12.929152000 11.283761000
H -5.730918000 13.962750000 10.470691000
C -5.594367000 11.881887000 9.934269000
H -5.838943000 10.909502000 10.400293000
H -6.239777000 12.001826000 9.060690000
N -4.916314000 11.959126000 6.967698000
C -4.987499000 11.428434000 5.604880000
H -4.854015000 10.344368000 5.642044000
H -4.168671000 11.836735000 4.987526000
C -6.333514000 11.785364000 4.974099000
H -6.372596000 11.395229000 3.949589000
H -7.132031000 11.290003000 5.541488000
C -6.556101000 13.299024000 4.984337000
H -7.554240000 13.547636000 4.604696000
H -5.834374000 13.772654000 4.303828000
C -6.356112000 13.861958000 6.392877000
H -6.407274000 14.957638000 6.382532000
H -7.161160000 13.507177000 7.050031000
C -5.011515000 13.421347000 6.972974000
H -4.191668000 13.863071000 6.380520000
H -4.891607000 13.774719000 7.999175000
N -4.118898000 9.587385000 7.882723000
C -3.129412000 8.553301000 7.627568000
H -2.150037000 9.026118000 7.551405000
H -3.349883000 8.071677000 6.657233000
C -3.136889000 7.490380000 8.727432000
H -2.783493000 7.951169000 9.657618000
H -2.426177000 6.694744000 8.471877000
C -4.541734000 6.913606000 8.921303000
H -4.559375000 6.205756000 9.758494000
H -4.825139000 6.342910000 8.024196000
C -5.563192000 8.032158000 9.142949000
H -6.581573000 7.625323000 9.186088000
H -5.367432000 8.523891000 10.104743000

C	-5.473793000	9.075697000	8.026061000
H	-5.786238000	8.602526000	7.076459000
H	-6.161538000	9.904845000	8.200038000
N	-1.043912000	12.939450000	3.212105000
C	-1.774225000	12.869484000	1.956116000
H	-1.912666000	11.820585000	1.684516000
H	-1.208105000	13.345588000	1.131812000
C	-3.126657000	13.575784000	2.068197000
H	-3.756005000	13.023289000	2.776776000
H	-3.629741000	13.552148000	1.093527000
C	-2.946178000	15.014659000	2.553676000
H	-3.918615000	15.506710000	2.674567000
H	-2.398311000	15.587759000	1.790896000
C	-2.161577000	15.034975000	3.865890000
H	-1.965668000	16.066105000	4.184609000
H	-2.751055000	14.555003000	4.655952000
C	-0.836529000	14.286580000	3.730851000
H	-0.164317000	14.860113000	3.064902000
H	-0.349766000	14.199455000	4.706082000
N	-0.615048000	10.245076000	3.113685000
C	-0.173202000	9.713897000	1.835530000
H	0.770827000	10.188634000	1.562659000
H	-0.899404000	9.948789000	1.033526000
C	-0.000555000	8.194848000	1.904718000
H	0.826955000	7.965992000	2.588052000
H	0.276778000	7.814200000	0.913818000
C	-1.280476000	7.524008000	2.406191000
H	-1.137562000	6.441004000	2.499776000
H	-2.080299000	7.671388000	1.665261000
C	-1.711163000	8.131520000	3.742470000
H	-2.667858000	7.706784000	4.070183000
H	-0.967801000	7.893693000	4.513678000
C	-1.838134000	9.651791000	3.640031000
H	-2.696706000	9.897010000	2.986890000
H	-2.031202000	10.090375000	4.622927000
N	1.506368000	11.996261000	3.135896000
C	1.713862000	12.615220000	1.836052000
H	0.795676000	13.119238000	1.530075000
H	1.937217000	11.854658000	1.063634000
C	2.876757000	13.607952000	1.875039000
H	2.608054000	14.443628000	2.533783000
H	3.036279000	14.019960000	0.870735000
C	4.143133000	12.926836000	2.393344000
H	4.968697000	13.645006000	2.464481000
H	4.458956000	12.157322000	1.673040000
C	3.875118000	12.274148000	3.749583000

H 4.756279000 11.718285000 4.090099000
H 3.670599000 13.049260000 4.498560000
C 2.675892000 11.327075000 3.694227000
H 2.941618000 10.443273000 3.084435000
H 2.418749000 10.983485000 4.700212000
N 1.981589000 10.750076000 7.687262000
P 3.033982000 9.607188000 7.997851000
N 2.976204000 9.042903000 9.629721000
C 2.854631000 10.066868000 10.665330000
H 2.301278000 10.910074000 10.247811000
H 3.856301000 10.430059000 10.966498000
C 2.133802000 9.511283000 11.893172000
H 1.099097000 9.288201000 11.612212000
H 2.101396000 10.284032000 12.670812000
C 2.823807000 8.249916000 12.414451000
H 2.262183000 7.816640000 13.250692000
H 3.818440000 8.511283000 12.805902000
C 2.984730000 7.229812000 11.286521000
H 3.553313000 6.355583000 11.628024000
H 1.996884000 6.873963000 10.967357000
C 3.697431000 7.857442000 10.087299000
H 4.728766000 8.115597000 10.392353000
H 3.767956000 7.145870000 9.261615000
N 2.906797000 8.083656000 7.182073000
C 3.278040000 8.042244000 5.766916000
H 4.169429000 8.655491000 5.616706000
H 2.475287000 8.471186000 5.141933000
C 3.531407000 6.595351000 5.342147000
H 3.800475000 6.568148000 4.278967000
H 4.390452000 6.207471000 5.904918000
C 2.301856000 5.724302000 5.609578000
H 2.512180000 4.673689000 5.376522000
H 1.488859000 6.037833000 4.939148000
C 1.837765000 5.876284000 7.059576000
H 0.892321000 5.344275000 7.221211000
H 2.579005000 5.428510000 7.734559000
C 1.658639000 7.350174000 7.422789000
H 0.841935000 7.778032000 6.813996000
H 1.372063000 7.471586000 8.469680000
N 4.625165000 10.094756000 7.568578000
C 4.915311000 11.494952000 7.298415000
H 3.960385000 12.017095000 7.201020000
H 5.442704000 11.566816000 6.332219000
C 5.795177000 12.119093000 8.383514000
H 5.225261000 12.168097000 9.320625000
H 6.046750000 13.149986000 8.104464000

C	7.068277000	11.294974000	8.590532000
H	7.674624000	11.710704000	9.404024000
H	7.685047000	11.350348000	7.681084000
C	6.723081000	9.830867000	8.873537000
H	7.633550000	9.221419000	8.936447000
H	6.217013000	9.757155000	9.844669000
C	5.804225000	9.268059000	7.784742000
H	6.373059000	9.211956000	6.839548000
H	5.490135000	8.248167000	8.019761000
N	0.341718000	13.584919000	8.108045000
P	0.801406000	15.046014000	8.490472000
N	1.493868000	15.109027000	10.074284000
C	0.897945000	14.218061000	11.069993000
H	0.588065000	13.301169000	10.565854000
H	-0.005401000	14.678325000	11.512729000
C	1.899869000	13.918812000	12.183947000
H	2.741771000	13.358589000	11.758010000
H	1.425100000	13.274170000	12.933228000
C	2.410004000	15.210273000	12.825083000
H	3.176754000	14.996922000	13.579310000
H	1.580387000	15.704914000	13.351293000
C	2.956015000	16.153421000	11.752377000
H	3.238753000	17.119532000	12.188591000
H	3.861676000	15.720566000	11.307924000
C	1.922954000	16.382149000	10.646827000
H	1.064675000	16.933681000	11.073711000
H	2.350808000	16.999720000	9.852873000
N	2.055335000	15.845043000	7.602622000
C	1.743620000	16.166594000	6.207646000
H	0.703983000	16.496657000	6.142020000
H	1.841102000	15.267878000	5.574580000
C	2.690577000	17.253278000	5.697824000
H	2.459889000	17.476472000	4.648869000
H	2.515895000	18.172675000	6.271524000
C	4.149749000	16.817649000	5.848001000
H	4.828970000	17.627959000	5.557621000
H	4.345721000	15.981807000	5.161290000
C	4.430244000	16.359882000	7.280929000
H	5.443217000	15.947055000	7.362907000
H	4.375336000	17.219462000	7.961889000
C	3.413841000	15.308164000	7.726103000
H	3.525380000	14.404100000	7.103617000
H	3.580601000	15.008932000	8.762609000
N	-0.480194000	16.178625000	8.332665000
C	-1.837708000	15.731502000	8.050705000
H	-1.849672000	14.639150000	8.044816000

H	-2.130353000	16.069981000	7.040164000
C	-2.826264000	16.304443000	9.067524000
H	-2.606670000	15.876155000	10.053988000
H	-3.845130000	15.998279000	8.801695000
C	-2.724179000	17.829913000	9.134044000
H	-3.392177000	18.233271000	9.904434000
H	-3.058585000	18.255104000	8.176014000
C	-1.279410000	18.261499000	9.395765000
H	-1.185327000	19.353949000	9.351323000
H	-0.980273000	17.950036000	10.404938000
C	-0.330523000	17.625422000	8.376551000
H	-0.557933000	18.047325000	7.379497000
H	0.709353000	17.877790000	8.592135000
O	-0.153487000	10.827337000	9.804487000

$[UO(P(pip)_3)_4]_2$ (s=1)

N	-0.301333000	13.175597000	12.037549000
N	-2.496240000	12.663978000	14.127988000
O	-0.384386000	12.994990000	16.425809000
U	-0.382910000	13.114684000	14.243019000
P	-4.037735000	12.450094000	13.829483000
P	-0.269315000	13.232918000	10.462944000
N	-5.011344000	12.617646000	15.260476000
C	-4.417609000	12.023360000	16.462614000
H	-3.362077000	12.302332000	16.501686000
H	-4.470888000	10.918884000	16.411584000
C	-5.149045000	12.498088000	17.713718000
H	-4.959249000	13.567203000	17.852697000
H	-4.715195000	11.993626000	18.581134000
C	-6.653883000	12.243692000	17.630611000
H	-7.168997000	12.661633000	18.504640000
H	-6.847090000	11.161421000	17.641171000
C	-7.216079000	12.830312000	16.338542000
H	-8.277283000	12.577738000	16.219415000
H	-7.142221000	13.925190000	16.358834000
C	-6.434637000	12.299940000	15.139351000
H	-6.585607000	11.206818000	15.080162000
H	-6.815824000	12.734144000	14.212371000
N	-4.939539000	13.496781000	12.790567000
C	-4.700700000	13.448299000	11.349682000
H	-4.445815000	12.428158000	11.062362000
H	-3.838114000	14.075230000	11.074682000
C	-5.955157000	13.917398000	10.608116000
H	-5.783190000	13.878797000	9.525591000
H	-6.777080000	13.221754000	10.823624000
C	-6.352037000	15.329032000	11.043249000
H	-7.290529000	15.634299000	10.565182000

H	-5.583465000	16.039008000	N	-1.319492000	14.432942000
10.706386000			9.735076000		
C	-6.469740000	15.403652000	C	-1.836243000	14.292396000
12.565985000			8.374406000		
H	-6.639983000	16.437528000	H	-2.077692000	13.245282000
12.891028000			8.199072000		
H	-7.336065000	14.815839000	H	-1.093520000	14.580464000
12.897026000			7.608765000		
C	-5.212081000	14.859671000	C	-3.085039000	15.140959000
13.246341000			8.138114000		
H	-4.356921000	15.518909000	H	-3.906249000	14.759145000
13.017918000			8.754248000		
H	-5.334030000	14.845564000	H	-3.387252000	15.033264000
14.329438000			7.089070000		
N	-4.381513000	10.918347000	C	-2.826127000	16.601616000
13.103939000			8.490921000		
C	-3.420935000	9.831060000	H	-3.728842000	17.206345000
13.211835000			8.344757000		
H	-2.584986000	10.177071000	H	-2.058146000	17.012573000
13.822904000			7.818942000		
H	-3.013048000	9.595278000	C	-2.342975000	16.686723000
12.217697000			9.936152000		
C	-4.056485000	8.562362000	H	-2.096954000	17.721717000
13.782274000			10.201896000		
H	-4.352235000	8.741153000	H	-3.147751000	16.363055000
14.824490000			10.607176000		
H	-3.311581000	7.758540000	C	-1.110939000	15.811941000
13.790412000			10.169925000		
C	-5.279220000	8.148601000	H	-0.263239000	16.275815000
12.962840000			9.631713000		
H	-5.757442000	7.261463000	H	-0.848891000	15.784594000
13.394724000			11.231318000		
H	-4.956812000	7.868543000	N	-0.738535000	11.748718000
11.948927000			9.662451000		
C	-6.270931000	9.307957000	C	-0.265497000	11.390516000
12.875183000			8.326225000		
H	-7.107407000	9.058792000	H	0.767249000	11.720002000
12.209820000			8.217925000		
H	-6.696044000	9.499573000	H	-0.844354000	11.889174000
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C	-5.585321000	10.576377000	C	-0.341057000	9.885266000
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H	-5.321776000	10.406327000	H	0.368467000	9.369333000
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H	-6.273044000	11.423469000	H	-0.029497000	9.689838000
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C	-1.748799000	9.357088000	8.330902000
H	-1.794301000	8.272349000	8.178215000
H	-2.449415000	9.806928000	7.611797000
C	-2.168336000	9.724351000	9.751556000
H	-3.199155000	9.404135000	9.944099000
H	-1.526165000	9.197990000	10.468250000
C	-2.062890000	11.229933000	9.995763000
H	-2.848516000	11.725234000	9.393686000
H	-2.257562000	11.469133000	11.045172000
N	1.300102000	13.592016000	9.780988000
C	1.466075000	14.216961000	8.470558000
H	0.666551000	14.941382000	8.324421000
H	1.390446000	13.485784000	7.645306000
C	2.813475000	14.925409000	8.334266000
H	2.844650000	15.782587000	9.016538000
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C	3.963876000	13.977926000	8.657031000
H	4.927615000	14.496772000	8.593188000
H	3.992745000	13.166886000	7.914185000
C	3.755664000	13.389172000	10.049864000
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C	2.393236000	12.706855000	10.174592000
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H	2.206520000	12.392378000	11.205457000
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C	2.384713000	10.057724000	16.590441000
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C	2.154427000	9.152809000	17.796178000
H	1.103559000	8.846433000	17.814202000
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C	3.056693000	7.919392000	17.766799000
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C	2.921017000	7.195053000	16.430368000
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C	3.175964000	8.169393000	15.283730000
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H 2.201316000 8.218620000 9.538569000
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C 0.809002000 6.798965000 12.385057000
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H 1.686941000 6.305365000 12.822264000
C 0.598797000 8.145518000 13.082071000
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H 0.524697000 8.015686000 14.162314000
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C 5.437906000 12.262926000 14.213473000
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C -0.178312000 19.122498000 12.962622000
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P 3.168799000 13.700741000 20.347091000
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N 3.891690000 14.431022000 18.943607000
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H	6.061251000	14.295194000	N	4.206828000	12.435670000
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C	5.643263000	15.800743000	C	3.791234000	11.046288000
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H	6.697578000	16.093577000	H	2.818623000	11.020069000
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H	5.042437000	16.713330000	H	3.650801000	10.630424000
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C	5.292738000	14.844143000	C	4.829532000	10.191198000
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H	5.964031000	13.968235000	H	4.889359000	10.509194000
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H	5.465673000	15.318984000	H	4.503199000	9.144725000
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N	3.556875000	14.949594000	C	6.202849000	10.324194000
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C	3.475152000	14.662061000	H	6.957399000	9.746848000
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H	3.737726000	13.617564000	H	6.158071000	9.899529000
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H	2.443963000	14.794089000	C	6.607532000	11.795372000
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C	4.431118000	15.583675000	H	7.547693000	11.909737000
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23.396830000			22.580798000		
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23.876620000			21.522356000		
H	3.134875000	17.297182000	N	-0.002523000	14.172519000
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21.693822000			26.025783000		
H	5.056195000	17.241629000	H	-0.171096000	14.076635000
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C	3.131710000	16.316262000	C	1.357659000	15.478500000
21.185805000			26.211789000		

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27.248089000			24.100540000		
C	0.486044000	16.703903000	H	2.556902000	12.305170000
25.957931000			24.722305000		
H	1.051771000	17.627496000	H	2.052904000	11.919687000
26.128018000			23.065943000		
H	-0.354244000	16.713075000	N	-2.013883000	12.311040000
26.668043000			24.510231000		
C	-0.051472000	16.651450000	C	-2.372769000	12.728292000
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H	-0.724943000	17.495680000	H	-1.982113000	13.729851000
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23.823428000			26.640507000		
C	-0.804041000	15.347773000	C	-3.884909000	12.737924000
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H	-1.740938000	15.372757000	H	-4.339483000	13.518218000
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H	-0.691505000	10.775941000	H	-4.104435000	10.613639000
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H	0.746874000	11.539615000	C	-4.138539000	11.044956000
26.624875000			24.291248000		
C	1.059209000	9.533323000	H	-4.526100000	10.056013000
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C	2.728968000	10.220922000	P	-1.644090000	9.288547000
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C	-1.337747000	8.442880000	16.217966000
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C	-1.706449000	6.960095000	16.162706000
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H	-0.203613000	6.253487000	17.550841000
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C	-3.349171000	17.936412000	21.761636000
H	-3.086290000	17.968306000	22.835892000
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C	0.248204000	6.037552000	-1.187201000
C	0.852019000	7.170881000	-0.354193000
C	2.303275000	6.852802000	0.013512000
C	2.400806000	5.478615000	0.680556000
P	-0.904868000	3.620722000	-0.299175000
N	-2.122428000	4.277355000	0.747434000
C	-1.951869000	4.005796000	2.173217000
C	-3.296345000	4.079613000	2.897010000
C	-3.972298000	5.430910000	2.661094000
C	-4.073525000	5.715854000	1.162434000
C	-2.706473000	5.588968000	0.487090000
N	-0.368003000	2.246474000	0.277145000
U	-0.128296000	0.127535000	-0.200612000
O	-0.550134000	0.462636000	-1.927016000
N	0.290749000	-0.239027000	1.772157000
P	0.656189000	-0.614628000	3.269753000
N	-0.765687000	-0.953216000	4.179768000
C	-2.034828000	-0.385566000	3.719657000
C	-3.206453000	-1.225455000	4.226805000
C	-3.165336000	-1.386143000	5.746833000
C	-1.809847000	-1.942931000	6.180074000
C	-0.670029000	-1.082672000	5.632788000
N	1.646706000	0.599747000	3.971953000
C	1.409889000	1.985394000	3.563576000
C	2.718191000	2.774207000	3.595135000
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H	1.758048000	18.279104000	H	-4.374755000	17.535919000
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C	1.406567000	16.386459000	H	-3.714008000	19.978784000
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H 4.974695000 15.210449000 19.931266000
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H 4.580611000 17.388908000 21.359318000
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26.581480000			26.387121000		
H	0.834650000	13.513084000	H	2.898920000	10.431825000
26.767869000			27.083932000		
H	-0.564527000	14.379083000	C	2.520311000	10.400650000
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26.653774000			24.704049000		
H	1.817386000	15.605948000	H	2.120203000	9.702447000
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C	0.093762000	16.856579000	H	2.280893000	12.478219000
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H	0.671557000	17.788077000	H	1.740821000	12.081656000
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H	-0.698969000	16.962281000	N	-2.314207000	12.177246000
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C	-0.534722000	16.636759000	C	-2.724063000	12.631051000
24.924373000			26.657233000		
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24.161814000			27.457108000		
C	-1.291693000	15.310066000	C	-4.245780000	12.690361000
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H	-2.193849000	15.389506000	H	-4.633343000	13.450481000
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H	-1.625170000	15.110484000	H	-4.506937000	13.005259000
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C	0.211178000	10.975610000	H	-5.957951000	11.378777000
26.619230000			26.509855000		

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C	-3.309708000	15.538187000	H	-8.084519000	14.370573000
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H	-2.576528000	14.734056000	H	-6.839591000	13.126781000
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H	-3.307220000	15.608272000	C	-5.776137000	13.831740000
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21.270236000
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20.758190000
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21.275583000
H -4.197072000 19.845282000
21.827614000
H -3.974293000 19.095614000
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21.909318000
H -3.557541000 17.816660000
22.986692000
H -4.835631000 17.412163000
21.839640000
O -1.458181000 12.970427000
16.612983000
O -1.461659000 12.144103000
17.765496000

Crystallographic Analyses

Crystals suitable for X-ray diffraction were covered in paratone oil in a glove box and transferred to the diffractometer in a 20-mL capped vial. Crystals were mounted on a loop with paratone oil on a Bruker D8 VENTURE diffractometer. The crystals were cooled and kept at T = 100(2) K during data collections. The structures were solved with the ShelXT structure solution program using the Intrinsic Phasing solution method and by using Olex2 as the graphical interface.[16, 17] The model was refined with version 2014/7 of XL using Least Squares minimization.[18] Structures were visualized in Mercury and graphics were generated with POV-ray.[19, 20] The molecular structure of **3-U** contains two distinct molecules – one is comprised of a full molecule with a US_3 core that represents the majority of the data and the bulk of the compound, and the other is comprised of a full molecule with a US_2 core that represents the minority of the data and is not representative of what is experimentally observed of the bulk. These co-crystalize on the same lattice site. The molecular structure of **3-U** showing containing both US_3 and US_2 molecules (Figure S17) is shown, followed by a separate molecular structure of **3-U** containing just the US_3 molecule (Figure S18) for clarity. Similarly, the molecular structure of **4-U** contains two distinct molecules – one is comprised of a full molecule with a USe_3 core that represents the majority of the data and the bulk of the compound, and the other is comprised of a full molecule with a USe_2 core that represents the minority of the data and is not representative of what is experimentally observed of the bulk. These co-crystalize on the same lattice site. The molecular structure of **4-U** showing containing both USe_3 and USe_2 molecules (Figure S19) is shown, followed by a separate molecular structure of **4-U** containing just the USe_3 molecule (Figure S20) for clarity.

The electron density for U, S and C, N and P (compound **3-U**) was calculated with a quantum-mechanical model using a TZVP basis set for the ligand atoms and with and all-electron scalar relativistic TZVP basis set for the U atom. An energy optimization was performed, and the model densities rapidly converged on a singlet ground state.

The electron density maps for this S_3 model, were subtracted from the electron densities calculated from the intensity data. The residual density maps are readily calculated by the software Olex2, and the results are shown below in Figure S17. The U atom with its 92 electrons gave the biggest difference between the two sets of the structure factors (the ligand S2 moves the U atom from its optimal position for binding the S3 ligand). This very large electron peak 0.49 Å from the U has a peak height of 32 electrons (1/3 of the total occupancy). Two more large peaks are shown with peak heights of 5 electrons, and a separation of 2.05 Å (i.e. a disulfide S4-S5). The energy optimization for the complex with the disulfide and identical parameters also rapidly converged on a singlet ground state (the SCF took a bit longer here than for the S3 ligand). These peaks cannot be a superoxide or any other O2 group due to their long distances, separation of 2.05 Å, and due to the number of integrated electrons in these regions (too large to be oxygen atoms).

It is worthwhile to point out that the S3, S2 and Se3, Se2 ligands in both complexes refine to exactly 2/3 and 1/3 site fractions, and the U is hexavalent with no unpaired spins for both the S3, S2 and Se3, Se2 ligands (these ligands can both be treated as 2- with no unpaired electrons).

The electron density contribution of the S2 ligand is of interest and helped us address the reviewer's comments about us potentially having misidentified the S2 ion. Fortunately, the strong scattering of the S atoms (compared with lighter oxygen atoms) allows for the unbiased determination of the ligand identities. The electron density in this region is far away from the U center (2.7 Å) and will also not be affected by the residual densities around the U nucleus.

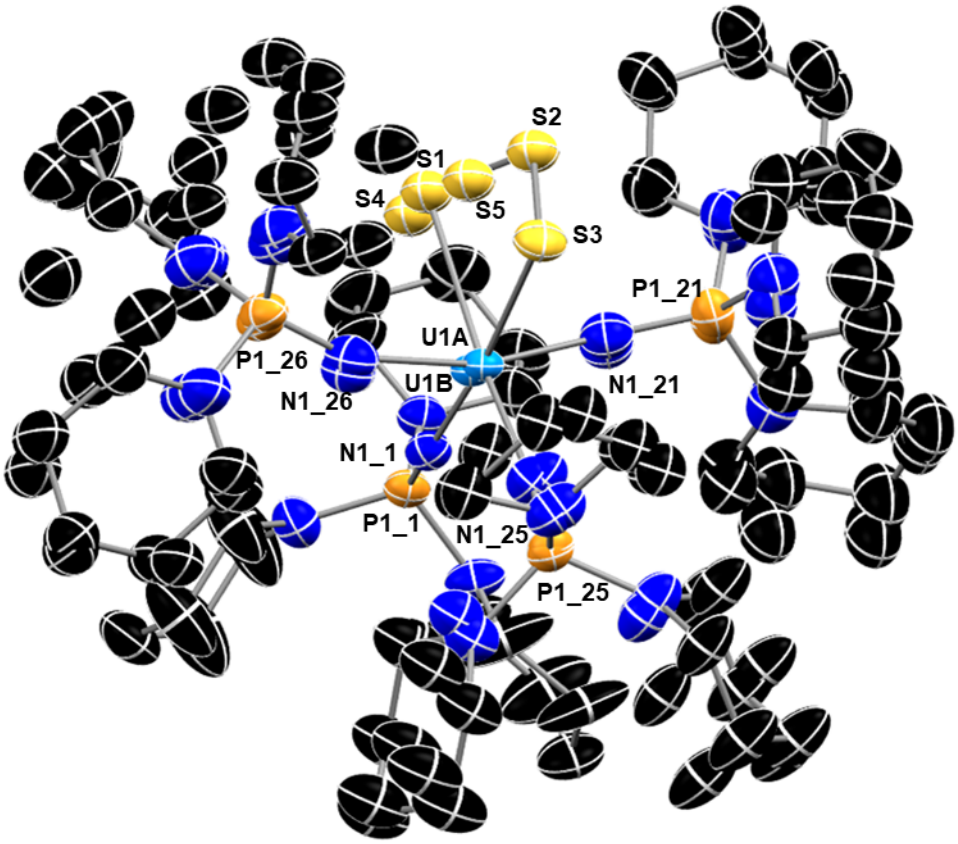

Figure S13. Molecular structure of **3-U** showing both US_3 (major) and US_2 (minor) molecules in the asymmetric unit cell with thermal ellipsoids shown at 50% probability; H atoms are omitted for clarity.

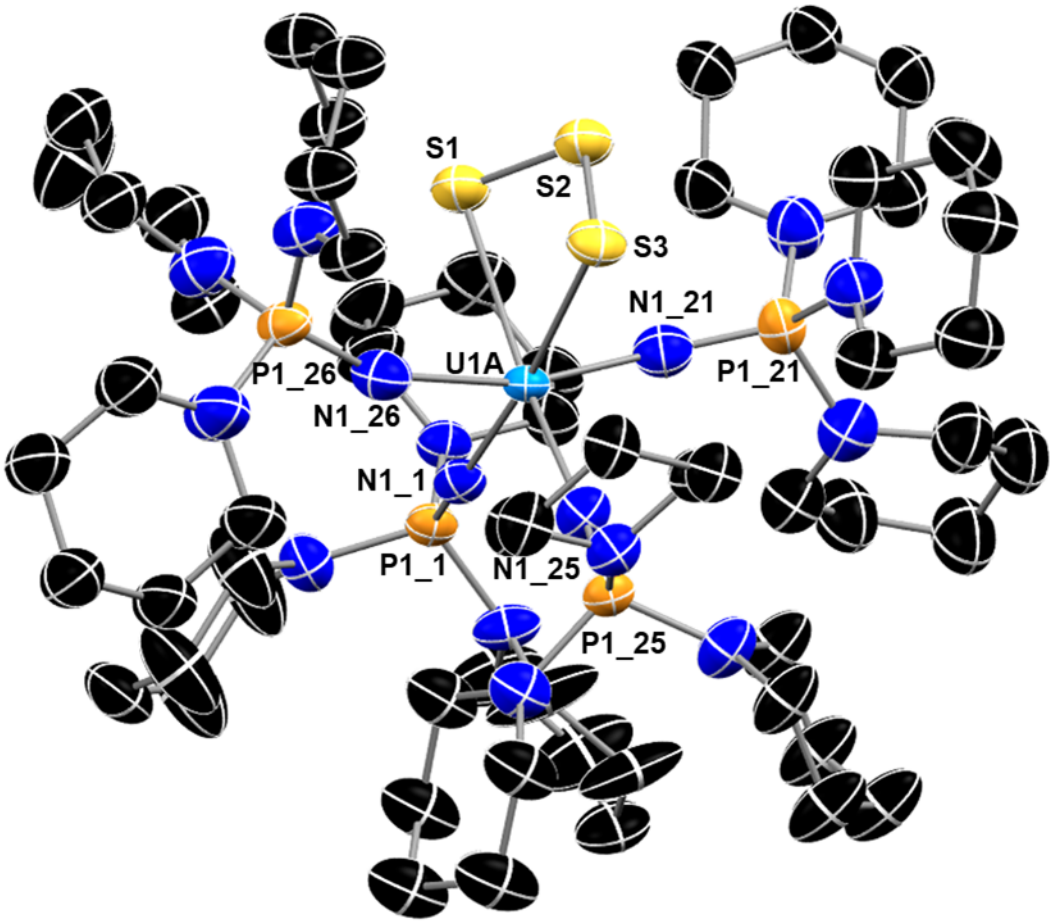

Figure S14. Molecular structure of **3-U** showing only the US_3 (major) molecule in the asymmetric unit cell with thermal ellipsoids shown at 50% probability; H atoms are omitted for clarity.

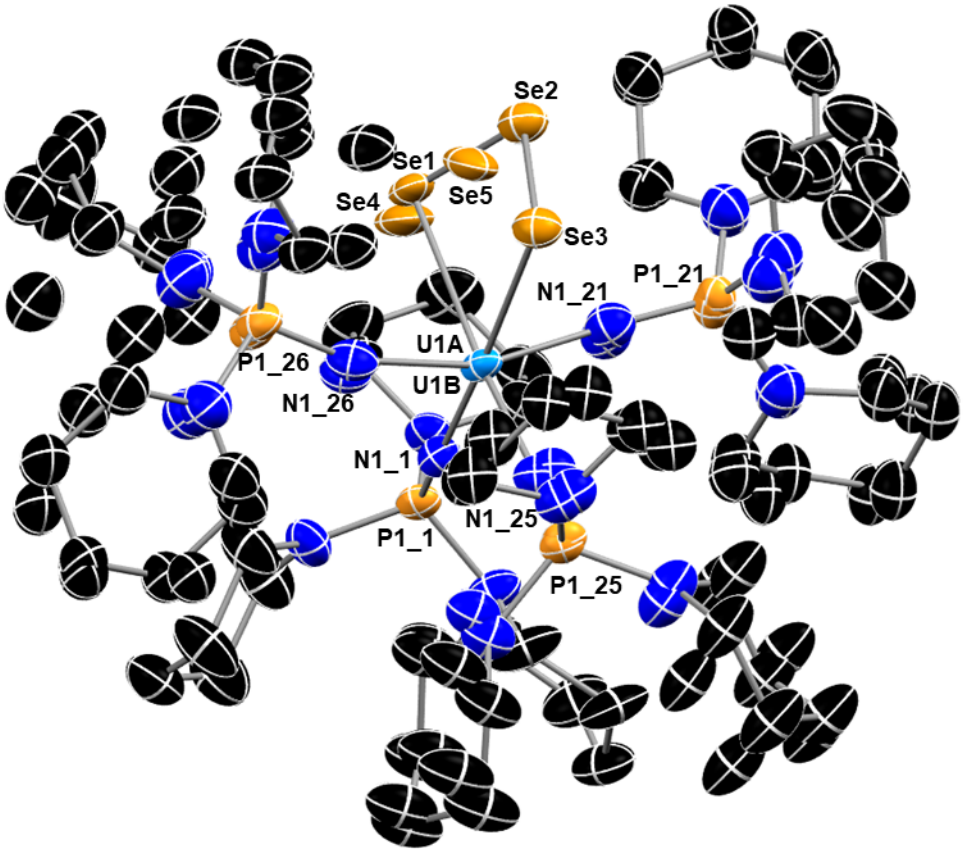

Figure S15. Molecular structure of **3-U** showing both USe_3 (major) and USe_2 (minor) cores in the asymmetric unit cell with thermal ellipsoids shown at 50% probability; H atoms are omitted for clarity.

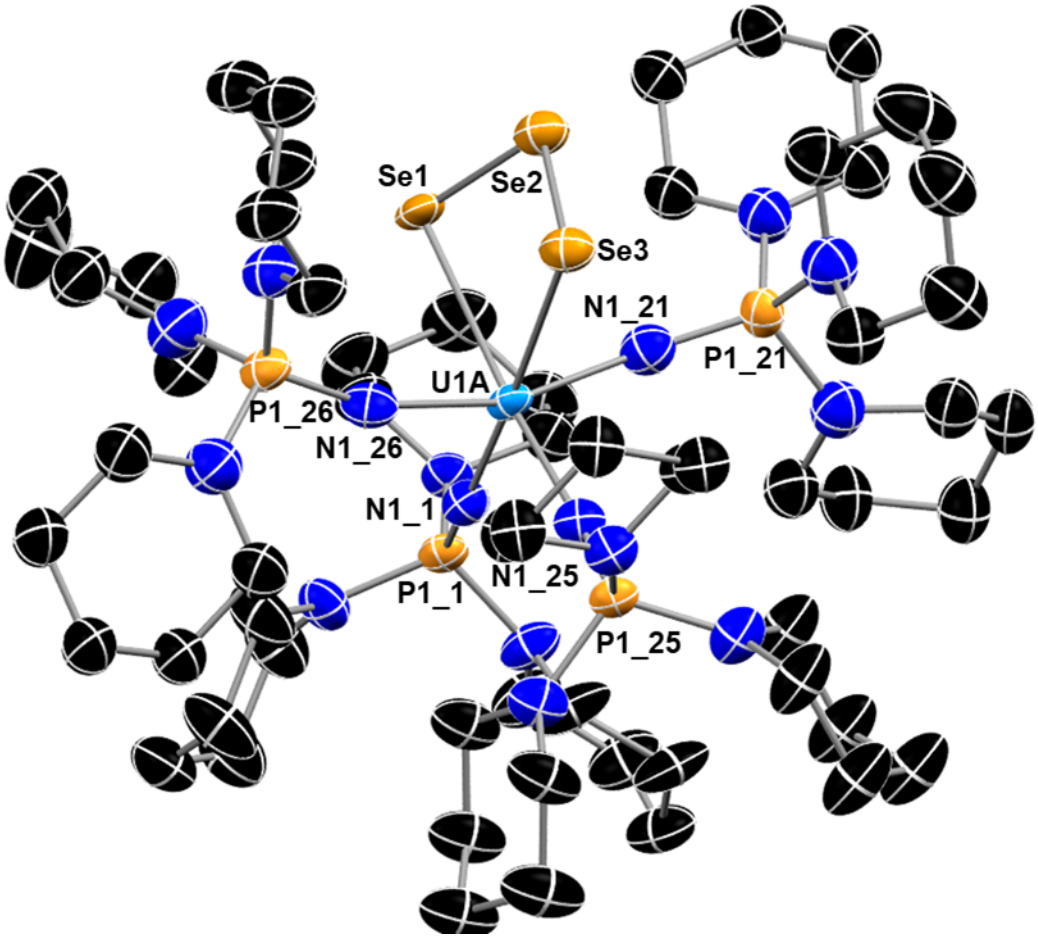

Figure S16. Molecular structure of **4-U** showing only the USe_3 (major) core in the asymmetric unit cell with thermal ellipsoids shown at 50% probability; H atoms are omitted for clarity.

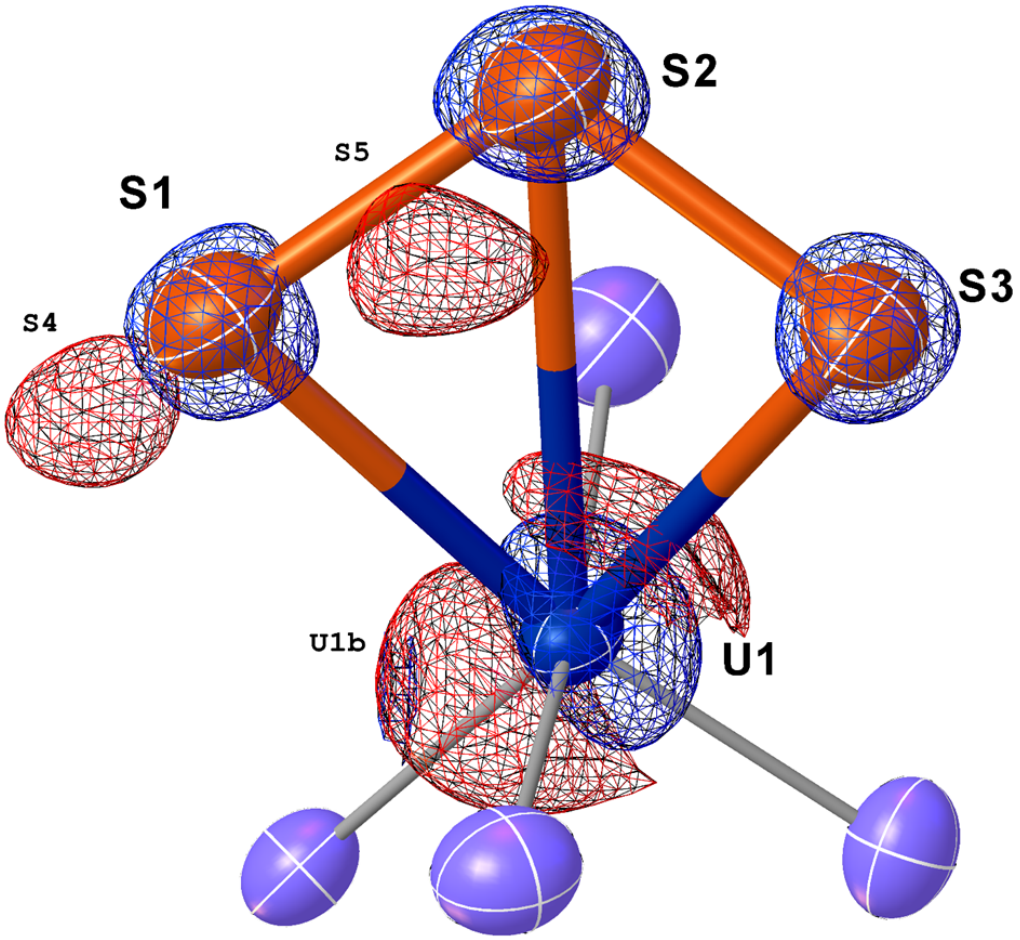

Figure S17. The residual electron density surfaces of the crystal structure with the structure factors of the S3 ligand (including its acceptor U) subtracted from the experimental structure factors for compound **3-U**. The S2 ligand (and its bound U atom) and clearly visible in this drawing. The S4-S5 distances refine to exactly 2.04(1) Å and the integration of the electron densities correspond to sulfur atoms (5.5 electrons for 1/3 S-atom). The population must be 1/3 for the overall population to be 1.

Table S3. Crystallographic Data and Structure Refinement for **3-U** and **4-U**.

	3-U	**4-U**
Empirical Formula	$C_{60}H_{120}N_{16}P_4S_{2.66}U$	$C_{60}H_{120}N_{16}P_4Se_{2.66}U$
Formula Weight	1512.98	1842.23
Temperature (K)	100(2)	100(2)
Crystal System	monoclinic	monoclinic
Space Group	$P2_1/n$	$P2_1/n$
a/Å	14.4586(9)	14.4586(9)
b/Å	27.1124(13)	27.1124(13)
c/Å	22.5764(12)	22.5764(12)
α/°	90	90
β/°	96.244(2)	96.244(2)
γ/°	90	90
Volume/Å3	8797.6(8)	8797.6(8)
Z	4	4
Z'	1	1
ρ(g/cm3)	1.142	1.391
μ(mm-1)	2.020	3.080
F(000)	3146.0	3786.0
Crystal Size/mm3	0.269 x 0.241 x 0.131	0.3 x 0.2 x 0.1
Radiation	MoKα (λ=0.71073)	MoKα (λ=0.71073)
2θ range for data collection(°)	3.63 to 49.384	3.834 to 49.426
Index Ranges	-16 ≤ h ≤ 16, -31 ≤ k ≤31, -26 ≤ 1 ≤ 26	-17 ≤ h ≤ 17, -31 ≤ k ≤31, -26 ≤ 1 ≤ 26
Reflections Collected	255364	208409
Independent Reflections	14727 [Rint = 0.1003, Rsigma = 0.0339]]	14932 [Rint = 0.1416, Rsigma = 0.0515]]
Data/Restraints/ Parameters	14727/3555/948	14932/3557/961
Goodness-of-Fit on F2	1.060	1.047
Final R Indexes [I>=2σ (I)]	R1=0.0759, wR2=0.1722	R1=0.0799, wR2=0.1629
Final R Indexes [all data]	R1=0.0898, wR2=0.1817	R1=0.1005, wR2=0.1746
Largest Diff. Peak/Hole/ (e Å3)	1.51/-1.76	1.45/-1.431
Flack Parameter	-	-
Completeness to 2θ	98.5	100

Table S4. Lengths for **3-U**.

Atom	Atom	Length/Å
U1A	S1	2.755(4)
U1A	S2	3.158(5)
U1A	S3	2.750(4)
U1A	N1_21	2.030(6)
U1A	N1_25	2.090(6)
U1A	N1_26	2.126(6)
U1A	N1_1	2.188(6)
S1	S2	2.048(4)
S2	S3	2.049(4)
U1B	S4	2.757(8)
U1B	S5	2.760(8)
U1B	N1_22	2.177(11)
U1B	N1_24	2.211(11)
U1B	N1_23	2.072(12)
U1B	N1_1	1.940(7)
S4	S5	2.040(11)
P1_21	N1_21	1.560(4)
P1_21	N2_21	1.659(3)
P1_21	N3_21	1.668(3)
P1_21	N4_21	1.667(3)
N2_21	C1_21	1.457(3)
N2_21	C5_21	1.458(3)
N3_21	C6_21	1.463(3)
N3_21	C10_21	1.461(2)
N4_21	C11_21	1.463(3)
N4_21	C15_21	1.464(3)
C1_21	C2_21	1.525(2)
C2_21	C3_21	1.524(2)
C3_21	C4_21	1.524(2)
C4_21	C5_21	1.525(2)
C6_21	C7_21	1.519(2)
C7_21	C8_21	1.524(2)
C8_21	C9_21	1.523(2)
C9_21	C10_21	1.519(2)
C11_21	C12_21	1.517(3)
C12_21	C13_21	1.524(3)
C13_21	C14_21	1.523(3)
C14_21	C15_21	1.520(3)

Atom	Atom	Length/Å
P1_25	N4_25	1.663(3)
N2_25	C1_25	1.466(3)
N2_25	C5_25	1.467(3)
N3_25	C6_25	1.459(2)
N3_25	C10_25	1.460(2)
N4_25	C11_25	1.461(2)
N4_25	C15_25	1.460(2)
C1_25	C2_25	1.523(3)
C2_25	C3_25	1.525(3)
C3_25	C4_25	1.525(3)
C4_25	C5_25	1.523(3)
C6_25	C7_25	1.515(3)
C7_25	C8_25	1.523(3)
C8_25	C9_25	1.523(3)
C9_25	C10_25	1.516(3)
C11_25	C12_25	1.516(3)
C12_25	C13_25	1.524(3)
C13_25	C14_25	1.522(3)
C14_25	C15_25	1.518(3)
P1_23	N1_23	1.559(4)
P1_23	N2_23	1.666(3)
P1_23	N3_23	1.663(3)
P1_23	N4_23	1.667(3)
N2_23	C1_23	1.462(3)
N2_23	C5_23	1.462(3)
N3_23	C6_23	1.459(3)
N3_23	C10_23	1.459(2)
N4_23	C11_23	1.464(3)
N4_23	C15_23	1.463(3)
C1_23	C2_23	1.525(3)
C2_23	C3_23	1.524(3)
C3_23	C4_23	1.525(3)
C4_23	C5_23	1.524(3)
C6_23	C7_23	1.516(3)
C7_23	C8_23	1.523(3)
C8_23	C9_23	1.523(3)
C9_23	C10_23	1.516(3)
C11_23	C12_23	1.517(3)

P1_22	N1_22	1.558(4)	C12_23	C13_23	1.524(3)
P1_22	N2_22	1.665(3)	C13_23	C14_23	1.523(3)
P1_22	N3_22	1.664(3)	C14_23	C15_23	1.519(3)
P1_22	N4_22	1.669(3)	P1_26	N1_26	1.559(4)
N2_22	C1_22	1.462(3)	P1_26	N2_26	1.662(3)
N2_22	C5_22	1.463(3)	P1_26	N3_26	1.666(3)
N3_22	C6_22	1.461(3)	P1_26	N4_26	1.666(3)
N3_22	C10_22	1.461(3)	N2_26	C1_26	1.459(3)
N4_22	C11_22	1.466(3)	N2_26	C5_26	1.460(3)
N4_22	C15_22	1.466(3)	N3_26	C6_26	1.461(3)
C1_22	C2_22	1.525(3)	N3_26	C10_26	1.462(3)
C2_22	C3_22	1.524(3)	N4_26	C11_26	1.460(3)
C3_22	C4_22	1.525(3)	N4_26	C15_26	1.461(3)
C4_22	C5_22	1.524(3)	C1_26	C2_26	1.526(3)
C6_22	C7_22	1.516(3)	C2_26	C3_26	1.524(3)
C7_22	C8_22	1.523(3)	C3_26	C4_26	1.524(3)
C8_22	C9_22	1.522(3)	C4_26	C5_26	1.526(3)
C9_22	C10_22	1.516(3)	C6_26	C7_26	1.517(3)
C11_22	C12_22	1.517(3)	C7_26	C8_26	1.523(3)
C12_22	C13_22	1.525(3)	C8_26	C9_26	1.523(3)
C13_22	C14_22	1.523(3)	C9_26	C10_26	1.517(3)
C14_22	C15_22	1.519(3)	C11_26	C12_26	1.517(3)
P1_24	N1_24	1.558(4)	C12_26	C13_26	1.524(3)
P1_24	N2_24	1.669(3)	C13_26	C14_26	1.523(3)
P1_24	N3_24	1.665(3)	C14_26	C15_26	1.520(3)
P1_24	N4_24	1.665(3)	P1_1	N1_1	1.554(4)
N2_24	C1_24	1.465(3)	P1_1	N2_1	1.669(3)
N2_24	C5_24	1.465(3)	P1_1	N3_1	1.674(3)
N3_24	C6_24	1.465(3)	P1_1	N4_1	1.663(3)
N3_24	C10_24	1.464(3)	N2_1	C1_1	1.469(3)
N4_24	C11_24	1.463(3)	N2_1	C5_1	1.466(3)
N4_24	C15_24	1.463(3)	N3_1	C6_1	1.470(3)
C1_24	C2_24	1.524(3)	N3_1	C10_1	1.470(3)
C2_24	C3_24	1.525(3)	N4_1	C11_1	1.461(2)
C3_24	C4_24	1.525(3)	N4_1	C15_1	1.461(2)
C4_24	C5_24	1.523(3)	C1_1	C2_1	1.523(3)
C6_24	C7_24	1.516(3)	C2_1	C3_1	1.525(3)
C7_24	C8_24	1.523(3)	C3_1	C4_1	1.524(3)
C8_24	C9_24	1.522(3)	C4_1	C5_1	1.523(3)
C9_24	C10_24	1.516(3)	C6_1	C7_1	1.511(3)
C11_24	C12_24	1.517(3)	C7_1	C8_1	1.523(3)

C12_24	C13_24	1.524(3)	C8_1	C9_1	1.523(3)
C13_24	C14_24	1.523(3)	C9_1	C10_1	1.512(3)
C14_24	C15_24	1.520(3)	C11_1	C12_1	1.519(2)
P1_25	N1_25	1.559(4)	C12_1	C13_1	1.525(2)
P1_25	N2_25	1.673(3)	C13_1	C14_1	1.523(2)
P1_25	N3_25	1.662(3)	C14_1	C15_1	1.521(2)

Table S5. Angles for **3-U**.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
S1	U1A	S2	39.79(8)	N4_24	C11_24	C12_24	113.1(4)
S3	U1A	S1	74.82(15)	C11_24	C12_24	C13_24	111.9(5)
S3	U1A	S2	39.84(8)	C14_24	C13_24	C12_24	112.3(5)
N1_21	U1A	S1	85.6(2)	C15_24	C14_24	C13_24	113.0(5)
N1_21	U1A	S2	69.5(2)	N4_24	C15_24	C14_24	112.2(4)
N1_21	U1A	S3	85.3(3)	N1_25	P1_25	N2_25	117.6(2)
N1_21	U1A	N1_25	96.2(3)	N1_25	P1_25	N3_25	112.6(2)
N1_21	U1A	N1_26	165.4(3)	N1_25	P1_25	N4_25	111.3(2)
N1_21	U1A	N1_1	95.6(3)	N3_25	P1_25	N2_25	102.65(19)
N1_25	U1A	S1	166.9(3)	N3_25	P1_25	N4_25	108.4(2)
N1_25	U1A	S2	129.1(3)	N4_25	P1_25	N2_25	103.40(19)
N1_25	U1A	S3	92.4(3)	P1_25	N1_25	U1A	164.3(4)
N1_25	U1A	N1_26	94.6(3)	C1_25	N2_25	P1_25	118.1(3)
N1_25	U1A	N1_1	93.6(3)	C1_25	N2_25	C5_25	113.1(4)
N1_26	U1A	S1	81.7(2)	C5_25	N2_25	P1_25	117.1(3)
N1_26	U1A	S2	96.0(2)	C6_25	N3_25	P1_25	118.2(3)
N1_26	U1A	S3	84.5(2)	C6_25	N3_25	C10_25	118.6(4)
N1_26	U1A	N1_1	93.5(3)	C10_25	N3_25	P1_25	123.1(3)
N1_1	U1A	S1	99.16(19)	C11_25	N4_25	P1_25	120.4(3)
N1_1	U1A	S2	135.00(17)	C15_25	N4_25	P1_25	123.2(3)
N1_1	U1A	S3	173.85(19)	C15_25	N4_25	C11_25	116.4(4)
S2	S1	U1A	80.77(14)	N2_25	C1_25	C2_25	110.9(4)
S1	S2	U1A	59.44(12)	C1_25	C2_25	C3_25	111.4(5)
S1	S2	S3	109.4(2)	C2_25	C3_25	C4_25	109.3(5)
S3	S2	U1A	59.29(12)	C5_25	C4_25	C3_25	112.0(5)
S2	S3	U1A	80.87(13)	N2_25	C5_25	C4_25	110.4(4)
S4	U1B	S5	43.4(2)	N3_25	C6_25	C7_25	115.4(4)
N1_22	U1B	S4	86.4(4)	C6_25	C7_25	C8_25	112.6(5)
N1_22	U1B	S5	85.0(4)	C9_25	C8_25	C7_25	112.9(5)
N1_22	U1B	N1_24	86.6(5)	C10_25	C9_25	C8_25	113.7(5)
N1_24	U1B	S4	167.8(5)	N3_25	C10_25	C9_25	115.4(4)

N1_24	U1B	S5	125.9(4)
N1_23	U1B	S4	89.4(5)
N1_23	U1B	S5	84.8(4)
N1_23	U1B	N1_22	168.8(5)
N1_23	U1B	N1_24	95.6(5)
N1_1	U1B	S4	90.8(3)
N1_1	U1B	S5	134.2(4)
N1_1	U1B	N1_22	93.7(4)
N1_1	U1B	N1_24	99.6(5)
N1_1	U1B	N1_23	96.8(5)
S5	S4	U1B	68.38(13)
S4	S5	U1B	68.22(13)
N1_21	P1_21	N2_21	118.5(2)
N1_21	P1_21	N3_21	112.1(2)
N1_21	P1_21	N4_21	110.9(2)
N2_21	P1_21	N3_21	102.9(2)
N2_21	P1_21	N4_21	103.68(19)
N4_21	P1_21	N3_21	107.9(2)
P1_21	N1_21	U1A	160.2(4)
C1_21	N2_21	P1_21	120.1(3)
C1_21	N2_21	C5_21	114.2(4)
C5_21	N2_21	P1_21	119.1(3)
C6_21	N3_21	P1_21	117.5(3)
C10_21	N3_21	P1_21	122.6(3)
C10_21	N3_21	C6_21	118.1(4)
C11_21	N4_21	P1_21	119.9(3)
C11_21	N4_21	C15_21	115.8(4)
C15_21	N4_21	P1_21	122.4(3)
N2_21	C1_21	C2_21	111.0(4)
C3_21	C2_21	C1_21	111.2(5)
C2_21	C3_21	C4_21	109.5(5)
C3_21	C4_21	C5_21	112.0(5)
N2_21	C5_21	C4_21	110.5(4)
N3_21	C6_21	C7_21	114.8(4)
C6_21	C7_21	C8_21	112.3(5)
C9_21	C8_21	C7_21	112.9(5)
C10_21	C9_21	C8_21	113.6(5)
N3_21	C10_21	C9_21	115.1(4)
N4_21	C11_21	C12_21	113.1(4)
C11_21	C12_21	C13_21	111.9(5)
C14_21	C13_21	C12_21	112.3(5)
N4_25	C11_25	C12_25	113.3(4)
C11_25	C12_25	C13_25	111.9(5)
C14_25	C13_25	C12_25	112.3(5)
C15_25	C14_25	C13_25	113.1(5)
N4_25	C15_25	C14_25	112.5(4)
N1_23	P1_23	N2_23	118.0(2)
N1_23	P1_23	N3_23	112.6(2)
N1_23	P1_23	N4_23	111.0(2)
N2_23	P1_23	N4_23	103.44(19)
N3_23	P1_23	N2_23	102.9(2)
N3_23	P1_23	N4_23	108.1(2)
P1_23	N1_23	U1B	152.1(6)
C1_23	N2_23	P1_23	119.1(3)
C1_23	N2_23	C5_23	113.6(4)
C5_23	N2_23	P1_23	118.2(3)
C6_23	N3_23	P1_23	118.1(3)
C6_23	N3_23	C10_23	118.7(4)
C10_23	N3_23	P1_23	123.1(3)
C11_23	N4_23	P1_23	119.8(3)
C15_23	N4_23	P1_23	122.5(3)
C15_23	N4_23	C11_23	115.9(4)
N2_23	C1_23	C2_23	110.9(4)
C3_23	C2_23	C1_23	111.3(5)
C2_23	C3_23	C4_23	109.5(5)
C5_23	C4_23	C3_23	112.0(5)
N2_23	C5_23	C4_23	110.4(4)
N3_23	C6_23	C7_23	115.3(4)
C6_23	C7_23	C8_23	112.6(5)
C9_23	C8_23	C7_23	112.9(5)
C10_23	C9_23	C8_23	113.7(5)
N3_23	C10_23	C9_23	115.5(4)
N4_23	C11_23	C12_23	113.1(4)
C11_23	C12_23	C13_23	111.9(5)
C14_23	C13_23	C12_23	112.3(5)
C15_23	C14_23	C13_23	113.0(5)
N4_23	C15_23	C14_23	112.2(4)
N1_26	P1_26	N2_26	118.2(2)
N1_26	P1_26	N3_26	112.4(2)
N1_26	P1_26	N4_26	111.0(2)
N2_26	P1_26	N3_26	102.82(19)
N2_26	P1_26	N4_26	103.58(19)

C15_21	C14_21	C13_21	112.9(5)	N3_26	P1_26	N4_26	108.0(2)
N4_21	C15_21	C14_21	112.1(4)	P1_26	N1_26	U1A	158.4(4)
N1_22	P1_22	N2_22	118.2(2)	C1_26	N2_26	P1_26	119.7(3)
N1_22	P1_22	N3_22	112.5(2)	C1_26	N2_26	C5_26	114.0(4)
N1_22	P1_22	N4_22	111.0(2)	C5_26	N2_26	P1_26	118.7(3)
N2_22	P1_22	N4_22	103.41(19)	C6_26	N3_26	P1_26	117.8(3)
N3_22	P1_22	N2_22	102.9(2)	C6_26	N3_26	C10_26	118.3(4)
N3_22	P1_22	N4_22	108.0(2)	C10_26	N3_26	P1_26	122.7(3)
P1_22	N1_22	U1B	157.7(6)	C11_26	N4_26	P1_26	120.3(3)
C1_22	N2_22	P1_22	119.0(3)	C11_26	N4_26	C15_26	116.4(4)
C1_22	N2_22	C5_22	113.5(4)	C15_26	N4_26	P1_26	122.9(3)
C5_22	N2_22	P1_22	118.1(3)	N2_26	C1_26	C2_26	110.9(4)
C6_22	N3_22	P1_22	117.8(3)	C3_26	C2_26	C1_26	111.3(5)
C10_22	N3_22	P1_22	122.9(3)	C2_26	C3_26	C4_26	109.6(5)
C10_22	N3_22	C6_22	118.3(4)	C3_26	C4_26	C5_26	111.9(5)
C11_22	N4_22	P1_22	119.5(3)	N2_26	C5_26	C4_26	110.4(4)
C15_22	N4_22	P1_22	122.0(3)	N3_26	C6_26	C7_26	115.0(4)
C15_22	N4_22	C11_22	115.5(4)	C6_26	C7_26	C8_26	112.5(5)
N2_22	C1_22	C2_22	110.8(4)	C7_26	C8_26	C9_26	112.9(5)
C3_22	C2_22	C1_22	111.3(5)	C10_26	C9_26	C8_26	113.6(5)
C2_22	C3_22	C4_22	109.4(5)	N3_26	C10_26	C9_26	115.1(4)
C5_22	C4_22	C3_22	112.0(5)	N4_26	C11_26	C12_26	113.2(4)
N2_22	C5_22	C4_22	110.4(4)	C11_26	C12_26	C13_26	111.9(5)
N3_22	C6_22	C7_22	115.1(4)	C14_26	C13_26	C12_26	112.3(5)
C6_22	C7_22	C8_22	112.5(5)	C15_26	C14_26	C13_26	112.9(5)
C9_22	C8_22	C7_22	112.9(5)	N4_26	C15_26	C14_26	112.2(4)
C10_22	C9_22	C8_22	113.7(5)	N1_1	P1_1	N2_1	118.1(2)
N3_22	C10_22	C9_22	115.3(4)	N1_1	P1_1	N3_1	112.4(2)
N4_22	C11_22	C12_22	113.0(4)	N1_1	P1_1	N4_1	111.5(2)
C11_22	C12_22	C13_22	111.8(5)	N2_1	P1_1	N3_1	102.47(19)
C14_22	C13_22	C12_22	112.2(5)	N4_1	P1_1	N2_1	103.51(18)
C15_22	C14_22	C13_22	112.9(5)	N4_1	P1_1	N3_1	107.8(2)
N4_22	C15_22	C14_22	112.1(4)	P1_1	N1_1	U1A	161.7(3)
N1_24	P1_24	N2_24	117.9(2)	P1_1	N1_1	U1B	161.3(4)
N1_24	P1_24	N3_24	112.5(2)	C1_1	N2_1	P1_1	117.9(3)
N1_24	P1_24	N4_24	111.2(2)	C5_1	N2_1	P1_1	117.3(3)
N3_24	P1_24	N2_24	102.7(2)	C5_1	N2_1	C1_1	112.8(4)
N4_24	P1_24	N2_24	103.40(19)	C6_1	N3_1	P1_1	116.0(3)
N4_24	P1_24	N3_24	108.2(2)	C6_1	N3_1	C10_1	117.0(4)
P1_24	N1_24	U1B	154.7(6)	C10_1	N3_1	P1_1	120.8(3)
C1_24	N2_24	P1_24	118.4(3)	C11_1	N4_1	P1_1	120.4(3)

C5_24	N2_24	P1_24	117.5(3)
C5_24	N2_24	C1_24	113.2(4)
C6_24	N3_24	P1_24	117.4(3)
C10_24	N3_24	P1_24	122.5(3)
C10_24	N3_24	C6_24	117.8(4)
C11_24	N4_24	P1_24	120.1(3)
C11_24	N4_24	C15_24	116.0(4)
C15_24	N4_24	P1_24	122.7(3)
N2_24	C1_24	C2_24	110.8(4)
C1_24	C2_24	C3_24	111.3(5)
C2_24	C3_24	C4_24	109.3(5)
C5_24	C4_24	C3_24	112.0(5)
N2_24	C5_24	C4_24	110.4(4)
N3_24	C6_24	C7_24	114.9(4)
C6_24	C7_24	C8_24	112.5(5)
C9_24	C8_24	C7_24	112.9(5)
C10_24	C9_24	C8_24	113.7(5)
N3_24	C10_24	C9_24	115.1(4)
C15_1	N4_1	P1_1	123.1(3)
C15_1	N4_1	C11_1	116.3(4)
N2_1	C1_1	C2_1	110.7(4)
C1_1	C2_1	C3_1	111.3(5)
C4_1	C3_1	C2_1	109.3(5)
C5_1	C4_1	C3_1	112.1(5)
N2_1	C5_1	C4_1	110.4(4)
N3_1	C6_1	C7_1	115.3(4)
C6_1	C7_1	C8_1	112.8(5)
C7_1	C8_1	C9_1	112.6(5)
C10_1	C9_1	C8_1	113.8(5)
N3_1	C10_1	C9_1	115.3(4)
N4_1	C11_1	C12_1	113.1(4)
C11_1	C12_1	C13_1	111.7(4)
C14_1	C13_1	C12_1	112.2(5)
C15_1	C14_1	C13_1	112.8(5)
N4_1	C15_1	C14_1	112.3(4)

Table S6. Lengths for **4-U**.

Atom	Atom	Length/Å
U1A	Se1	2.9153(15)
U1A	Se3	2.9441(14)
U1A	N1_21	2.057(5)
U1A	N1_25	2.113(5)
U1A	N1_26	2.089(5)
U1A	N1_1	2.095(5)
Se1	Se2	2.336(2)
Se2	Se3	2.3381(18)
U1B	Se4	2.859(3)
U1B	Se5	2.857(3)
U1B	N1_1	2.095(5)
U1B	N1_22	2.058(5)
U1B	N1_23	2.089(5)
U1B	N1_24	2.114(5)
Se4	Se5	2.300(6)
P1_21	N1_21	1.561(4)
P1_21	N2_21	1.658(3)
P1_21	N3_21	1.662(3)
P1_21	N4_21	1.664(3)
N2_1	C1_1	1.470(3)
N2_1	C5_1	1.467(3)
N3_1	C6_1	1.473(3)
N3_1	C10_1	1.473(3)
N4_1	C11_1	1.462(3)
N4_1	C15_1	1.462(3)
C1_1	C2_1	1.522(3)
C2_1	C3_1	1.526(3)
C3_1	C4_1	1.526(3)
C4_1	C5_1	1.523(3)
C6_1	C7_1	1.514(3)
C7_1	C8_1	1.524(3)
C8_1	C9_1	1.524(3)
C9_1	C10_1	1.514(3)
C11_1	C12_1	1.520(2)
C12_1	C13_1	1.524(2)
C13_1	C14_1	1.523(2)
C14_1	C15_1	1.521(2)
P1_22	N1_22	1.559(4)

N2_21	C1_21	1.460(3)
N2_21	C5_21	1.461(3)
N3_21	C6_21	1.463(3)
N3_21	C10_21	1.462(3)
N4_21	C11_21	1.466(3)
N4_21	C15_21	1.466(3)
C1_21	C2_21	1.525(2)
C2_21	C3_21	1.525(2)
C3_21	C4_21	1.525(2)
C4_21	C5_21	1.525(2)
C6_21	C7_21	1.521(2)
C7_21	C8_21	1.524(2)
C8_21	C9_21	1.523(2)
C9_21	C10_21	1.519(2)
C11_21	C12_21	1.518(3)
C12_21	C13_21	1.524(3)
C13_21	C14_21	1.523(3)
C14_21	C15_21	1.520(3)
P1_25	N1_25	1.559(4)
P1_25	N2_25	1.668(3)
P1_25	N3_25	1.658(3)
P1_25	N4_25	1.660(3)
N2_25	C1_25	1.467(3)
N2_25	C5_25	1.468(3)
N3_25	C6_25	1.460(3)
N3_25	C10_25	1.461(3)
N4_25	C11_25	1.462(3)
N4_25	C15_25	1.462(3)
C1_25	C2_25	1.523(3)
C2_25	C3_25	1.525(3)
C3_25	C4_25	1.526(3)
C4_25	C5_25	1.523(3)
C6_25	C7_25	1.517(3)
C7_25	C8_25	1.524(3)
C8_25	C9_25	1.522(3)
C9_25	C10_25	1.516(3)
C11_25	C12_25	1.517(3)
C12_25	C13_25	1.524(3)
C13_25	C14_25	1.522(3)
C14_25	C15_25	1.518(3)
P1_26	N1_26	1.560(4)
P1_22	N2_22	1.662(3)
P1_22	N3_22	1.661(3)
P1_22	N4_22	1.663(3)
N2_22	C1_22	1.463(3)
N2_22	C5_22	1.464(3)
N3_22	C6_22	1.463(3)
N3_22	C10_22	1.462(3)
N4_22	C11_22	1.465(3)
N4_22	C15_22	1.466(3)
C1_22	C2_22	1.524(3)
C2_22	C3_22	1.525(3)
C3_22	C4_22	1.525(3)
C4_22	C5_22	1.525(3)
C6_22	C7_22	1.518(3)
C7_22	C8_22	1.524(3)
C8_22	C9_22	1.523(3)
C9_22	C10_22	1.516(3)
C11_22	C12_22	1.518(3)
C12_22	C13_22	1.524(3)
C13_22	C14_22	1.523(3)
C14_22	C15_22	1.520(3)
P1_23	N1_23	1.559(4)
P1_23	N2_23	1.662(3)
P1_23	N3_23	1.658(3)
P1_23	N4_23	1.665(3)
N2_23	C1_23	1.463(3)
N2_23	C5_23	1.463(3)
N3_23	C6_23	1.460(3)
N3_23	C10_23	1.460(3)
N4_23	C11_23	1.466(3)
N4_23	C15_23	1.466(3)
C1_23	C2_23	1.524(3)
C2_23	C3_23	1.525(3)
C3_23	C4_23	1.525(3)
C4_23	C5_23	1.525(3)
C6_23	C7_23	1.517(3)
C7_23	C8_23	1.524(3)
C8_23	C9_23	1.523(3)
C9_23	C10_23	1.516(3)
C11_23	C12_23	1.518(3)
C12_23	C13_23	1.524(3)

P1_26	N2_26	1.658(3)	C13_23	C14_23	1.523(3)
P1_26	N3_26	1.662(3)	C14_23	C15_23	1.519(3)
P1_26	N4_26	1.662(3)	P1_24	N1_24	1.559(4)
N2_26	C1_26	1.459(3)	P1_24	N2_24	1.665(3)
N2_26	C5_26	1.460(3)	P1_24	N3_24	1.662(3)
N3_26	C6_26	1.462(3)	P1_24	N4_24	1.661(3)
N3_26	C10_26	1.463(3)	N2_24	C1_24	1.466(3)
N4_26	C11_26	1.461(3)	N2_24	C5_24	1.465(3)
N4_26	C15_26	1.461(3)	N3_24	C6_24	1.465(3)
C1_26	C2_26	1.525(3)	N3_24	C10_24	1.465(3)
C2_26	C3_26	1.524(3)	N4_24	C11_24	1.463(3)
C3_26	C4_26	1.525(3)	N4_24	C15_24	1.464(3)
C4_26	C5_26	1.526(3)	C1_24	C2_24	1.523(3)
C6_26	C7_26	1.518(3)	C2_24	C3_24	1.525(3)
C7_26	C8_26	1.524(3)	C3_24	C4_24	1.525(3)
C8_26	C9_26	1.523(3)	C4_24	C5_24	1.524(3)
C9_26	C10_26	1.517(3)	C6_24	C7_24	1.517(3)
C11_26	C12_26	1.518(3)	C7_24	C8_24	1.524(3)
C12_26	C13_26	1.524(3)	C8_24	C9_24	1.522(3)
C13_26	C14_26	1.523(3)	C9_24	C10_24	1.517(3)
C14_26	C15_26	1.520(3)	C11_24	C12_24	1.518(3)
P1_1	N1_1	1.556(4)	C12_24	C13_24	1.524(3)
P1_1	N2_1	1.665(3)	C13_24	C14_24	1.522(3)
P1_1	N3_1	1.671(3)	C14_24	C15_24	1.520(3)
P1_1	N4_1	1.659(3)			

Table S7. Angles for **4-U**.

Atom	**Atom**	**Atom**	**Angle/˚**	**Atom**	**Atom**	**Atom**	**Angle/˚**
Se1	U1A	Se3	79.48(5)	N4_26	C15_26	C14_26	113.5(4)
N1_21	U1A	Se1	84.9(2)	N1_1	P1_1	N2_1	117.8(2)
N1_21	U1A	Se3	82.0(2)	N1_1	P1_1	N3_1	112.1(2)
N1_21	U1A	N1_25	95.6(3)	N1_1	P1_1	N4_1	111.7(2)
N1_21	U1A	N1_26	161.5(3)	N2_1	P1_1	N3_1	102.6(2)
N1_21	U1A	N1_1	97.6(3)	N4_1	P1_1	N2_1	103.23(19)
N1_25	U1A	Se1	168.4(2)	N4_1	P1_1	N3_1	108.6(2)
N1_25	U1A	Se3	89.1(2)	P1_1	N1_1	U1A	164.4(3)
N1_26	U1A	Se1	82.5(2)	P1_1	N1_1	U1B	164.4(3)
N1_26	U1A	Se3	82.4(2)	C1_1	N2_1	P1_1	117.4(3)
N1_26	U1A	N1_25	94.1(2)	C5_1	N2_1	P1_1	117.6(3)
N1_26	U1A	N1_1	97.4(3)	C5_1	N2_1	C1_1	113.0(4)

N1_1	U1A	Se1	97.11(15)	C6_1	N3_1	P1_1	116.5(3)
N1_1	U1A	Se3	176.58(15)	C6_1	N3_1	C10_1	115.8(4)
N1_1	U1A	N1_25	94.3(3)	C10_1	N3_1	P1_1	120.8(3)
Se2	Se1	U1A	81.97(6)	C11_1	N4_1	P1_1	120.1(3)
Se1	Se2	Se3	106.55(9)	C11_1	N4_1	C15_1	116.3(4)
Se2	Se3	U1A	81.30(5)	C15_1	N4_1	P1_1	123.6(3)
Se5	U1B	Se4	47.47(12)	N2_1	C1_1	C2_1	109.9(4)
N1_1	U1B	Se4	84.09(18)	C1_1	C2_1	C3_1	110.0(5)
N1_1	U1B	Se5	131.53(18)	C4_1	C3_1	C2_1	110.4(5)
N1_1	U1B	N1_24	97.1(4)	C5_1	C4_1	C3_1	110.5(5)
N1_22	U1B	Se4	84.3(4)	N2_1	C5_1	C4_1	110.2(4)
N1_22	U1B	Se5	83.8(4)	N3_1	C6_1	C7_1	113.8(4)
N1_22	U1B	N1_1	90.7(4)	C6_1	C7_1	C8_1	111.6(5)
N1_22	U1B	N1_23	168.9(5)	C9_1	C8_1	C7_1	111.5(5)
N1_22	U1B	N1_24	90.4(5)	C10_1	C9_1	C8_1	112.3(5)
N1_23	U1B	Se4	84.7(4)	N3_1	C10_1	C9_1	114.5(4)
N1_23	U1B	Se5	87.7(3)	N4_1	C11_1	C12_1	112.7(4)
N1_23	U1B	N1_1	89.4(4)	C11_1	C12_1	C13_1	111.2(5)
N1_23	U1B	N1_24	100.7(5)	C14_1	C13_1	C12_1	111.8(5)
N1_24	U1B	Se4	174.5(4)	C15_1	C14_1	C13_1	111.5(5)
N1_24	U1B	Se5	130.9(4)	N4_1	C15_1	C14_1	113.3(4)
Se5	Se4	U1B	66.21(7)	N1_22	P1_22	N2_22	117.7(3)
Se4	Se5	U1B	66.32(7)	N1_22	P1_22	N3_22	112.2(2)
N1_21	P1_21	N2_21	117.9(2)	N1_22	P1_22	N4_22	111.2(2)
N1_21	P1_21	N3_21	112.0(2)	N2_22	P1_22	N4_22	103.1(2)
N1_21	P1_21	N4_21	111.1(2)	N3_22	P1_22	N2_22	102.9(2)
N2_21	P1_21	N3_21	102.9(2)	N3_22	P1_22	N4_22	108.9(2)
N2_21	P1_21	N4_21	103.3(2)	P1_22	N1_22	U1B	154.9(6)
N3_21	P1_21	N4_21	108.9(2)	C1_22	N2_22	P1_22	118.4(3)
P1_21	N1_21	U1A	165.6(4)	C1_22	N2_22	C5_22	113.8(4)
C1_21	N2_21	P1_21	119.1(3)	C5_22	N2_22	P1_22	118.2(3)
C1_21	N2_21	C5_21	114.2(4)	C6_22	N3_22	P1_22	118.4(3)
C5_21	N2_21	P1_21	118.8(3)	C10_22	N3_22	P1_22	123.0(3)
C6_21	N3_21	P1_21	118.4(3)	C10_22	N3_22	C6_22	117.4(4)
C10_21	N3_21	P1_21	123.0(3)	C11_22	N4_22	P1_22	119.5(3)
C10_21	N3_21	C6_21	117.4(4)	C11_22	N4_22	C15_22	115.8(4)
C11_21	N4_21	P1_21	119.4(3)	C15_22	N4_22	P1_22	122.8(3)
C15_21	N4_21	P1_21	122.8(3)	N2_22	C1_22	C2_22	110.0(4)
C15_21	N4_21	C11_21	115.7(4)	C1_22	C2_22	C3_22	110.0(5)
N2_21	C1_21	C2_21	110.0(4)	C4_22	C3_22	C2_22	110.5(5)
C3_21	C2_21	C1_21	109.9(5)	C5_22	C4_22	C3_22	110.5(5)

C4_21	C3_21	C2_21	110.7(5)
C3_21	C4_21	C5_21	110.5(5)
N2_21	C5_21	C4_21	110.2(4)
N3_21	C6_21	C7_21	113.5(4)
C6_21	C7_21	C8_21	111.2(5)
C9_21	C8_21	C7_21	111.8(5)
C10_21	C9_21	C8_21	112.1(5)
N3_21	C10_21	C9_21	114.6(4)
N4_21	C11_21	C12_21	112.7(4)
C11_21	C12_21	C13_21	111.3(5)
C14_21	C13_21	C12_21	111.9(5)
C15_21	C14_21	C13_21	111.6(5)
N4_21	C15_21	C14_21	113.2(4)
N1_25	P1_25	N2_25	117.3(2)
N1_25	P1_25	N3_25	112.4(2)
N1_25	P1_25	N4_25	111.4(2)
N3_25	P1_25	N2_25	102.7(2)
N3_25	P1_25	N4_25	109.2(2)
N4_25	P1_25	N2_25	103.1(2)
P1_25	N1_25	U1A	165.2(4)
C1_25	N2_25	P1_25	117.6(3)
C1_25	N2_25	C5_25	113.3(4)
C5_25	N2_25	P1_25	117.3(3)
C6_25	N3_25	P1_25	118.9(3)
C6_25	N3_25	C10_25	117.8(4)
C10_25	N3_25	P1_25	123.2(3)
C11_25	N4_25	P1_25	120.1(3)
C15_25	N4_25	P1_25	123.6(3)
C15_25	N4_25	C11_25	116.4(4)
N2_25	C1_25	C2_25	109.9(4)
C1_25	C2_25	C3_25	110.0(5)
C2_25	C3_25	C4_25	110.5(5)
C5_25	C4_25	C3_25	110.5(5)
N2_25	C5_25	C4_25	110.1(4)
N3_25	C6_25	C7_25	114.1(4)
C6_25	C7_25	C8_25	111.5(5)
C9_25	C8_25	C7_25	111.8(5)
C10_25	C9_25	C8_25	112.3(5)
N3_25	C10_25	C9_25	114.9(4)
N4_25	C11_25	C12_25	112.9(4)
C11_25	C12_25	C13_25	111.3(5)
N2_22	C5_22	C4_22	110.2(4)
N3_22	C6_22	C7_22	113.8(4)
C6_22	C7_22	C8_22	111.3(5)
C9_22	C8_22	C7_22	111.7(5)
C10_22	C9_22	C8_22	112.3(5)
N3_22	C10_22	C9_22	114.8(4)
N4_22	C11_22	C12_22	112.7(4)
C11_22	C12_22	C13_22	111.3(5)
C14_22	C13_22	C12_22	111.8(5)
C15_22	C14_22	C13_22	111.6(5)
N4_22	C15_22	C14_22	113.3(4)
N1_23	P1_23	N2_23	117.6(2)
N1_23	P1_23	N3_23	112.4(2)
N1_23	P1_23	N4_23	111.1(2)
N2_23	P1_23	N4_23	103.1(2)
N3_23	P1_23	N2_23	102.9(2)
N3_23	P1_23	N4_23	108.9(2)
P1_23	N1_23	U1B	154.7(6)
C1_23	N2_23	P1_23	118.5(3)
C1_23	N2_23	C5_23	113.9(4)
C5_23	N2_23	P1_23	118.3(3)
C6_23	N3_23	P1_23	118.9(3)
C6_23	N3_23	C10_23	117.8(4)
C10_23	N3_23	P1_23	123.3(3)
C11_23	N4_23	P1_23	119.3(3)
C15_23	N4_23	P1_23	122.7(3)
C15_23	N4_23	C11_23	115.7(4)
N2_23	C1_23	C2_23	110.0(4)
C1_23	C2_23	C3_23	110.0(5)
C2_23	C3_23	C4_23	110.6(5)
C5_23	C4_23	C3_23	110.5(5)
N2_23	C5_23	C4_23	110.2(4)
N3_23	C6_23	C7_23	114.0(4)
C6_23	C7_23	C8_23	111.4(5)
C9_23	C8_23	C7_23	111.7(5)
C10_23	C9_23	C8_23	112.3(5)
N3_23	C10_23	C9_23	114.9(4)
N4_23	C11_23	C12_23	112.7(4)
C11_23	C12_23	C13_23	111.3(5)
C14_23	C13_23	C12_23	111.8(5)
C15_23	C14_23	C13_23	111.6(5)

C14_25	C13_25	C12_25	111.9(5)
C15_25	C14_25	C13_25	111.8(5)
N4_25	C15_25	C14_25	113.6(4)
N1_26	P1_26	N2_26	117.9(2)
N1_26	P1_26	N3_26	112.1(2)
N1_26	P1_26	N4_26	111.1(2)
N2_26	P1_26	N3_26	102.9(2)
N2_26	P1_26	N4_26	103.2(2)
N4_26	P1_26	N3_26	108.8(2)
P1_26	N1_26	U1A	161.7(4)
C1_26	N2_26	P1_26	119.3(3)
C1_26	N2_26	C5_26	114.4(4)
C5_26	N2_26	P1_26	119.1(3)
C6_26	N3_26	P1_26	118.5(3)
C6_26	N3_26	C10_26	117.4(4)
C10_26	N3_26	P1_26	122.7(3)
C11_26	N4_26	P1_26	120.1(3)
C11_26	N4_26	C15_26	116.6(4)
C15_26	N4_26	P1_26	123.4(3)
N2_26	C1_26	C2_26	110.0(4)
C3_26	C2_26	C1_26	110.0(5)
C2_26	C3_26	C4_26	110.7(5)
C3_26	C4_26	C5_26	110.4(5)
N2_26	C5_26	C4_26	110.2(4)
N3_26	C6_26	C7_26	113.8(4)
C6_26	C7_26	C8_26	111.4(5)
C9_26	C8_26	C7_26	111.7(5)
C10_26	C9_26	C8_26	112.2(5)
N3_26	C10_26	C9_26	114.6(4)
N4_26	C11_26	C12_26	113.0(4)
C11_26	C12_26	C13_26	111.3(5)
C14_26	C13_26	C12_26	111.9(5)
C15_26	C14_26	C13_26	111.6(5)
N4_23	C15_23	C14_23	113.3(4)
N1_24	P1_24	N2_24	117.5(2)
N1_24	P1_24	N3_24	112.2(2)
N1_24	P1_24	N4_24	111.4(2)
N3_24	P1_24	N2_24	102.8(2)
N4_24	P1_24	N2_24	103.1(2)
N4_24	P1_24	N3_24	109.0(2)
P1_24	N1_24	U1B	155.7(6)
C1_24	N2_24	P1_24	117.9(3)
C5_24	N2_24	P1_24	117.8(3)
C5_24	N2_24	C1_24	113.5(4)
C6_24	N3_24	P1_24	118.1(3)
C10_24	N3_24	P1_24	122.6(3)
C10_24	N3_24	C6_24	117.0(4)
C11_24	N4_24	P1_24	119.9(3)
C11_24	N4_24	C15_24	116.2(4)
C15_24	N4_24	P1_24	123.3(3)
N2_24	C1_24	C2_24	109.9(4)
C1_24	C2_24	C3_24	109.9(5)
C4_24	C3_24	C2_24	110.5(5)
C5_24	C4_24	C3_24	110.5(5)
N2_24	C5_24	C4_24	110.2(4)
N3_24	C6_24	C7_24	113.7(4)
C6_24	C7_24	C8_24	111.4(5)
C9_24	C8_24	C7_24	111.8(5)
C10_24	C9_24	C8_24	112.3(5)
N3_24	C10_24	C9_24	114.6(4)
N4_24	C11_24	C12_24	112.8(4)
C11_24	C12_24	C13_24	111.3(5)
C14_24	C13_24	C12_24	111.9(5)
C15_24	C14_24	C13_24	111.6(5)
N4_24	C15_24	C14_24	113.3(4)

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