Construction of Heterometallic Clusters with Multiple Uranium-Metal Bonds by Dianionic Nitrogen-Phosphorus Ligands

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1. Experimental Procedures

All operations were carried out using an inert atmosphere glove box with dry argon (<1 ppm O2/H2O). Solvents were dried and deoxygenated before use through a commercial solvent drying system. Samples were carefully checked for purity and data reproducibility. All NMR spectra were recorded on Bruker AVQ-400 or DRX 500 spectrometers with tetramethylsilane (TMS) as the internal standard at room temperature.

CHN microanalyses were performed on a Vario EL III elemental analyser at Shanghai Institute of Organic Chemistry, the Chinese Academy of Sciences, and the samples were treated under high vacuum for 24 hours at room temperature. The powder X-ray diffraction pattern (PXRD) measurements were obtained on a Philips X'pert MPD Pro X-ray diffractometer using Cu Kα radiation (λ = 0.15418 nm), and the X-ray tube was operated at 40 kV and 40 mA at room temperature. Magnetic susceptibility measurements on crystalline samples were carried out on a SQUID magnetometer at 0.1 T in the temperature range from 1.8 to 300 K.

UV-Vis-NIR spectra were recorded on a Lambda 750 spectrometer at room temperature. Pt(COD)2 was synthesized according to a published method.51

L1 and L2. 2'-Oxydiethanamine (1.00 g, 9.6 mmol) and Et3N (9.70 g, 96.0 mmol) were dissolved in THF (150 mL). Chlorodiisopropylphosphine (2.93 g, 19.2 mmol) was then added dropwise and the mixture was stirred overnight at room temperature. Volatiles were removed in vacuo and the residual white solid was extracted with hexane. After filtration, the solvents were removed in vacuo leaving L1 as a colorless oil (3.0 g 93%). 1H NMR (500 MHz, CD63, ppm): δ 3.26 (t, J1JH = 5.5 Hz, 4H, -OCH2), 3.10-3.07 (m, 4H, -CH2,NH+), 1.49-1.43 (m, 4H,-CHMe2), 1.22-1.19 (m, 4H, -NH-), 1.06-1.00 (m, 24H, -CH3). 31P NMR (202 MHz, CD63, ppm): δ 65.23. 13C NMR (126 MHz, CD63, ppm): δ 72.09 (d, 1JCP = 7.6 Hz, -CH2O-), 47.65 (d, 1JCP = 31.5 Hz, -CH2NH-), 25.71 (d, 1JCP = 16.4 Hz, -CH(CH3)2-) 18.23, (d, 1JCP = 26.5 Hz, -CH3-), 16.36 (d, 1JCP = 11.3 Hz, -CH3-). The synthesis of ligand L2 (91% yield) was accomplished by the same method except that 2, 2'- (ethylenedioxy)diethylamine was used. 1H NMR (500 MHz, CD63, ppm): δ 3.40 (s, 4H, -OCH2), 3.30 (t, J1JH = 5.5 Hz, 4H, -OCH2CH2NH-), 3.11-3.06 (m, 4H, -OCH2CH2NH-), 1.47–1.43 (m, 4H, -CHMe2), 1.30–1.27 (m, 24H, -NH-), 1.05–0.99 (m, 24H, -CH3). 31P NMR (202 MHz, CD63, ppm): δ 65.26. 13C NMR (126 MHz, CD63, ppm): δ 73.18 (d, 1JCP = 8.8 Hz, -OCH2CH2NH-), 70.26 (s, -OCH2-) 48.43 (d, 1JCP = 31.5 Hz, -CH2NH-) 26.49 (d, 1JCP = 16.4 Hz, -CH(CH3)2) 19.03 (d, 1JCP = 26.5 Hz, -CH3-) 17.17 (d, 1JCP = 11.3 Hz, -CH3-).

Ligand L1 (336 mg, 1.00 mmol) was dissolved in 5 mL THF and pre-cooled at -30°C. n-BuLi (2.4 M, 0.83 mL, 2.00 mmol) was then added dropwise. Three hours later, UCl4 (380 mg, 1.00 mmol) in 5 mL THF was added at -30°C. The reaction mixture warmed to room temperature and then stirred for 6 h. Volatile materials were removed under reduced pressure and the mixture was extracted with toluene. Gray-green crystals of 1 (415 mg, 58%) were isolated from toluene solution by storage at -30 °C for 24 h. Anal. Calcd (%) for C30H24Cl2N2O2P2U: C, 33.58; H, 6.20; N, 3.92. Found: C, 33.45; H, 6.30; N, 3.94. 1H NMR (500 MHz, CD63, ppm): δ 66.67 (s, 4H), 61.18 (s, 4H), 30.00 (s, 12H), 29.21 (s, 12H), -22.36 (s, 4H, THF), -47.72 (s, 4H), -53.20 (s, 4H, THF). The synthesis of complex 2 (65% yield) was accomplished by the same method except that ligand L2 was used. Anal. Calcd (%) for C18H40Cl2N2O2P2U: C, 31.45; H, 5.87; N, 4.08. Found: C, 31.00; H, 6.19; N, 4.06.
$^1$H NMR (500 MHz, C$_6$D$_6$, ppm): $\delta$ 184.93 (s, 4H), 45.34 (s, 4H), 40.69 (s, 12H), 20.82 (s, 12H), -5.94 (s, 12H), -70.98 (s, 4H).

3-U$_2$Ni$_2$. To a solution of complex 1 (120 mg, 0.17 mmol) dissolved in 2 mL THF, a 2 mL THF solution containing Ni(COD)$_2$ (46.0 mg, 0.17 mmol) was added. After shaking several times to get a clear black solution, the resulting mixture was allowed to stand undisturbed at room temperature for 24 h. Storing the solution at $-30^\circ$C for 24 h yielded product 3-U$_2$Ni$_2$ (71 mg, 60%) as black crystals. Anal. Calcd (%) for C$_{44}$H$_{96}$Cl$_4$N$_4$Ni$_2$O$_5$P$_4$U$_2$: C, 32.61; H, 5.97; N, 3.46. Found: C, 28.16; H, 5.20; N, 4.11. The carbon content for this species is consistently lower than the calculated values, which probably due to the loss of solvent molecules or due to the inadequate combustion of these air and moisture sensitive species. $^1$H NMR (500 MHz, C$_6$D$_6$, ppm): $\delta$ 65.52 (s, 4H), 58.82 (s, 4H), 52.20 (s, 4H), 44.87 (s, 4H), 36.94 (s, 12H), 36.16 (s, 12H), 13.46 (s, 12H), 0.59 (s, 12H), -28.78 (s, 4H), -38.45 (s, 4H).

4-U$_2$Pd$_2$. To a solution of complex 1 (120 mg, 0.17 mmol) dissolved in 2 mL THF, a 5 mL THF solution containing Pd(PPh$_3$)$_4$ (193 mg, 0.17 mmol) was added. After shaking several times to get a clear orange solution, the resulting mixture was allowed to stand undisturbed at room temperature for 24 h. Orange-red crystals were grown from the THF solution at $-30^\circ$C. Washing the crystals with cooled THF afforded pure 4-U$_2$Pd$_2$ (65 mg, 47%). Anal. Calcd (%) for C$_{40}$H$_{88}$Cl$_4$N$_4$O$_4$P$_4$Pd$_2$U$_2$: C, 29.23; H, 5.40; N, 3.41. Found: C, 27.98; H, 5.23; N, 3.39. The carbon content for this species is consistently lower than the calculated values, which probably due to the loss of solvent molecules or due to the inadequate combustion of these air and moisture sensitive species.

5-(UNi)$_n$. To a solution of complex 2 (103 mg, 0.15 mmol) dissolved in 2 mL THF, a 3 mL THF solution containing Ni(COD)$_2$ (41 mg, 0.15 mmol) was added. The resulting clear solution was allowed to stand undisturbed at room temperature for 24 h. The product of 5-(UNi)$_n$ (76 mg, 68%) was obtained as black crystals after storage the THF solution at $-30^\circ$C for 24 hours. Anal. Calcd (%) for C$_{22}$H$_{48}$Cl$_2$N$_2$O$_4$NiO$_3$P$_2$U: C, 32.30; H, 5.91; N, 3.42. Found: C, 30.37; H, 5.45; N, 3.62. The carbon content for this species is consistently lower than the calculated values, which probably due to the loss of solvent molecules or due to the inadequate combustion of these air and moisture sensitive species.

6-UPd. To a solution of complex 2 (41 mg, 0.06 mmol) dissolved in 2 mL THF, a 5 mL THF solution containing Pd(PPh$_3$)$_4$ (68 mg, 0.06 mmol) was added. The resulting clear solution was allowed to stand undisturbed at room temperature for 24 h. The product of 6-UPd (31 mg, 49%) was obtained as orange crystals after storage the THF solution at $-30^\circ$C for 24 h. Anal. Calcd (%) for C$_{40}$H$_{63}$Cl$_2$N$_2$O$_3$P$_3$PdU: C, 42.58; H, 5.63; N, 2.48. Found: C, 42.58; H, 5.56; N, 2.52.

7-U$_2$Pt$_3$. To a solution of complex 2 (83 mg, 0.12 mmol) dissolved in 2 mL THF, a 2 mL THF solution containing Pt(COD)$_2$ (74 mg, 0.018 mmol) was added. The resulting clear solution was allowed to stand undisturbed at room temperature for 24 h. The product of 7-U$_2$Pt$_3$ (62 mg, 52%) was obtained as black crystals after storage the THF solution at $-30^\circ$C for 24 h. Anal. Calcd (%) for C$_{44}$H$_{96}$Cl$_4$N$_4$O$_6$P$_4$Pt$_3$U$_2$: C, 25.11; H, 4.60; N, 2.66. Found: C, 23.74; H, 4.47; N, 2.53. The carbon content for this species is consistently lower
than the calculated values, which probably due to the loss of solvent molecules or due to the inadequate combustion of these air and moisture sensitive species.
2. NMR spectra

Fig. S1 $^1$H NMR spectrum of ligand L1 in benzene-$D_6$.

Fig. S2 $^{31}$P NMR spectrum of ligand L1 in benzene-$D_6$. 
Fig. S3 $^{13}$C NMR spectrum of ligand L1 in benzene-D$_6$.

Fig. S4 $^1$H NMR spectrum of ligand L2 in benzene-D$_6$. 
**Fig. S5** $^{31}$P NMR spectrum of ligand L2 in benzene-D$_6$.

**Fig. S6** $^{13}$C NMR spectrum of ligand L2 in benzene-D$_6$. 
Fig. S7 $^1$H NMR spectrum of complex 1 in benzene-$D_6$. 

Fig. S8 $^1$H NMR spectrum of complex 2 in benzene-$D_6$. 
Fig. S9 $^1$H NMR spectrum of cluster $\text{3-U}_2\text{Ni}_2$ in benzene-D$_6$. 
3. Powder X-ray diffraction

Fig. S10 Powder X-ray diffraction patterns for 4-\textit{U}_2\textit{Pd}_2 from 5° to 50° (a) and 5° to 20° (b).
Fig. S11 Powder X-ray diffraction patterns for $5\text{-}(\text{UNi})_n$ from 5° to 50° (a) and 5° to 20° (b).
Fig. S12 Powder X-ray diffraction patterns for 6-UPd from 5° to 50° (a) and 5° to 20° (b).
Fig. S13 Powder X-ray diffraction patterns for 7-U$_2$Pt$_3$ from 5° to 50° (a) and 5° to 20° (b).
4. X-ray Crystallographic data

Single-crystal X-ray diffraction data for complexes 1, 2, 3-U₂Ni₂, 4-U₂Pd₂, 5-(UNi)ₙ, 6-UPd, and 7-U₂Pt₃ were collected on BRUKER D8 VENTURE PHOTON II detectors with a radiation source of Mo(Kα) (0.71073 Å) or Ga(Kα) (1.34139 Å). Integrations, cell refinement and data reduction were performed with the SAINT program. The crystal system was determined by Laue symmetry, and the space groups were assigned on the basis of systematic absences by using XPREP. All structures were solved by directed methods and refined on $F^2$ using full-matrix least-squares methods with SHELXTL version 6.10. All non-hydrogen atoms were refined on $F^2$ by full-matrix least-squares procedures with the use of anisotropic displacement parameters. Evaluation of the CIF using the CheckCIF routine at www.checkcif.iucr.org gave no A or B alert for complexes 1, 2, 4-U₂Pd₂, 6-UPd, and 7-U₂Pt₃. An alert level B of low bond precision on C-C bonds was found when checking the CIF files of complexes 3-U₂Ni₂ and 5-(UNi)ₙ. The quality of these two crystals was poor but they represented the best products obtained from multiple recrystallization attempts. CCDC-1979169 (1), 1979170 (2), 1979171 (3-U₂Ni₂), 1979172 (4-U₂Pd₂), 1979173 (5-(UNi)ₙ), 1979174 (6-UPd), and 1979175 (7-U₂Pt₃) contain the crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre (www.ccdc.cam.ac.uk/data-request/cif). Details of the data collection and refinement for theses complexes are given in Tables S1 and S2.

| Complex | 1 | 2 | 3-U₂Ni₂ | 4-U₂Pd₂ |
|---------|---|---|---------|---------|
| Formula | C₂₀H₄₄Cl₂N₂₂O₂P₂U | C₁₈H₄₀Cl₂N₂₂O₂P₂ | C₄₄H₈₈Cl₄N₄Ni₂O₄P₂ | C₆₀H₈₈Cl₄N₄O₄P₄ |
| $M_r$ [g/mol] | 715.44 | 687.39 | 1620.40 | 1643.68 |
| Temp. [K] | 173(2) | 173(2) | 173(2) | 173(2) |
| Crystal system | Monoclinic | Monoclinic | Monoclinic | Orthorhombic |
| Space group | $P2_1/c$ | $P2_1/c$ | $P2_1/n$ | $Pccn$ |
| $a$ [Å] | 12.7105(10) | 14.480(2) | 14.5223(19) | 16.3226(16) |
| $b$ [Å] | 28.115(2) | 14.590(2) | 15.8953(18) | 22.813(2) |
| $c$ [Å] | 8.1727(7) | 12.5668(18) | 27.339(3) | 14.7718(15) |
| α [°]  | 90 | 90 | 90 | 90 |
|--------|----|----|----|----|
| β [°]  | 105.391 | 102.290(4) | 103.728(3) | 90 |
| γ [°]  | 90 | 90 | 90 | 90 |
| Volume [Å³] | 2815.8(4) | 2594.0(6) | 6130.5(13) | 5500.6(10) |
| Z/D<sub>calcd.</sub> [g/cm³] | 4/1.688 | 4/1.760 | 4/1.756 | 4/1.985 |
| μ [mm⁻¹] | 6.085 | 15.343 | 6.192 | 17.973 |
| F(000) | 1400 | 1336 | 3184 | 3168 |
| θ range [°] | 2.205 to 27.594 | 3.786 to 63.448 | 1.930 to 25.000 | 2.896 to 54.027 |
| Index ranges | -16 ≤ h ≤ 16 | 0 ≤ h ≤ 19 | -17 ≤ h ≤ 14 | -19 ≤ h ≤ 19 |
| | -25 ≤ k ≤ 36 | -19 ≤ k ≤ 0 | -18 ≤ k ≤ 18 | -27 ≤ k ≤ 27 |
| | -10 ≤ l ≤ 10 | -16 ≤ l ≤ 16 | -27 ≤ l ≤ 32 | -17 ≤ l ≤ 17 |
| Completeness | 99.8 % | 98.7 % | 99.9 % | 100.0 % |
| Data/parameters | 6512 / 270 | 6110 / 253 | 10800 / 581 | 5045 / 279 |
| GOF on F² | 1.091 | 1.125 | 1.002 | 1.013 |
| Final R indices [I>2σ(I)] | R<sub>1</sub> = 0.0474 | R<sub>1</sub> = 0.0647 | R<sub>1</sub> = 0.0465 | R<sub>1</sub> = 0.0332 |
| | R<sub>2</sub> = 0.1391 | R<sub>2</sub> = 0.1935 | R<sub>2</sub> = 0.1383 | R<sub>2</sub> = 0.0685 |
| R indices (all data) | R<sub>1</sub> = 0.0541 | R<sub>1</sub> = 0.0776 | R<sub>1</sub> = 0.0591 | R<sub>1</sub> = 0.0554 |
| | R<sub>2</sub> = 0.1439 | R<sub>2</sub> = 0.2195 | R<sub>2</sub> = 0.1495 | R<sub>2</sub> = 0.0776 |
| Largest diff. peak and hole [e·Å⁻³] | 4.911 and -3.682 | 2.719 and -4.676 | 2.691 and -2.743 | 0.945 and -0.817 |

**Table S2.** Crystal data and structure refinements for complexes 5-(UNi)<sub>n</sub>, 6-UPd and 7-U₂Pt₃.

| Complex | 5-(UNi)<sub>n</sub> | 6-UPd | 7-U₂Pt₃ |
|---------|--------------------|-------|---------|
| Formula | C<sub>22</sub>H<sub>48</sub>Cl₂N₂NiO₃P₃U | C<sub>40</sub>H<sub>60</sub>Cl₂N₂O₃P₃PdU | C<sub>64</sub>H<sub>96</sub>Cl₄N₄O₆P₄Pt₅U₂ |
| Mr [g/mol] | 818.20 | 1128.16 | 2104.25 |
| Property                      | Value 1          | Value 2          | Value 3          |
|-------------------------------|------------------|------------------|------------------|
| Temp. [K]                     | 173(2)           | 173(2)           | 173(2)           |
| Crystal system                | Monoclinic       | Triclinic        | Monoclinic       |
| Space group                   | $P2_1/n$         | $P\bar{1}$       | $C2/c$           |
| $a$ [Å]                       | 11.3508(18)      | 12.208(3)        | 12.6630(8)       |
| $b$ [Å]                       | 12.914(2)        | 12.209(3)        | 21.4809(13)      |
| $c$ [Å]                       | 20.597(4)        | 17.048(4)        | 23.0838(17)      |
| $\alpha$ [°]                 | 90               | 108.557(7)       | 90               |
| $\beta$ [°]                  | 95.165(7)        | 90.701(8)        | 99.354(2)        |
| $\gamma$ [°]                 | 90               | 108.839(7)       | 90               |
| Volume [Å³]                   | 3006.9(9)        | 2261.0(10)       | 6195.6(7)        |
| $Z$/Density [g/cm³]           | 4/1.807          | 2/1.657          | 4/2.256          |
| $\mu$ [mm⁻¹]                 | 16.624           | 11.277           | 21.368           |
| F(000)                        | 1608             | 1116             | 3928             |
| $\theta$ range/deg           | 3.518 to 54.617  | 2.398 to 54.402  | 3.376 to 63.565  |
| Index ranges                  | -13 ≤ h ≤ 13     | -14 ≤ h ≤ 14     | -16 ≤ h ≤ 16     |
|                               | -15 ≤ k ≤ 15     | -14 ≤ k ≤ 14     | -27 ≤ k ≤ 28     |
|                               | -22 ≤ l ≤ 24     | -20 ≤ l ≤ 20     | -30 ≤ l ≤ 20     |
| Completeness                  | 97.1 %           | 99.3             | 99.2 %           |
| Data/parameters               | 5406 / 277       | 8233 / 477       | 7657 / 311       |
| GOF on $F^2$                  | 1.112            | 1.042            | 1.066            |
| Final R indices               | $R_1 = 0.0977$   | $R_1 = 0.0344$   | $R_1 = 0.0376$   |
|                               | $R_2 = 0.2146$   | $R_2 = 0.0940$   | $R_2 = 0.0948$   |
| R indices (all data)          | $R_1 = 0.1126$   | $R_1 = 0.0359$   | $R_1 = 0.0439$   |
|                               | $R_2 = 0.2235$   | $R_2 = 0.0956$   | $R_2 = 0.0985$   |
| Largest diff. peak and hole   | 4.361 and -2.234 | 1.154 and -1.831 | 1.667 and -2.406 |
**Fig. S14** Crystal structure of complex 1. Thermal ellipsoids are drawn at 50 % probability. Hydrogen atoms are omitted for clarity.

**Table S3.** Selected bond lengths [Å] and angles [°] for complex 1.

| Bond                  | Length/Distance |
|-----------------------|-----------------|
| U(1)-N(2)             | 2.227(5)        |
| U(1)-Cl(2)            | 2.6653(17)      |
| U(1)-N(1)             | 2.245(5)        |
| U(1)-P(2)             | 3.0466(18)      |
| U(1)-O(1)             | 2.485(5)        |
| U(1)-P(1)             | 3.0747(19)      |
| U(1)-O(2)             | 2.485(5)        |
| U(1)-Cl(1)            | 2.6441(17)      |
| P(2)-N(2)             | 1.678(6)        |
| P(2)-C(14)            | 1.865(8)        |
| O(2)-C(17)            | 1.455(8)        |
| P(2)-C(11)            | 1.869(7)        |
| O(2)-C(20)            | 1.468(8)        |
| P(1)-N(1)             | 1.671(6)        |
| P(1)-C(8)             | 1.855(9)        |
| P(1)-C(5)             | 1.869(9)        |
| N(2)-C(4)             | 1.451(8)        |
| C(11)-C(12)           | 1.525(10)       |
| C(11)-C(13)           | 1.537(10)       |
| C(2)-C(1)             | 1.508(11)       |
| Bond                  | Length (Å) | Bond                  | Length (Å) | Bond                  | Length (Å) |
|----------------------|------------|----------------------|------------|----------------------|------------|
| C(4)-C(3)            | 1.508(10)  | C(17)-C(18)          | 1.505(11)  | C(20)-C(19)          | 1.502(10)  |
| C(5)-C(6)            | 1.512(14)  |                             |            |                           |            |
| N(2)-U(1)-N(1)       | 129.2(2)   | O(1)-U(1)-O(2)        | 171.33(16) |                           |            |
| N(2)-U(1)-O(1)       | 64.66(18)  | N(2)-U(1)-Cl(1)       | 89.92(16)  |                           |            |
| N(1)-U(1)-O(1)       | 64.98(19)  | N(1)-U(1)-Cl(1)       | 94.73(15)  |                           |            |
| N(2)-U(1)-O(2)       | 119.13(18) | O(1)-U(1)-Cl(1)       | 87.91(13)  |                           |            |
| N(1)-U(1)-O(2)       | 111.70(18) | O(2)-U(1)-Cl(1)       | 84.36(11)  |                           |            |
| N(2)-U(1)-Cl(2)      | 89.63(15)  | N(2)-U(1)-P(2)        | 32.66(14)  |                           |            |
| N(1)-U(1)-Cl(2)      | 93.25(15)  | N(1)-U(1)-P(2)        | 159.94(15) |                           |            |
| O(1)-U(1)-Cl(2)      | 100.86(12) | O(1)-U(1)-P(2)        | 97.22(11)  |                           |            |
| O(2)-U(1)-Cl(2)      | 87.18(11)  | O(2)-U(1)-P(2)        | 87.21(11)  |                           |            |
| Cl(1)-U(1)-Cl(2)     | 170.05(6)  | Cl(1)-U(1)-P(2)       | 93.71(5)   |                           |            |
| Cl(2)-U(1)-P(2)      | 80.63(5)   | Cl(1)-U(1)-P(1)       | 92.16(6)   |                           |            |
| N(2)-U(1)-P(1)       | 161.21(15) | Cl(2)-U(1)-P(1)       | 91.46(6)   |                           |            |
| N(1)-U(1)-P(1)       | 32.04(15)  | P(2)-U(1)-P(1)        | 165.03(5)  |                           |            |
| O(1)-U(1)-P(1)       | 96.74(11)  | N(2)-P(2)-C(14)       | 106.1(3)   |                           |            |
| O(2)-U(1)-P(1)       | 79.67(11)  | N(2)-P(2)-C(11)       | 104.7(3)   |                           |            |
| N(2)-P(2)-U(1)       | 45.74(19)  | C(8)-P(1)-C(5)        | 100.6(4)   |                           |            |
| C(14)-P(2)-U(1)      | 118.8(2)   | N(1)-P(1)-U(1)        | 45.47(19)  |                           |            |
| C(11)-P(2)-U(1)      | 130.6(2)   | C(8)-P(1)-U(1)        | 129.3(4)   |                           |            |
| N(1)-P(1)-C(8)       | 111.5(4)   | C(5)-P(1)-U(1)        | 127.6(3)   |                           |            |
| N(1)-P(1)-C(5)       | 107.2(3)   | C(17)-O(2)-C(20)      | 108.7(5)   |                           |            |
| C(17)-O(2)-U(1)      | 122.2(4)   | C(2)-N(1)-P(1)        | 129.9(5)   |                           |            |
| C(20)-O(2)-U(1)      | 123.1(4)   | C(2)-N(1)-U(1)        | 127.3(4)   |                           |            |
| C(3)-O(1)-C(1)       | 113.7(5)   | P(1)-N(1)-U(1)        | 102.5(3)   |                           |            |
| C(3)-O(1)-U(1)       | 115.3(4)   | C(4)-N(2)-P(2)        | 129.6(5)   |                           |
Fig. S15 Crystal structure of complex 2. Thermal ellipsoids are drawn at 50 % probability. Hydrogen atoms are omitted for clarity.

Table S4. Selected bond lengths [Å] and angles [°] for complex 2.

| Bond/Angle | Length/Distance | Bond/Angle | Length/Distance |
|------------|----------------|------------|----------------|
| C(1)-O(1)-U(1) | 115.7(4) | C(4)-N(2)-U(1) | 128.3(4) |
| P(2)-N(2)-U(1) | 101.6(3) |              |              |
| U(1)-N(2) | 2.237(8) | U(1)-O(2) | 2.559(7) |
| U(1)-N(1) | 2.242(7) | U(1)-Cl(2) | 2.683(2) |
| U(1)-O(3) | 2.547(6) | U(1)-Cl(1) | 2.686(3) |
| U(1)-P(1) | 2.885(3) | N(1)-P(2) | 1.636(9) |
| U(1)-P(2) | 2.894(2) | C(1)-O(3) | 1.443(12) |
| N(1)-C(7) | 1.500(13) | C(1)-C(6) | 1.498(16) |
| P(1)-N(2) | 1.651(8) | P(1)-C(2) | 1.844(12) |
| P(1)-C(14) | 1.883(11) |              |              |
| N(2)-U(1)-N(1) | 167.4(3) | N(2)-U(1)-O(2) | 127.9(3) |
| N(2)-U(1)-O(3) | 64.4(3) | N(1)-U(1)-O(2) | 64.7(3) |
| Bond/Angle | Value   | Bond/Angle | Value   |
|------------|---------|------------|---------|
| N(1)-U(1)-O(3) | 128.2(3) | O(3)-U(1)-O(2) | 63.6(2) |
| N(2)-U(1)-Cl(2) | 89.4(2) | N(1)-U(1)-Cl(1) | 89.6(2) |
| N(1)-U(1)-Cl(2) | 92.5(2) | O(3)-U(1)-Cl(1) | 84.46(17) |
| O(3)-U(1)-Cl(2) | 80.35(17) | O(2)-U(1)-Cl(1) | 80.69(17) |
| O(2)-U(1)-Cl(2) | 84.22(17) | Cl(2)-U(1)-Cl(1) | 162.18(8) |
| N(2)-U(1)-Cl(1) | 92.4(2) | N(2)-U(1)-P(1) | 34.8(2) |
| N(1)-U(1)-P(1) | 132.9(2) | N(2)-U(1)-P(2) | 133.4(2) |
| O(3)-U(1)-P(1) | 98.43(16) | N(1)-U(1)-P(2) | 34.3(2) |
| O(2)-U(1)-P(1) | 159.72(16) | O(3)-U(1)-P(2) | 159.43(16) |
| Cl(2)-U(1)-P(1) | 102.65(8) | O(2)-U(1)-P(2) | 98.19(16) |
| Cl(1)-U(1)-P(1) | 88.70(8) | Cl(2)-U(1)-P(2) | 88.80(8) |
| Cl(1)-U(1)-P(2) | 102.64(8) | C(7)-N(1)-U(1) | 128.0(7) |
| P(1)-U(1)-P(2) | 100.99(6) | P(2)-N(1)-U(1) | 95.2(3) |
| C(7)-N(1)-P(2) | 136.2(7) | O(3)-C(1)-C(6) | 105.1(9) |

**Fig. S16** Crystal structure of complex 3-\textsubscript{U$_2$Ni$_2$}. Thermal ellipsoids are drawn at 50 % probability. Hydrogen atoms are omitted for clarity.

**Table S5.** Selected bond lengths [Å] and angles [°] for complex 3-\textsubscript{U$_2$Ni$_2$}.

| Bond   | Value   |
|--------|---------|
| U(1)-N(1) | 2.243(7) |
| U(1)-Cl(4) | 2.8696(19) |
| Bond | Length (Å) | Bond | Length (Å) |
|------|-----------|------|-----------|
| U(1)-N(2) | 2.248(7) | U(1)-Ni(1) | 3.0477(11) |
| U(1)-O(1) | 2.532(7) | U(1)-P(1) | 3.160(2) |
| U(1)-Cl(1) | 2.633(3) | U(1)-Ni(2) | 3.1615(11) |
| U(1)-Cl(3) | 2.867(2) | U(1)-P(2) | 3.178(2) |
| U(2)-N(4) | 2.252(7) | U(2)-Cl(4) | 2.835(2) |
| U(2)-N(3) | 2.256(7) | U(2)-Ni(2) | 3.0358(10) |
| U(2)-O(2) | 2.502(6) | U(2)-Ni(1) | 3.1421(10) |
| U(2)-Cl(2) | 2.653(2) | U(2)-P(4) | 3.146(2) |
| U(2)-Cl(3) | 2.8145(19) | U(2)-P(3) | 3.159(2) |
| Ni(1)-P(3) | 2.162(3) | N(1)-C(1) | 1.462(12) |
| Ni(1)-P(1) | 2.173(2) | N(1)-P(1) | 1.679(8) |
| Ni(1)-Cl(4) | 2.257(2) | N(2)-C(4) | 1.427(12) |
| Ni(2)-P(2) | 2.157(3) | N(2)-P(2) | 1.689(8) |
| Ni(2)-P(4) | 2.175(2) | N(3)-C(5) | 1.464(11) |
| Ni(2)-Cl(3) | 2.286(2) | N(3)-P(3) | 1.672(7) |
| O(1)-C(2) | 1.272(14) | O(1)-C(3) | 1.442(13) |
| O(2)-C(6) | 1.415(11) | P(1)-C(12) | 1.851(12) |
| O(2)-C(7) | 1.460(10) | P(1)-C(9) | 1.877(9) |
| O(4)-C(37) | 1.39(4) | P(2)-C(18) | 1.864(9) |
| O(4)-C(40) | 1.47(5) | P(2)-C(15) | 1.866(10) |
| O(5)-C(44) | 1.31(3) | P(3)-C(21) | 1.863(8) |
| O(5)-C(41) | 1.42(4) | P(3)-C(24) | 1.876(8) |
| P(4)-C(30) | 1.848(9) | P(4)-C(27) | 1.864(9) |

| Bond | Angle (°) | Bond | Angle (°) |
|------|----------|------|----------|
| N(1)-U(1)-N(2) | 119.8(3) | N(1)-U(1)-Cl(3) | 130.7(2) |
| N(1)-U(1)-O(1) | 62.3(3) | N(2)-U(1)-Cl(3) | 109.4(2) |
| N(2)-U(1)-O(1) | 64.1(3) | O(1)-U(1)-Cl(3) | 154.9(2) |
| Bond                        | Angle (°) | Bond                        | Angle (°) |
|-----------------------------|-----------|-----------------------------|-----------|
| N(1)-U(1)-Cl(1)            | 93.2(2)   | Cl(1)-U(1)-Cl(3)            | 78.85(8)  |
| N(2)-U(1)-Cl(1)            | 101.6(2)  | N(1)-U(1)-Cl(4)             | 97.6(2)   |
| O(1)-U(1)-Cl(1)            | 79.0(3)   | N(2)-U(1)-Cl(4)             | 94.1(2)   |
| O(1)-U(1)-Cl(4)            | 127.6(3)  | Cl(1)-U(1)-Ni(1)            | 118.15(9) |
| Cl(1)-U(1)-Cl(4)           | 153.29(9) | Cl(3)-U(1)-Ni(1)            | 70.20(4)  |
| Cl(3)-U(1)-Cl(4)           | 75.59(6)  | Cl(4)-U(1)-Ni(1)            | 44.71(4)  |
| N(1)-U(1)-Ni(1)            | 71.54(19) | N(1)-U(1)-P(1)              | 30.62(19) |
| N(2)-U(1)-Ni(1)            | 138.6(2)  | N(2)-U(1)-P(1)              | 138.2(2)  |
| O(1)-U(1)-Ni(1)            | 131.76(19)| O(1)-U(1)-P(1)              | 92.07(18) |
| Cl(1)-U(1)-P(1)            | 107.04(9) | Cl(4)-U(1)-P(1)             | 73.07(6)  |
| Cl(3)-U(1)-P(1)            | 105.64(6) | Ni(1)-U(1)-P(1)             | 40.93(4)  |
| N(1)-U(1)-Ni(2)            | 156.09(19)| Ni(1)-U(1)-Ni(2)            | 86.86(3)  |
| N(2)-U(1)-Ni(2)            | 70.34(19) | P(1)-U(1)-Ni(2)             | 126.99(4) |
| O(1)-U(1)-Ni(2)            | 134.16(17)| N(1)-U(1)-P(2)              | 146.9(3)  |
| Cl(1)-U(1)-Ni(2)           | 106.31(7) | N(2)-U(1)-P(2)              | 30.6(2)   |
| Cl(3)-U(1)-Ni(2)           | 44.24(4)  | O(1)-U(1)-P(2)              | 94.47(18) |
| Cl(4)-U(1)-Ni(2)           | 58.95(5)  | Cl(1)-U(1)-P(2)             | 105.76(9) |
| Cl(3)-U(1)-P(2)            | 80.35(6)  | N(4)-U(2)-O(2)              | 63.9(2)   |
| Cl(4)-U(1)-P(2)            | 77.55(6)  | N(3)-U(2)-O(2)              | 64.6(2)   |
| Ni(1)-U(1)-P(2)            | 119.32(4) | N(4)-U(2)-Cl(2)             | 92.81(18) |
| P(1)-U(1)-P(2)             | 147.21(6) | N(3)-U(2)-Cl(2)             | 99.20(19) |
| Ni(2)-U(1)-P(2)            | 39.78(5)  | O(2)-U(2)-Cl(2)             | 84.03(17) |
| N(4)-U(2)-N(3)             | 125.2(3)  | N(4)-U(2)-Cl(3)             | 94.80(17) |
| N(3)-U(2)-Cl(3)            | 94.19(18) | N(3)-U(2)-Cl(4)             | 113.32(19)|
| O(2)-U(2)-Cl(3)            | 118.91(16)| O(2)-U(2)-Cl(4)             | 163.73(16)|
| Cl(2)-U(2)-Cl(3)           | 156.84(7) | Cl(2)-U(2)-Cl(4)            | 80.39(7)  |
| N(4)-U(2)-Cl(4)            | 121.4(2)  | Cl(3)-U(2)-Cl(4)            | 76.97(6)  |
| Bond | Angle | Error |
|------|-------|-------|
| N(4)-U(2)-Ni(2) | 72.14(18) |
| N(3)-U(2)-Ni(2) | 139.75(18) |
| Cl(3)-U(2)-Ni(2) | 45.82(4) |
| Cl(4)-U(2)-Ni(2) | 60.86(5) |
| O(2)-U(2)-Ni(2) | 132.03(14) |
| N(4)-U(2)-Ni(1) | 139.75(18) |
| Cl(3)-U(2)-Ni(1) | 69.47(4) |
| Cl(4)-U(2)-Ni(1) | 97.26(6) |
| N(3)-U(2)-P(4) | 148.7(2) |
| Cl(4)-U(2)-P(4) | 31.53(18) |
| Ni(2)-U(2)-P(4) | 94.94(14) |
| Ni(2)-U(2)-P(3) | 30.56(18) |
| Ni(2)-U(2)-P(3) | 94.89(14) |
| Ni(2)-U(2)-P(3) | 154.3(2) |
| Cl(4)-U(2)-P(3) | 128.78(9) |
| Ni(2)-U(2)-P(3) | 108.58(9) |
| Ni(1)-U(2)-P(3) | 135.69(7) |
| P(1)-Ni(1)-P(4) | 63.46(5) |
| P(3)-Ni(1)-P(4) | 123.10(9) |
| P(3)-Ni(1)-P(4) | 108.31(9) |
| Cl(4)-Ni(1)-P(4) | 149.93(8) |
| U(1)-Ni(1)-U(2) | 72.32(6) |
| U(2)-Ni(1)-U(2) | 72.13(6) |
| U(2)-Ni(1)-U(2) | 61.98(5) |
| C(1)-N(1)-U(1) | 70.52(7) |
| C(1)-N(1)-U(1) | 128.7(6) |
| C(1)-N(1)-U(1) | 106.5(4) |
| C(1)-N(1)-U(1) | 124.8(7) |
| C(1)-N(1)-U(1) | 127.8(6) |
| Bond/Angle | Length/Angle [Å/°] |
|------------|--------------------|
| C(1)-N(1)-P(1) | 124.4(6) |
| C(5)-N(3)-P(3) | 127.1(6) |
| C(5)-N(3)-U(2) | 126.4(5) |
| P(3)-N(3)-U(2) | 106.1(4) |
| C(8)-N(4)-P(4) | 127.8(6) |
| C(8)-N(4)-U(2) | 127.5(5) |
| P(4)-N(4)-U(2) | 104.6(3) |
| C(2)-O(1)-C(3) | 120.8(9) |
| C(2)-O(1)-U(1) | 121.5(8) |
| C(3)-O(1)-U(1) | 115.0(6) |
| C(6)-O(2)-C(7) | 115.9(7) |
| N(1)-P(1)-C(12) | 104.1(5) |
| N(1)-P(1)-C(9) | 106.4(4) |
| Ni(2)-Cl(3)-U(2) | 72.21(6) |
| Ni(2)-Cl(3)-U(1) | 74.73(7) |
| Ni(1)-Cl(4)-U(2) | 71.83(6) |
| Ni(1)-Cl(4)-U(1) | 103.03(7) |
| C(1)-P(1)-C(9) | 104.0(5) |
| C(1)-P(1)-C(12) | 113.6(3) |
| N(1)-P(1)-Ni(1) | 118.0(3) |
| N(1)-P(1)-N(1) | 42.9(3) |
| P(1)-Ni(1)-U(2) | 3.2655(6) |
| P(1)-Ni(1)-Pd(1) | 3.2992(6) |

**Fig. S17** Crystal structure of complex 4-Undoped. Thermal ellipsoids are drawn at 50% probability. Hydrogen atoms are omitted for clarity.

**Table S6.** Selected bond lengths [Å] and angles [°] for complex 4-Undoped.

| Bond/Distance | Length [Å] |
|---------------|------------|
| U(1)-N(1)     | 2.246(5)   |
| U(1)-N(2)     | 2.271(5)   |
| U(1)-Pd(1)    | 3.2655(6)  |
| U(1)-Pd(1)#1  | 3.2992(6)  |
| Bond                  | Distance (Å) | Bond                  | Distance (Å) | Bond                  | Distance (Å) |
|----------------------|--------------|----------------------|--------------|----------------------|--------------|
| U(1)-O(1)            | 2.520(4)     | Pd(1)-P(2)           | 2.2825(17)   | U(1)-O(1)            | 2.520(4)     |
| U(1)-Cl(1)           | 2.6928(16)   | Pd(1)-P(1)#1         | 2.3101(17)   | U(1)-Cl(1)           | 2.6928(16)   |
| U(1)-O(2)            | 2.757(4)     | Pd(1)-Cl(2)          | 2.6893(16)   | U(1)-O(2)            | 2.757(4)     |
| U(1)-Cl(2)#1         | 2.8339(16)   | Pd(1)-U(1)#1         | 3.2992(6)    | U(1)-Cl(2)#1         | 2.8339(16)   |
| U(1)-Cl(2)           | 2.9229(15)   | Cl(2)-U(1)#1         | 2.8340(16)   | U(1)-Cl(2)           | 2.9229(15)   |
| U(1)-P(1)            | 3.2069(17)   | N(1)-C(1)            | 1.479(8)     | U(1)-P(1)            | 3.2069(17)   |
| U(1)-P(2)            | 3.2251(16)   | N(1)-P(1)            | 1.673(5)     | U(1)-P(2)            | 3.2251(16)   |
| N(2)-P(2)            | 1.671(5)     | N(2)-C(4)            | 1.464(8)     | N(2)-P(2)            | 1.671(5)     |
| N(2)-P(2)            | 1.671(5)     | P(1)-Pd(1)#1         | 2.3100(17)   | N(2)-P(2)            | 1.671(5)     |
| N(2)-P(2)            | 1.671(5)     | P(2)-C(8)            | 1.854(7)     | N(2)-P(2)            | 1.671(5)     |
| N(2)-P(2)            | 1.671(5)     | P(2)-C(5)            | 1.862(6)     | N(2)-P(2)            | 1.671(5)     |
| N(2)-P(2)            | 1.671(5)     | C(1)-C(2)            | 1.512(9)     | N(2)-P(2)            | 1.671(5)     |
| N(2)-P(2)            | 1.671(5)     | N(2)-P(2)            | 1.671(5)     | N(2)-P(2)            | 1.671(5)     |
| N(1)-U(1)-N(2)       | 130.73(18)   | O(1)-U(1)-Cl(1)      | 75.10(10)    | N(1)-U(1)-N(2)       | 130.73(18)   |
| N(1)-U(1)-O(1)       | 65.63(15)    | N(1)-U(1)-O(2)       | 80.38(16)    | N(1)-U(1)-O(1)       | 65.63(15)    |
| N(2)-U(1)-O(1)       | 65.61(16)    | N(2)-U(1)-O(2)       | 79.57(16)    | N(2)-U(1)-O(1)       | 65.61(16)    |
| N(1)-U(1)-Cl(1)      | 86.40(14)    | O(1)-U(1)-O(2)       | 73.35(13)    | N(1)-U(1)-Cl(1)      | 86.40(14)    |
| N(2)-U(1)-Cl(1)      | 87.87(13)    | Cl(1)-U(1)-O(2)      | 148.44(10)   | N(2)-U(1)-Cl(1)      | 87.87(13)    |
| N(1)-U(1)-Cl(2)#1    | 108.13(13)   | N(1)-U(1)-Cl(2)#1    | 111.90(13)   | N(1)-U(1)-Cl(2)#1    | 108.13(13)   |
| N(2)-U(1)-Cl(2)#1    | 106.67(14)   | N(2)-U(1)-Cl(2)#1    | 112.50(12)   | N(2)-U(1)-Cl(2)#1    | 106.67(14)   |
| O(1)-U(1)-Cl(2)#1    | 143.86(10)   | O(1)-U(1)-Cl(2)#1    | 146.98(10)   | O(1)-U(1)-Cl(2)#1    | 143.86(10)   |
| Cl(1)-U(1)-Cl(2)#1   | 141.04(5)    | Cl(1)-U(1)-Cl(2)#1   | 71.88(5)     | Cl(1)-U(1)-Cl(2)#1   | 141.04(5)    |
| O(2)-U(1)-Cl(2)#1    | 70.51(10)    | O(2)-U(1)-Cl(2)#1    | 139.67(10)   | O(2)-U(1)-Cl(2)#1    | 70.51(10)    |
| Cl(2)#1-U(1)-Cl(2)   | 69.16(5)     | Cl(2)#1-U(1)-P(1)    | 84.26(4)     | Cl(2)#1-U(1)-Cl(2)   | 69.16(5)     |
| N(1)-U(1)-P(1)       | 29.56(13)    | Cl(2)-U(1)-P(1)      | 87.51(4)     | N(1)-U(1)-P(1)       | 29.56(13)    |
| N(2)-U(1)-P(1)       | 159.44(13)   | N(1)-U(1)-P(2)       | 160.03(13)   | N(2)-U(1)-P(1)       | 159.44(13)   |
| Bond                  | Bond Angle 1  | Bond Angle 2  | Bond Angle 3  |
|----------------------|--------------|--------------|--------------|
| O(1)-U(1)-P(1)       | 95.19(10)    | N(2)-U(1)-P(2) | 29.36(13)    |
| Cl(1)-U(1)-P(1)      | 94.34(5)     | O(1)-U(1)-P(2) | 94.82(10)    |
| O(2)-U(1)-P(1)       | 88.14(10)    | Cl(1)-U(1)-P(2) | 92.57(5)    |
| O(2)-U(1)-P(2)       | 90.42(10)    | Cl(2)-U(1)-P(2) | 85.01(4)    |
| Cl(2)-U(1)-P(2)      | 86.56(4)     | O(2)-U(1)-P(2) | 104.67(9)    |
| P(1)-U(1)-P(2)       | 169.03(4)    | Cl(2)-U(1)-Pd(1) | 56.29(3)    |
| N(1)-U(1)-Pd(1)      | 158.61(12)   | Cl(2)-U(1)-Pd(1) | 51.15(3)    |
| N(2)-U(1)-Pd(1)      | 70.53(13)    | P(1)-U(1)-Pd(1) | 129.07(3)    |
| O(1)-U(1)-Pd(1)      | 135.75(9)    | P(2)-U(1)-Pd(1) | 41.17(3)    |
| Cl(1)-U(1)-Pd(1)     | 98.07(4)     | N(1)-U(1)-Pd(1)#1 | 71.11(12) |
| N(2)-U(1)-Pd(1)#1    | 156.24(13)   | P(2)-Pd(1)-P(1)#1 | 131.21(6) |
| O(1)-U(1)-Pd(1)#1    | 136.69(9)    | P(2)-Pd(1)-Cl(2) | 115.94(6) |
| Cl(1)-U(1)-Pd(1)#1   | 104.69(4)    | P(1)#1-Pd(1)-Cl(2) | 108.43(6) |
| O(2)-U(1)-Pd(1)#1    | 97.94(9)     | P(2)-Pd(1)-U(1) | 68.46(4)    |
| Cl(2)#1-U(1)-Pd(1)#1 | 51.33(3)     | P(1)#1-Pd(1)-U(1) | 159.38(5) |
| Cl(2)-U(1)-Pd(1)#1   | 55.20(3)     | Cl(2)-Pd(1)-U(1) | 57.83(3)    |
| P(1)-U(1)-Pd(1)#1    | 41.56(3)     | P(2)-Pd(1)-U(1)#1 | 158.94(4) |
| P(2)-U(1)-Pd(1)#1    | 128.11(3)    | P(1)#1-Pd(1)-U(1)#1 | 67.08(4) |
| Pd(1)-U(1)-Pd(1)#1   | 87.551(14)   | Cl(2)-Pd(1)-U(1)#1 | 55.36(3) |
| U(1)-Pd(1)-U(1)#1    | 92.449(14)   | Pd(1)-Cl(2)-U(1) | 71.02(4)    |
| Pd(1)-Cl(2)-U(1)#1   | 73.30(4)     | U(1)#1-Cl(2)-U(1) | 110.84(5) |

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1
Fig. S18 Crystal structure of complex 5-(UNi)$_n$. Thermal ellipsoids are drawn at 50 % probability. Hydrogen atoms are omitted for clarity.

Table S7. Selected bond lengths [Å] and angles [°] for complex 5-(UNi)$_n$.

| Bond                                      | Length/Distance | Bond                                      | Length/Distance |
|-------------------------------------------|-----------------|-------------------------------------------|-----------------|
| Ni(1)-P(2)                                | 2.224(5)        | U(1)-N(1)                                 | 2.241(16)       |
| Ni(1)-P(1)                                | 2.226(5)        | U(1)-O(2)                                 | 2.523(13)       |
| Ni(1)-Cl(2)                               | 2.409(5)        | U(1)-O(1)                                 | 2.548(15)       |
| Ni(1)-U(1)                                | 2.620(3)        | U(1)-Cl(1)                                | 2.711(5)        |
| U(1)-N(2)                                 | 2.236(17)       | U(1)-Cl(2)#1                              | 2.820(5)        |
| U(1)-P(1)                                 | 2.969(5)        | N(2)-C(6)                                 | 1.51(3)         |
| U(1)-P(2)                                 | 2.994(5)        | N(2)-P(2)                                 | 1.656(17)       |
| Cl(2)-U(1)#2                              | 2.820(5)        | O(1)-C(3)                                 | 1.42(3)         |
| N(1)-C(1)                                 | 1.44(3)         | O(1)-C(2)                                 | 1.45(3)         |
| N(1)-P(1)                                 | 1.648(16)       | O(2)-C(4)                                 | 1.43(3)         |
| O(2)-C(5)                                 | 1.46(2)         | P(2)-C(16)                                | 1.83(2)         |
| P(1)-C(7)                                 | 1.85(2)         | P(2)-C(13)                                | 1.83(2)         |
| P(1)-C(10)                                | 1.87(2)         | C(1)-C(2)                                 | 1.55(3)         |
| P(2)-Ni(1)-P(1)                           | 150.6(2)        | Cl(2)-Ni(1)-U(1)                          | 170.77(18)      |
| P(2)-Ni(1)-Cl(2)                          | 109.2(2)        | N(2)-U(1)-N(1)                            | 158.6(6)        |
| P(1)-Ni(1)-Cl(2)                          | 100.2(2)        | N(2)-U(1)-O(2)                            | 67.1(5)         |
P(2)-Ni(1)-U(1)  75.85(15)  N(1)-U(1)-O(2)  134.0(5)
P(1)-Ni(1)-U(1)  75.06(16)  N(2)-U(1)-O(1)  134.1(5)
N(1)-U(1)-O(1)  67.3(5)  N(2)-U(1)-Ni(1)  79.1(4)
O(2)-U(1)-O(1)  67.1(5)  N(1)-U(1)-Ni(1)  79.7(4)
O(2)-U(1)-Ni(1)  146.2(3)  N(2)-U(1)-Cl(1)  91.8(5)
O(1)-U(1)-Ni(1)  146.5(3)  N(1)-U(1)-Cl(1)  95.2(5)
O(2)-U(1)-Cl(1)  80.1(3)  O(2)-U(1)-Cl(2)#1  79.2(3)
O(1)-U(1)-Cl(1)  77.7(4)  O(1)-U(1)-Cl(2)#1  79.7(4)
Ni(1)-U(1)-Cl(1)  100.70(14)  Ni(1)-U(1)-Cl(2)#1  105.42(13)
N(2)-U(1)-Cl(2)#1  94.6(5)  Cl(1)-U(1)-Cl(2)#1  153.83(17)
N(1)-U(1)-Cl(2)#1  88.0(5)  N(2)-U(1)-P(1)  125.5(4)
N(1)-U(1)-P(1)  33.3(4)  Cl(2)#1-U(1)-P(1)  97.58(15)
O(2)-U(1)-P(1)  167.4(3)  N(2)-U(1)-P(2)  33.1(4)
O(1)-U(1)-P(1)  100.4(3)  N(1)-U(1)-P(2)  125.7(4)
Ni(1)-U(1)-P(1)  46.43(11)  O(2)-U(1)-P(2)  100.2(3)
Cl(1)-U(1)-P(1)  99.25(16)  O(1)-U(1)-P(2)  167.0(3)
Ni(1)-U(1)-P(2)  46.09(11)  P(1)-U(1)-P(2)  92.44(14)
Cl(1)-U(1)-P(2)  98.41(16)  Ni(1)-Cl(2)-U(1)#2  167.2(2)
Cl(2)#1-U(1)-P(2)  100.74(15)

Symmetry transformations used to generate equivalent atoms:

#1  -x+3/2,y-1/2,-z+1/2  #2  -x+3/2,y+1/2,-z+1/2
Fig. S19 Crystal structure of complex 6-UPd. Thermal ellipsoids are drawn at 50 % probability. Hydrogen atoms are omitted for clarity.

Table S8. Selected bond lengths [Å] and angles [°] for complex 6-UPd.

| Bond                  | Length [Å]     | Bond                  | Length [Å]     |
|-----------------------|----------------|-----------------------|----------------|
| U(1)-N(2)             | 2.216(4)       | U(1)-Cl(2)            | 2.7008(13)     |
| U(1)-N(1)             | 2.222(4)       | U(1)-Pd(1)            | 2.9041(6)      |
| U(1)-O(1)             | 2.481(3)       | U(1)-P(2)             | 3.0551(12)     |
| U(1)-O(2)             | 2.510(3)       | U(1)-P(1)             | 3.0617(14)     |
| U(1)-Cl(1)            | 2.7002(14)     | Pd(1)-P(1)            | 2.3770(12)     |
| Pd(1)-P(2)            | 2.4053(12)     | P(2)-C(16)            | 1.852(5)       |
| Pd(1)-P(3)            | 2.4295(12)     | P(2)-C(13)            | 1.859(5)       |
| P(1)-N(1)             | 1.657(4)       | P(3)-C(31)            | 1.825(5)       |
| P(1)-C(10)            | 1.857(5)       | P(3)-C(25)            | 1.835(5)       |
| P(1)-C(7)             | 1.860(5)       | P(3)-C(19)            | 1.851(5)       |
| O(1)-C(3)             | 1.445(6)       | O(3)-C(40)            | 1.439(11)      |
| O(1)-C(2)             | 1.455(7)       | N(1)-C(1)             | 1.469(6)       |
| O(2)-C(5)             | 1.427(6)       | N(2)-C(6)             | 1.465(6)       |
| O(2)-C(4)             | 1.434(6)       | C(1)-C(2)             | 1.500(8)       |
| O(3)-C(37)            | 1.365(12)      |                       |                |
| Bond Configuration | Distance (Å) | Bond Configuration | Distance (Å) |
|--------------------|-------------|--------------------|-------------|
| N(2)-U(1)-N(1)     | 158.14(15)  | O(1)-U(1)-Cl(1)    | 79.55(9)    |
| N(2)-U(1)-O(1)     | 133.92(13)  | O(2)-U(1)-Cl(1)    | 82.11(9)    |
| N(1)-U(1)-O(1)     | 67.94(13)   | N(2)-U(1)-Cl(2)    | 93.78(10)   |
| N(2)-U(1)-O(2)     | 67.07(12)   | N(1)-U(1)-Cl(2)    | 90.46(11)   |
| N(1)-U(1)-O(2)     | 134.72(13)  | O(1)-U(1)-Cl(2)    | 79.78(9)    |
| O(1)-U(1)-O(2)     | 66.94(12)   | O(2)-U(1)-Cl(2)    | 78.18(9)    |
| N(2)-U(1)-Cl(1)    | 91.45(10)   | Cl(1)-U(1)-Cl(2)   | 155.73(5)   |
| N(1)-U(1)-Cl(1)    | 93.44(11)   | N(2)-U(1)-Pd(1)    | 79.60(10)   |
| N(1)-U(1)-Pd(1)    | 78.61(10)   | O(1)-U(1)-Pd(1)    | 146.23(9)   |
| O(2)-U(1)-Pd(1)    | 146.67(8)   | Cl(2)-U(1)-Pd(1)   | 105.66(4)   |
| Cl(1)-U(1)-Pd(1)   | 98.60(4)    | N(2)-U(1)-P(2)     | 32.07(10)   |
| N(1)-U(1)-P(2)     | 126.11(11)  | O(1)-U(1)-P(1)     | 99.69(9)    |
| O(1)-U(1)-P(2)     | 165.70(9)   | O(2)-U(1)-P(1)     | 166.38(8)   |
| O(2)-U(1)-P(2)     | 99.15(8)    | Cl(1)-U(1)-P(1)    | 98.50(4)    |
| Cl(1)-U(1)-P(2)    | 95.75(4)    | Cl(2)-U(1)-P(1)    | 97.38(4)    |
| Cl(2)-U(1)-P(2)    | 101.23(4)   | Cl(2)-U(1)-P(1)    | 97.38(4)    |
| Pd(1)-U(1)-P(2)    | 47.53(2)    | Pd(1)-U(1)-P(1)    | 46.87(2)    |
| N(2)-U(1)-P(1)     | 126.37(10)  | Pd(1)-Pd(1)-P(2)   | 139.43(4)   |
| N(1)-U(1)-P(1)     | 31.78(11)   | P(1)-Pd(1)-P(3)    | 110.62(4)   |
| P(2)-Pd(1)-P(3)    | 109.95(4)   | N(1)-P(1)-Pd(1)    | 107.95(14)  |
| P(1)-Pd(1)-U(1)    | 70.05(4)    | C(10)-P(1)-Pd(1)   | 118.33(19)  |
| P(2)-Pd(1)-U(1)    | 69.53(3)    | C(7)-P(1)-Pd(1)    | 111.27(18)  |
| P(3)-Pd(1)-U(1)    | 175.64(3)   | N(1)-P(1)-U(1)     | 44.94(13)   |
| N(1)-P(1)-C(10)    | 105.12(2)   | C(10)-P(1)-U(1)    | 124.48(18)  |
| N(1)-P(1)-C(7)     | 108.9(2)    | C(7)-P(1)-U(1)     | 127.2(2)    |
| C(10)-P(1)-C(7)    | 104.8(3)    | Pd(1)-P(1)-U(1)    | 63.08(3)    |
Figure S20 Crystal structure of complex 7-U₂Pt₃. Thermal ellipsoids are drawn at 50% probability. Hydrogen atoms are omitted for clarity.

Table S9. Selected bond lengths [Å] and angles [°] for complex 7-U₂Pt₃.

| Bond/Angle               | Value     | Bond/Angle               | Value     |
|--------------------------|-----------|--------------------------|-----------|
| U(1)-N(1)                | 2.286(5)  | U(1)-Cl(2)               | 2.6865(16)|
| U(1)-N(2)                | 2.343(5)  | U(1)-Pt(1)               | 2.7584(4) |
| U(1)-O(2)                | 2.541(4)  | U(1)-P(1)                | 3.1082(15)|
| U(1)-O(1)                | 2.600(4)  | Pt(1)-P(1)               | 2.2161(14)|
| U(1)-Cl(1)               | 2.6725(16)| Pt(1)-Pt(2)              | 2.6074(4) |
| Pt(1)-Pt(1)#1            | 2.8317(5) | N(1)-P(1)                | 1.630(5)  |
| Pt(2)-P(2)               | 2.3060(15)| N(2)-C(6)                | 1.485(7)  |
| Pt(2)-P(2)#1             | 2.3060(15)| N(2)-P(2)                | 1.640(5)  |
| Pt(2)-Pt(1)#1            | 2.6074(4) | O(1)-C(3)                | 1.424(8)  |
| N(1)-C(1)                | 1.463(7)  | O(1)-C(2)                | 1.439(8)  |
| O(2)-C(5)                | 1.427(8)  | O(3)-C(19)               | 1.555(17) |
| O(2)-C(4)                | 1.433(7)  | P(1)-C(10)               | 1.843(6)  |
| O(3)-C(22)               | 1.494(15) | P(1)-C(7)                | 1.850(6)  |
| P(2)-C(16)               | 1.845(6)  | P(2)-C(13)               | 1.866(6)  |
| C(1)-C(2)                | 1.508(9)  |                          |           |
| N(1)-U(1)-N(2)           | 166.60(18)| O(2)-U(1)-O(1)           | 61.51(14) |
| Bond                  | Distance (Å) | Bond Angle (°) |
|-----------------------|--------------|----------------|
| N(1)-U(1)-O(2)        | 125.74(16)   | N(1)-U(1)-Cl(1) 93.94(14) |
| N(2)-U(1)-O(2)        | 67.53(15)    | N(2)-U(1)-Cl(1) 90.78(13) |
| N(1)-U(1)-O(1)        | 64.22(15)    | O(2)-U(1)-Cl(1) 78.14(11) |
| N(2)-U(1)-O(1)        | 129.02(15)   | O(1)-U(1)-Cl(1) 80.94(11) |
| N(1)-U(1)-Cl(2)       | 91.03(14)    | N(1)-U(1)-Pt(1) 74.52(13) |
| N(2)-U(1)-Cl(2)       | 89.85(13)    | N(2)-U(1)-Pt(1) 92.42(12) |
| O(2)-U(1)-Cl(2)       | 79.44(11)    | O(2)-U(1)-Pt(1) 159.34(9)  |
| O(1)-U(1)-Cl(2)       | 79.65(11)    | O(1)-U(1)-Pt(1) 138.47(10) |
| Cl(1)-U(1)-Cl(2)      | 155.44(6)    | Cl(1)-U(1)-Pt(1) 97.97(4)  |
| N(1)-U(1)-P(1)        | 30.63(13)    | Cl(2)-U(1)-Pt(1) 106.53(4) |
| N(2)-U(1)-P(1)        | 136.23(12)   | P(1)-Pt(1)-Pt(2) 163.89(4) |
| O(2)-U(1)-P(1)        | 156.16(10)   | P(1)-Pt(1)-U(1)  76.47(4)  |
| O(1)-U(1)-P(1)        | 94.75(10)    | Pt(2)-Pt(1)-U(1) 102.594(9) |
| Cl(1)-U(1)-P(1)       | 96.94(5)     | P(1)-Pt(1)-Pt(1)#1 138.02(4) |
| Cl(2)-U(1)-P(1)       | 99.51(5)     | Pt(2)-Pt(1)-Pt(1)#1 57.111(7) |
| Pt(1)-U(1)-P(1)       | 43.89(3)     | U(1)-Pt(1)-Pt(1)#1 116.123(15) |
| P(2)-Pt(2)-Pt(1)      | 95.94(4)     | P(2)-Pt(2)-P(2)#1 160.59(8) |
| P(2)#1-Pt(2)-Pt(1)    | 100.35(4)    | P(2)#1-Pt(2)-Pt(1)#1 95.94(4) |
| P(2)-Pt(2)-Pt(1)#1    | 100.35(4)    | Pt(1)-Pt(2)-Pt(1)#1 65.777(14) |
| C(1)-N(1)-P(1)        | 128.8(4)     | C(6)-N(2)-P(2) 119.0(4)  |
| C(1)-N(1)-U(1)        | 127.4(4)     | C(6)-N(2)-U(1) 116.9(4)  |
| P(1)-N(1)-U(1)        | 103.8(2)     | P(2)-N(2)-U(1) 123.6(3)  |

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z+3/2
6. Magnetic measurements data

**Fig. S21** Variable temperature SQUID data plotted of complex \(3\text{-U}_2\text{Ni}_2\) as \(\chi\) vs \(T\) (a), \(1/\chi\) vs \(T\) (b), \(\mu_{\text{eff}}\) vs \(T\) per molecule (c), and field-dependent SQUID magnetization at 1.8 K (d).

**Fig. S22** Variable temperature SQUID data plotted of complex \(4\text{-U}_2\text{Pd}_2\) as \(\chi\) vs \(T\) (a), \(1/\chi\) vs \(T\) (b), \(\mu_{\text{eff}}\) vs \(T\) per molecule (c), and field-dependent SQUID magnetization at 1.8 K (d).
Fig. S23 Variable temperature SQUID data plotted of complex 5-(UNi)$_n$ $\chi$ vs T (a), $1/\chi$ vs T (b), $\mu_{\text{eff}}$ vs T per uranium ion (c), and field-dependent SQUID magnetization at 1.8 K (d).

Fig. S24 Variable temperature SQUID data plotted of complex 6-UPd as $\chi$ vs T (a), $1/\chi$ vs T (b), $\mu_{\text{eff}}$ vs T per uranium ion (c), and field-dependent SQUID magnetization at 1.8 K (d).
5. Computational Section.

The Gaussian09 program suite was used for all quantum-chemical calculations.\textsuperscript{54} We used Becke’s 3-parameter hybrid version,\textsuperscript{55} combined with the non-local correlation functional provided by Perdew/Wang,\textsuperscript{56} denoted as B3PW91. The relativistic energy-consistent small-core pseudopotential of the Stuttgart-Köln ECP library was used in combination with its adapted segmented basis set to represent a uranium atom\textsuperscript{57-59} For phosphorus, chlorine and nickel, palladium and platinum the quasi-relativistic energy-adjusted \textit{ab-initio} pseudopotentials were used, along with their corresponding energy-optimized valence basis sets.\textsuperscript{510,511} For all the atoms, the 6-31G(d) basis set was used.\textsuperscript{512,513} In all computations no constraints were imposed on the geometry. A full geometry optimization was performed for each structure using Schlegel’s analytical gradient method\textsuperscript{514} and the attainment of the energy minimum was verified by calculating the vibrational frequencies that result in the absence of imaginary eigenvalues. All stationary points have been identified for the minimum (number of imaginary frequencies, Nimag = 0). The NBO analysis\textsuperscript{515} was carried out on the optimized structures using the module included in the Gaussian package. Finally, the Chemcraft graphical program was used for the 3D representations of the structures and the orbital plots.\textsuperscript{516}
Fig. S26 Optimized structure of complex 3-U$_2$Ni$_2$.

Table S10. The WBI of the complex 3-U$_2$Ni$_2$ with regards to the bonding surround the U atoms.

|            | WBI  |            | WBI  |
|------------|------|------------|------|
| U28 – Ni7  | 0.4  | U11 – N23  | 0.8  |
| U11 – Ni19 | 0.3  | U28 – N34  | 0.8  |
| U11 – Ni7  | 0.3  | U11 – O12  | 0.3  |
| U28 – Ni19 | 0.3  | U28 – O29  | 0.3  |
| U11 – Cl27 | 0.6  | Ni7 – P8   | 0.4  |
| U11 – Cl33 | 0.6  | Ni19 – P20 | 0.4  |
| U28 – Cl27 | 0.7  | Ni7 – P4   | 0.4  |
| U28 – Cl33 | 0.6  | Ni19 – P16 | 0.4  |

Table S11. NBO analysis summary for complex 3-U$_2$Ni$_2$.

|            | U(28) | Ni(7) |
|------------|-------|-------|
| 1st Bond   |       |       |
| U(28)      | 11.62%| 88.38%|
| Ni(7)      |       |       |
| s          | 12.04%| 0.19% |
| p          | 6.94% | 0.50% |
| d          | 27.58%| 99.31%|
| f          | 53.43%| 0.00% |

|            | U(11) | Ni(19) |
|------------|-------|--------|
| 1st Bond   |       |        |
| U(11)      | 10.09%| 89.91% |
| Ni(19)     |       |        |
| s          | 13.07%| 0.08%  |
| p          | 6.59% | 0.51%  |
| d          | 29.10%| 99.41% |
| f          | 54.54%| 0.00%  |

|            | U(11) | N(15) |
|------------|-------|-------|
| 1st Bond   |       |       |
| U(11)      | 12.91%| 87.09%|
| N(15)      |       |       |
| s          | 15.05%| 45.79%|
| p          | 5.21% | 54.21%|
| d          | 54.54%| 0.01% |
| f          | 25.17%| 0.00% |

|            | U(11) | N(15) |
|------------|-------|-------|
| 2nd Bond   |       |       |
| 1st Bond   |       |       |
| U(11)      | 12.63%| 87.37%|
| N(15)      |       |       |
| s          | 15.05%| 45.79%|
| p          | 5.21% | 54.21%|
| d          | 54.54%| 0.01% |
| f          | 25.17%| 0.00% |
|   | 1st Bond |  | 2nd Bond |  | 1st Bond |  | 2nd Bond |  | 1st Bond |  | 2nd Bond |  |
|---|---------|---|----------|---|---------|---|----------|---|---------|---|----------|---|
|   | U(11)   | N(23) |         |    | U(28)   | N(32) |         |    | U(28)   | N(34) |         |    |
|   | 14.19%  | 85.81% |         |    | 14.56%  | 85.44% |         |    | 12.94%  | 87.06% |         |    |
|   | 5.29%   | 3.78%  | 53.20%  | 37.70% | 45.47%  | 54.52% | 0.01%   | 0.00% | 6.98%   | 3.49%  | 53.00%  | 36.49% | 44.81%  | 55.19% | 0.01%   | 0.00% |
|   | 12.74%  | 87.26% |         |    | 13.29%  | 86.71% |         |    | 13.15%  | 5.78%  | 51.67%  | 29.36% | 46.03%  | 53.96% | 0.00%   | 0.00% |
|   | 0.01%   | 11.98% | 40.01%  | 47.98% | 0.03%   | 99.96% | 0.01%   | 0.00% | 0.01%   | 11.39% | 41.38%  | 47.21% | 0.02%   | 99.97% | 0.01%   | 0.00% |
|   |         |        |         |    |         |        |         |    |         |        |         |    |         |        |         |    |
|   | 15.47%  | 84.53% |         |    | 11.84%  | 88.16% |         |    |         |        |         |    |         |        |         |    |
|   | 14.75%  | 26.68% | 39.11%  | 19.45% | 53.37%  | 46.63% | 0.00%   | 0.00% |         |        |         |    |         |        |         |    |
|   | 14.42%  | 11.63% | 48.79%  | 25.16% | 30.93%  | 69.07% | 0.00%   | 0.00% |         |        |         |    |         |        |         |    |
|   |         |        |         |    |         |        |         |    |         |        |         |    |         |        |         |    |
|   | U(11)   | Cl(26) |         |    | U(11)   | Cl(27) |         |    | U(11)   | Cl(33) |         |    |
| s | p       | d       | f       |    | s       | p       | d       | f    | s       | p       | d       | f    | s       | p       | d       | f    |
| 1st Bond | 12.07% | 87.93% |
|----------|--------|--------|
| s        | p      | d      | f      | s     | p     | d     | f     |
| 15.30%   | 22.33% | 34.47% | 27.89% | 32.66%| 67.34%| 0.00% | 0.00% |

| 1st Bond | 12.66% | 87.34% |
|----------|--------|--------|
| s        | p      | d      | f      | s     | p     | d     | f     |
| 14.83%   | 23.82% | 32.86% | 28.49% | 34.69%| 65.31%| 0.00% | 0.00% |

| 1st Bond | 12.30% | 87.70% |
|----------|--------|--------|
| s        | p      | d      | f      | s     | p     | d     | f     |
| 11.59%   | 12.68% | 51.03% | 24.70% | 32.32%| 67.68%| 0.00% | 0.00% |

| 1st Bond | 15.90% | 84.10% |
|----------|--------|--------|
| s        | p      | d      | f      | s     | p     | d     | f     |
| 14.27%   | 27.96% | 37.28% | 20.49% | 54.26%| 45.74%| 0.00% | 0.00% |

Fig. S27 Unpaired spin density plot for complex $3\text{U}_2\text{Ni}_2$. 

![Unpaired spin density plot](image.png)
Fig. S28 Optimized structure of complex 6-UPd.

Table S12. The WBI of the complex 6-UPd with regards to the bonding surround the U atoms.

| Bonding coordinate | WBI |
|--------------------|-----|
| U15 – Pd14         | 0.4 |
| U15 – Cl16         | 0.8 |
| U15 – Cl40         | 0.9 |
| U15 – N18          | 0.6 |
| U15 – N27          | 0.6 |
| U15 – O21          | 0.3 |
| U15 – O24          | 0.3 |
| Pd14 – P28         | 0.4 |
| Pd14 – P17         | 0.4 |
| Pd14 – P7          | 0.4 |
| N18 – P17          | 0.9 |
| N27 – P28          | 0.9 |

Table S13. NBO analysis summary of the complex 6-UPd.

| 1st Bond | U(15) | P(17) |
|----------|-------|-------|
| s p d f  | 13.09 | 86.91 |
| s p d f  | 7.64% | 20.38%| 52.42%| 19.55%| 35.01%| 64.90%| 0.09%| 0.00% |
| s p d f  | 12.05 | 87.95 |
| s p d f  | 6.78% | 22.04%| 52.15%| 19.04%| 35.75%| 64.18%| 0.07%| 0.00% |
| s p d f  | 25.25 | 74.75 |
| s p d f  | 46.04%| 9.84% | 44.12%| 0.00%| 31.31%| 68.55%| 0.14%| 0.00% |
Evidently, there is no ‘bond’ reported for U – Pd interactions. Likewise, the O atoms from the ligand are not observed with regards to the NBOs. Having said this, analysis of donations and electron localizations can be analyzed in order to further understand the covalency of the various atomic interactions. Lone pairs are present throughout the system and an outline is as follows: two on each O atom occupying hybrid s/p orbitals, each Cl atom presents four lone pairs with one occupying a hybrid s/p orbital and the others in a p orbital. Additionally, three lone pairs are found in the f orbitals of the U atom and finally two found on the N atoms with one occupying a mixture of s and p orbitals, whilst the other is restricted to a p orbital.

The donation of these lone pairs are evident and firstly a large donation of density (113.13 a.u) is observed from the lone pair on the P(7) atom to the Pd atom. Furthermore the bond between U(15) – P(28) seems to donate to the Rydberg antibonding orbitals of P(7) ~47 a.u. Small donations from the lone pairs on the O atoms (a p to f orbital donation) is seen from the O – U atoms. Additionally, both N and Cl atoms donate relatively more density to the f orbitals of the U atoms too (an p and s/p interaction respectively). For O, N and Cl atoms, the U interactions are purely donations and this would explain the small WBI values.

Concerning the U – Pd bonding or the apparent lack of in the NBO analysis can be further understood due to the covalent nature of the bonding and the donation of density across the U – Pd – P coordinate. Furthermore, there are large donations from the U – P(28) and U – P(17) bonds towards the anti-bonding Rydberg orbitals of the Pd atom. Taking the beta spin orbitals into account, donations
are observed between the P(7) – Pd(14) bond towards the anti-bonding orbitals of the U atom. After the fact the donations are similar regardless of the alpha or beta spin.

Although a large donation is not observed, all lone pairs on the Pd atom donate some density towards the U atom. A total of ~45 a.u. Moreover, when examining the covalency of the interaction/donation between the two atoms, the average value for this interaction is 0.04 which suggests a very high degree of overlap between the d and f orbitals of the two metallic atoms. An example of this interaction is shown in the table below.

| Bonding Coordinate | Donation | Orbital Energy Difference | Overall Covalence contribution |
|--------------------|----------|---------------------------|-------------------------------|
| Lone Pair (1) Pd(14) to U(15) | 2.88 | 0.96 | 0.067 |
| Lone Pair (5) Pd(14) to U(15) | 0.03 | 39.84 | 0.046 |

This table shows two donations from the Pd atom to the various Ry* orbitals of the U atom. The donations individually are small but I have highlighted that the covalency is very small indicating a strong overlap between the d and f orbitals of the metals. Furthermore, both donations above differ in the difference in energy between the overlapping orbitals. Regardless of the difference in energy, the overlap or covalency is still very strong. This is suggestive of a strong covalent bond between the d and f orbitals of the U and Pd atoms.

Fig. S29 Unpaired spin density plot for complex 6-UPd.
Table S14. The WBI of the complex 7-U2Pt3 with regards to the bonding surround the U atoms.

| Bonding coordinate | WBI | Bonding coordinate | WBI |
|--------------------|-----|--------------------|-----|
| U9 – Pt24          | 0.8 | Pt24 – Pt40        | 0.2 |
| U9 – O16           | 0.3 | Pt25 – Pt40        | 0.3 |
| U9 – O13           | 0.3 | U135 – Pt40        | 0.8 |
| U9 – N8            | 0.8 | U135 – O33         | 0.3 |
| U9 – N19           | 0.7 | U135 – O30         | 0.3 |
| U9 – Cl10          | 1.1 | U135 – N27         | 0.7 |
| U9 – Cl23          | 1.1 | U135 – N36         | 0.8 |
| Pt24 – P2          | 0.6 | N36 – P37          | 0.8 |
| Pt25 – P20         | 0.5 | N27 – P26          | 0.8 |
| Pt24 – Pt25        | 0.3 | Pt40 – P37         | 0.6 |
| Pt25 – P26         | 0.5 |                   |     |

Table S15. NBO analysis summary of the complex 7-U2Pt3.

| Bond     | U(9)       | Cl(10)      |
|----------|------------|-------------|
| 1st Bond | 15.96%     | 84.04%      |

|         | s   | p   | d   | f   | s   | p   | d   | f   |
|---------|-----|-----|-----|-----|-----|-----|-----|-----|
| 10.55% | 21.55% | 43.54% | 24.36% | 54.85% | 45.15% | 0.00% | 0.00% |

| Bond     | U(9)       | Cl(23)     |
|----------|------------|------------|
| 1st Bond | 15.43%     | 84.57%     |

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|        | s      | p  | d     | f  | s      | p  | d     | f  |
|--------|--------|----|-------|----|--------|----|-------|----|
| U(135) | 13.84% | 22.59% | 40.16% | 23.41% | 56.68% | 43.32% | 0.00% | 0.00% |
| Cl(16) |        |     |       |    |        |     |       |    |
| 1st Bond | 15.93% |     |       |    |       |     |       |    |
|         | 84.07% |     |       |    |        |     |       |    |
| U(135) | 9.60% | 21.69% | 45.18% | 23.53% | 54.87% | 45.13% | 0.00% | 0.00% |
| Cl(17) |        |     |       |    |        |     |       |    |
| 1st Bond | 15.67% |     |       |    |       |     |       |    |
|         | 84.33% |     |       |    |        |     |       |    |
| U(9)   | 8.96% | 22.35% | 45.53% | 23.15% | 56.57% | 43.43% | 0.00% | 0.00% |
| N(8)   |        |     |       |    |        |     |       |    |
| 1st Bond | 13.54% |     |       |    |       |     |       |    |
|         | 86.48% |     |       |    |        |     |       |    |
|         | 11.57% |     |       |    |       |     |       |    |
|         | 88.43% |     |       |    |        |     |       |    |
| U(9)   | 0.00% | 8.14% | 47.55% | 44.29% | 0.05% | 99.93% | 0.02% | 0.00% |
| N(19)  |        |     |       |    |        |     |       |    |
| 1st Bond | 12.89% |     |       |    |       |     |       |    |
|         | 87.11% |     |       |    |        |     |       |    |
|         | 9.37% | 5.41% | 38.16% | 44.18% | 46.62% | 53.37% | 0.01% | 0.00% |
|         | 90.63% |     |       |    |        |     |       |    |
|         | 0.03% | 7.33% | 50.81% | 41.82% | 0.01% | 99.96% | 0.03% | 0.00% |
|       |       |       | U(135) |       |       | N(27) |
|-------|-------|-------|--------|-------|-------|-------|
| 1st   |       |       | 13.05% |       |       | 86.95%|
| Bond  | s     | p     | d      | f     | s     | p     | d     | f     |
|       | 7.71% | 5.65% | 42.63% | 43.98%| 46.99%| 53.00%| 0.01% | 0.00% |
| 2nd   |       |       | 9.71%  |       |       | 90.29%|
| Bond  | s     | p     | d      | f     | s     | p     | d     | f     |
|       | 0.07% | 7.81% | 50.67% | 41.44%| 0.21% | 99.76%| 0.02% | 0.00% |
| 1st   |       |       | 14.18% |       |       | 85.82%|
| Bond  | s     | p     | d      | f     | s     | p     | d     | f     |
|       | 5.06% | 4.03% | 43.67% | 47.21%| 44.61%| 55.38%| 0.01% | 0.00% |
| 2nd   |       |       | 11.63% |       |       | 88.37%|
| Bond  | s     | p     | d      | f     | s     | p     | d     | f     |
|       | 0.03% | 7.82% | 47.49% | 44.65%| 0.06% | 99.93%| 0.02% | 0.00% |
| 1st   |       |       | 8.96%  |       |       | 91.04%|
| Bond  | s     | p     | d      | f     | s     | p     | d     | f     |
|       | 26.02%| 12.11%| 44.88% | 16.98%| 6.52% | 93.25%| 0.00% |
| 1st   |       |       | 45.26% |       |       | 54.74%|
| Bond  | s     | p     | d      | f     | s     | p     | d     | f     |
|       | 34.65%| 65.02%| 0.33%  | 0.00% | 3.76% | 1.29% | 94.95%| 0.00% |
| 1st   |       |       | 36.63% |       |       | 63.37%|
| Bond | s   | p   | d   | f   | s   | p   | d   | f   |
|------|-----|-----|-----|-----|-----|-----|-----|-----|
|      | 22.28% | 76.94% | 0.78% | 0.00% | 22.48% | 77.46% | 0.06% | 0.00% |

| 1st Bond | s   | p   | d   | f   |
|----------|-----|-----|-----|-----|
| P(26)    | 5.37% |
| Pt(40)   | 94.63% |

| Bond | s   | p   | d   | f   | s   | p   | d   | f   |
|------|-----|-----|-----|-----|-----|-----|-----|-----|
|      | 32.85% | 66.88% | 0.27% | 0.00% | 3.01% | 0.31% | 96.68% | 0.00% |

**Fig. S31** Unpaired spin density plot for complex 7-U₂Pt₃.

**Fig. S32** Optimized structure of complex 4-U₂Pd₂.
Fig. S33 Bonding U-Pd Molecular Orbital depiction complex 4-U₂Pd₂.

Table S16. The WBI of the complex 4-U₂Pd₂ with regards to the bonding surround the U atoms.

| Bonding coordinate | WBI | Bonding coordinate | WBI |
|--------------------|-----|--------------------|-----|
| U25 – O7           | 0.3 | U19 – Pd27         | 0.3 |
| U25 – N10          | 0.8 | U19 – Pd17         | 0.3 |
| U25 – N4           | 0.8 | U19 – N33          | 0.8 |
| U25 – Cl141        | 1.1 | U19 – N39          | 0.8 |
| U25 – Cl18         | 0.9 | U19 – O36          | 0.3 |
| U25 – Cl26         | 0.6 | U19 – Cl18         | 0.3 |
| U25 – O136         | 0.0 | U19 – Cl26         | 0.6 |
| U25 – Pd27         | 0.2 | U19 – O123         | 0.3 |
| U25 – Pd17         | 0.2 | U19 – Cl20         | 1.1 |
| Pd27 – P28         | 0.5 | Pd17 – P22         | 0.4 |
| Pd27 – P11         | 0.4 | Pd17 – P3          | 0.4 |
| N10 – P11          | 0.8 | N4 – P3            | 0.8 |
| N39 – P28          | 0.8 | N33 – P22          | 0.8 |

Table S17. NBO analysis summary of the complex 4-U₂Pd₂.

| Bond     | N(4)  | U(25)  |
|----------|-------|--------|
| 1st Bond |       |        |
|          | 86.04%| 13.96% |
| s        | 45.84%| 5.83%  |
| p        | 54.16%| 4.51%  |
| d        | 0.01% | 52.76% |
| f        | 0.00% | 36.86% |
| 2nd Bond |       |        |
|          | 87.36%| 12.64% |
| s        | 0.01% | 0.14%  |
| p        | 99.98%| 11.84% |
| d        | 0.01% | 43.53% |
| f        | 0.00% | 44.47% |

N(10)

U(25)
| 1st Bond | 86.14% | 13.86% |
|----------|--------|--------|
| s | p | d | f | s | p | d | f |
| 45.61% | 54.38% | 0.01% | 0.00% | 7.02% | 3.59% | 51.43% | 37.93% |
| 2nd Bond | 87.80% | 12.20% |
| s | p | d | f | s | p | d | f |
| 0.01% | 99.98% | 0.01% | 0.00% | 0.18% | 12.80% | 46.80% | 40.21% |

| 1st Bond | Cl(18) | U(25) |
|----------|--------|-------|
| 87.15% | 12.85% |
| s | p | d | f | s | p | d | f |
| 25.53% | 74.47% | 0.00% | 0.00% | 7.50% | 16.77% | 39.48% | 36.25% |
| 2nd Bond | 92.55% | 7.45% |
| s | p | d | f | s | p | d | f |
| 33.29% | 66.71% | 0.00% | 0.00% | 1.59% | 14.00% | 53.42% | 30.99% |

| 1st Bond | U(19) | Cl(20) |
|----------|--------|-------|
| 15.37% | 84.63% |
| s | p | d | f | s | p | d | f |
| 9.33% | 15.10% | 59.43% | 16.13% | 54.92% | 45.08% | 0.00% | 0.00% |

| 1st Bond | U(19) | Cl(26) |
|----------|--------|-------|
| 12.06% | 87.94% |
| s | p | d | f | s | p | d | f |
| 3.93% | 11.73% | 58.13% | 26.19% | 35.54% | 64.46% | 0.00% | 0.00% |

| 1st Bond | U(19) | N(33) |
|----------|--------|-------|
| 13.43% | 86.57% |
| s | p | d | f | s | p | d | f |
| 4.27% | 3.24% | 48.60% | 43.85% | 45.19% | 54.81% | 0.01% | 0.00% |
| 2nd Bond | 12.89% | 87.11% |
| s | p | d | f | s | p | d | f |
| 0.02% | 4.80% | 45.30% | 49.87% | 0.06% | 99.93% | 0.01% | 0.00% |
|       | U(19)       | N(39)       |
|-------|-------------|-------------|
| Bond  | 1st Bond    | 2nd Bond    |
|       | 13.36%      | 12.24%      |
| s     | 4.15%       | 0.07%       |
| p     | 3.58%       | 5.64%       |
| d     | 50.59%      | 48.57%      |
| f     | 41.66%      | 45.71%      |
| s     | 45.21%      | 0.00%       |
| p     | 54.79%      | 99.99%      |
| d     | 0.01%       | 0.01%       |
| f     | 0.00%       | 0.00%       |

|       | U(25)       | Cl(26)      |
|-------|-------------|-------------|
| Bond  | 1st Bond    | 2nd Bond    |
|       | 13.12%      | 12.11%      |
| s     | 12.11%      | 12.04%      |
| p     | 12.04%      | 50.26%      |
| d     | 50.26%      | 25.59%      |
| f     | 25.59%      | 35.69%      |
| s     | 35.69%      | 64.31%      |
| p     | 64.31%      | 0.00%       |
| d     | 0.00%       | 0.00%       |
| f     | 0.00%       | 0.00%       |

|       | U(25)       | Cl(41)      |
|-------|-------------|-------------|
| Bond  | 1st Bond    | 2nd Bond    |
|       | 16.10%      | 15.60%      |
| s     | 15.60%      | 27.51%      |
| p     | 27.51%      | 35.91%      |
| d     | 35.91%      | 20.98%      |
| f     | 20.98%      | 53.19%      |
| s     | 53.19%      | 46.81%      |
| p     | 46.81%      | 0.00%       |
| d     | 0.00%       | 0.00%       |
| f     | 0.00%       | 0.00%       |

Fig. S34 Unpaired density plot of complex 4-U₂Pd₂.
Fig. S35 Optimized structure of complex 5-UNi.

**SI – Coordinates:**

**Complex 3 3-U$_2$Ni$_2$**

SCF Energy: -3014.75479135,

| Element | X      | Y      | Z      | SCF Energy |
|---------|--------|--------|--------|------------|
| C       | 6.543413 | -0.060730 | -0.229981 | 0.389372 |
| C       | 5.121032 | -0.480003 | -0.612451 | 0.177394 |
| C       | 4.794041 | -0.105406 | -2.058715 | 0.394893 |
| P       | 3.685450 | 0.096666 | 0.504552 | 10.394158 |
| C       | 4.477792 | 0.233961 | 2.228359 | 0.168361 |
| C       | 4.850349 | -1.138206 | 2.786917 | 0.404274 |
| Ni      | 1.848238 | -1.097266 | 0.419661 | 9.720762 |
| P       | 1.761374 | -3.097377 | -0.411229 | 10.383076 |
| C       | 2.615116 | -4.433969 | 0.630181 | 0.162612 |
| C       | 2.047899 | -4.442176 | 2.048424 | 0.406008 |
| U       | 1.170394 | 1.934233 | -0.324684 | 61.097953 |
| O       | 2.453133 | 4.113254 | 0.184772 | -0.522163 |
| C       | 1.693316 | 5.273320 | -0.153865 | 0.11519 |
| C       | 0.356243 | 5.065965 | 0.527069 | 0.101743 |
| O       | -0.075168 | 3.700406 | 0.275208 | -0.702608 |
| P       | -1.727082 | 3.181876 | 0.296194 | 10.372577 |
| C       | -2.577394 | 4.358366 | -0.923411 | 0.159245 |
| C       | -4.100599 | 4.270407 | -0.847281 | 0.395984 |
| Ni      | -1.894338 | 1.076799 | -0.190917 | 9.744450 |
| P       | -3.743463 | -0.109080 | -0.155035 | 10.401901 |
| C       | -5.046580 | 0.031489 | 1.214783 | -0.165257 |
| C       | -4.405126 | -0.276727 | 2.566485 | -0.414282 |
| N       | 3.366938 | 1.743635 | 0.082282 | -0.705583 |
| C       | 4.378617 | 2.783739 | 0.178790 | -0.093288 |
| C       | 3.781742 | 4.080593 | -0.336175 | 0.016028 |
| Cl      | 1.634343 | 2.750619 | -2.807138 | 9.518509 |
| Cl      | -0.417461 | -0.057369 | -1.734105 | 9.795902 |
| U       | -1.166617 | -1.990000 | 0.225118 | 61.029528 |
| O       | -2.385024 | -4.130962 | -0.522791 | 0.525152 |
| C       | -3.709157 | -4.180836 | 0.011635 | -0.015923 |
| C       | -4.335580 | -2.857332 | -0.386715 | -0.095672 |
| N       | -3.360638 | -1.802314 | -0.163071 | 0.712281 |
| Cl      | 0.208760 | 0.104436 | 1.706002 | 9.809704 |
| N       | 0.134610 | -3.648133 | -0.558398 | 0.698710 |
| C       | -0.264252 | -4.975868 | -0.994605 | -0.105414 |
| Element | X         | Y         | Z         | Energy   |
|---------|-----------|-----------|-----------|----------|
| C       | -1.594750 | -5.305729 | -0.344969 | -0.344969 -0.009152 |
| Cl      | -1.523167 | -3.066950 | 2.628129  | 9.515228 |
| C       | -2.558700 | 5.225310  | 2.239968  | -0.391000 |
| C       | 2.564631  | -3.324122 | -2.123062 | -1.747441 -0.174830 |
| C       | -6.153659 | -0.382220 | -1.826165 | -0.391658 |
| C       | 3.553691  | 0.977822  | 3.191623  | -0.411206 |
| C       | -1.608368 | 3.052931  | 3.104193  | -0.404677 |
| C       | -2.075942 | 4.082234  | -2.339812 | -0.413337 |
| C       | 1.812016  | -2.501590 | -3.167468 | -0.402961 |
| C       | 4.134853  | -4.270749 | 0.634408  | -0.396689 |
| C       | -3.909391 | -0.165882 | -2.968721 | -0.402980 |
| C       | -5.739489 | 1.392834  | 1.222663  | -0.396201 |
| H       | 4.712322  | 2.922179  | 1.219053  | 0.130761 |
| H       | 5.271975  | 2.560486  | -0.419177 | 0.125835 |
| H       | 4.341402  | 4.955939  | 0.020109  | 0.125046 |
| H       | 3.735190  | 4.093463  | -1.432489 | 0.183256 |
| H       | 1.585614  | 5.325034  | -1.245398 | 0.179577 |
| H       | 2.207556  | 6.172771  | 0.211313  | 0.124133 |
| H       | 0.476053  | 5.252115  | 1.605322  | 0.135067 |
| H       | -0.350642 | 5.816447  | 0.146987  | 0.123147 |
| H       | 0.459548  | -5.755033 | -0.718573 | 0.121623 |
| H       | -0.381904 | -5.018425 | -2.088589 | 0.137544 |
| H       | -2.089330 | -6.160808 | -0.826028 | 0.124026 |
| H       | -1.478414 | -5.502497 | 0.729223  | 0.178534 |
| H       | -3.651622 | -4.291533 | 1.101994  | 0.183677 |
| H       | -4.251111 | -5.033496 | -0.419340 | 0.123935 |
| H       | -4.621652 | -2.910254 | -1.447643 | 0.133381 |
| H       | -5.260233 | -2.717706 | 0.191556  | 0.126600 |
| H       | 5.056281  | -1.571857 | -0.519325 | 0.144276 |
| H       | 7.258524  | -0.524697 | -0.920893 | 0.131525 |
| H       | 6.821974  | -0.374055 | 0.779991  | 0.132953 |
| H       | 6.692849  | 1.020776  | -0.296481 | 0.126126 |
| H       | 4.860012  | 0.974658  | -2.220007 | 0.152809 |
| H       | 3.780123  | -0.407303 | -2.336345 | 0.171759 |
| H       | 5.494871  | -0.592404 | -2.747427 | 0.123914 |
| H       | 5.395820  | 0.820536  | 2.094061  | 0.129719 |
| H       | 2.616859  | 0.432561  | 3.341360  | 0.189215 |
| H       | 3.304128  | 1.981310  | 2.834195  | 0.147572 |
| H       | 4.041365  | 1.083589  | 4.168702  | 0.130592 |
| H       | 5.326863  | -1.031195 | 3.769108  | 0.132715 |
| H       | 5.549209  | -1.680796 | 2.143018  | 0.133954 |
|        |         |         |         |         |
|--------|---------|---------|---------|---------|
| H      | 3.958124| -1.759226| 2.917106| 0.171450|
| H      | -3.417088| 3.276241| 1.987597| 0.142031|
| H      | -0.581024| 3.432947| 3.130116| 0.139849|
| H      | -1.555472| 1.969281| 2.972872| 0.185408|
| H      | -2.063932| 3.258779| 4.080632| 0.128882|
| H      | -3.092828| 5.390387| 3.184224| 0.130939|
| H      | -3.121560| 5.740312| 1.456309| 0.128336|
| H      | -1.586807| 5.717217| 2.333871| 0.127552|
| H      | -2.272443| 5.372825|-0.632738| 0.124491|
| H      | -2.383134| 3.084950|-2.673815| 0.172248|
| H      | -0.985968| 4.125112|-2.411187| 0.185066|
| H      | -2.493301| 4.816231|-3.040551| 0.122566|
| H      | -4.554286| 4.961122|-1.568520| 0.131962|
| H      | -4.494731| 4.521001| 0.141942| 0.129690|
| H      | -4.442740| 3.261521|-1.096458| 0.153362|
| H      | 3.556527 | -2.875095|-1.981905| 0.142134|
| H      | 2.318357 | -2.566457|-4.138314| 0.129566|
| H      | 1.742555 | -1.447766|-2.889843| 0.183831|
| H      | 0.789596 | -2.872216|-3.298161| 0.146628|
| H      | 1.796368 | -5.246675|-2.832079| 0.130716|
| H      | 3.288182 | -5.396736|-1.892945| 0.127163|
| H      | 3.334298 | -4.764136|-3.537204| 0.131349|
| H      | 2.372171 | -5.393157| 0.153230| 0.125304|
| H      | 4.417949 | -3.307302| 1.066014| 0.154454|
| H      | 4.573670 | -4.334686|-0.365935| 0.128686|
| H      | 4.596386 | -5.055154| 1.246784| 0.131888|
| H      | 2.507196 | -5.247371| 2.635644| 0.122134|
| H      | 0.964764 | -4.585636| 2.061202| 0.180596|
| H      | 2.249195 | -3.495023| 2.560698| 0.165540|
| H      | -4.845361| 1.309979|-1.736979| 0.148387|
| H      | -3.707485| -1.242488|-2.991376| 0.139800|
| H      | -2.944845| 0.347466|-2.976326| 0.193362|
| H      | -4.444461| 0.092875|-3.890673| 0.128796|
| H      | -6.665505| 0.011545|-2.713335| 0.132507|
| H      | -6.775398| -0.138959|-0.960674| 0.129882|
| H      | -6.131733| -1.470140|-1.927102| 0.127514|
| H      | -5.797039| -0.740286| 0.996822| 0.125676|
| H      | -6.489915| 1.428355| 2.021644| 0.130601|
| H      | -6.248573| 1.620664| 0.281680| 0.130543|
| H      | -5.020477| 2.194558| 1.411627| 0.148961|
| H      | -3.623308| 0.453505| 2.803129| 0.164823|
| H      | -3.946404| -1.268788| 2.590608| 0.186966|
| H      | -5.158284| -0.232884| 3.363039| 0.123027|

Complex 4 4-U$_2$Pd$_2$
| SCF Energy: -3393.53670131 |
|-----------------------------|
| C  | 3.320602 | 5.121915   | 0.113195  |
| C  | 4.453904 | 5.527088   | 1.058937  |
| P  | 3.989843 | 6.261637   | 2.750020  |
| N  | 3.075574 | 5.086113   | 3.631796  |
| C  | 1.746099 | 4.654398   | 3.214888  |
| C  | 1.442595 | 3.342228   | 3.903091  |
| O  | 1.811621 | 3.551844   | 5.270014  |
| C  | 1.621015 | 2.411711   | 6.116483  |
| C  | 2.004402 | 2.881662   | 7.504967  |
| N  | 3.207337 | 3.697335   | 7.412705  |
| P  | 4.119322 | 4.139068   | 8.817813  |
| C  | 2.880492 | 4.834513   | 10.084915 |
| C  | 2.124635 | 6.008534   | 9.462254  |
| C  | 5.445503 | 4.380081   | 1.253363  |
| C  | 2.695052 | 7.576357   | 2.324538  |
| C  | 2.171796 | 8.235160   | 3.600535  |
| Pd | 5.927661 | 6.945649   | 3.890767  |
| Cl | 4.258344 | 7.184300   | 6.429866  |
| U  | 7.681745 | 7.721221   | 6.582812  |
| Cl | 6.418137 | 10.056942  | 6.735737  |
| C  | 3.230062 | 8.623710   | 1.350082  |
| P  | 7.867590 | 8.084404   | 3.376426  |
| C  | 9.034009 | 7.079319   | 2.262345  |
| C  | 9.408053 | 5.768305   | 2.947998  |
| U  | 4.117567 | 4.583490   | 5.553766  |
| Cl | 6.933106 | 4.993888   | 5.837489  |
| Pd | 5.796459 | 5.753217   | 8.330017  |
| P  | 7.172692 | 6.960203   | 9.705657  |
| C  | 8.234789 | 5.885413   | 10.857339 |
| C  | 9.055955 | 4.903554   | 10.028584 |
| C  | 7.631356 | 9.673934   | 2.374991  |
| C  | 7.099115 | 9.342219   | 0.979401  |
| N  | 8.764559 | 8.537963   | 4.786249  |
| C  | 9.897394 | 9.451455   | 4.767835  |
| C  | 9.861387 | 10.293245  | 6.028457  |
| O  | 9.631003 | 9.374160   | 7.098408  |
| C  | 9.477893 | 9.986530   | 8.382375  |
| C  | 9.218657 | 8.846178   | 9.345228  |
| N  | 8.231362 | 7.950310   | 8.765092  |
| C  | 6.711311 | 10.639867  | 3.117401  |
| Cl | 4.878489 | 2.200455   | 4.636209  |
| C  | 4.667738 | 2.498336   | 9.584261  |
| C   | 5.564114 | 1.746634 | 8.602269 |
| C   | 5.381108 | 2.740606 | 10.914830 |
| C   | 6.340024 | 8.148604 | 10.924082 |
| C   | 5.603492 | 7.389306 | 12.028517 |
| C   | 5.396044 | 9.085417 | 10.174652 |
| C   | 1.934259 | 3.850294 | 10.778055 |
| C   | 10.277861 | 7.812598 | 1.756445 |
| C   | 9.104378 | 6.608950 | 11.888406 |
| H   | 0.980994 | 5.395526 | 3.496254 |
| H   | 1.663923 | 4.507282 | 2.132262 |
| H   | 0.380939 | 3.072418 | 3.853386 |
| H   | 2.058264 | 2.530610 | 3.492402 |
| H   | 2.278973 | 1.604633 | 5.769020 |
| H   | 0.571918 | 2.098335 | 6.061526 |
| H   | 1.170215 | 3.463450 | 7.924236 |
| H   | 2.136215 | 1.997633 | 8.146266 |
| H   | 9.884073 | 10.129889 | 3.904437 |
| H   | 10.854356 | 8.909712 | 4.724207 |
| H   | 10.810628 | 10.821996 | 6.196266 |
| H   | 9.035598 | 11.014759 | 5.998333 |
| H   | 8.626308 | 10.676326 | 8.342131 |
| H   | 10.393924 | 10.537596 | 8.638017 |
| H   | 10.167405 | 8.319450 | 9.535695 |
| H   | 8.897937 | 9.275434 | 10.304932 |
| H   | 4.996283 | 6.370250 | 0.608109 |
| H   | 3.726941 | 4.930689 | -0.887995 |
| H   | 2.548286 | 5.890212 | 0.007974 |
| H   | 2.841038 | 4.193800 | 0.439056 |
| H   | 4.981085 | 3.529464 | 1.762119 |
| H   | 6.302341 | 4.696848 | 1.856583 |
| H   | 5.817405 | 4.030818 | 0.281805 |
| H   | 1.870778 | 7.034309 | 1.841243 |
| H   | 2.968860 | 8.776462 | 4.118757 |
| H   | 1.766813 | 7.505426 | 4.306768 |
| H   | 1.375436 | 8.948474 | 3.353324 |
| H   | 2.451604 | 9.365318 | 1.132514 |
| H   | 3.548457 | 8.194172 | 0.395215 |
| H   | 4.081270 | 9.155239 | 1.785792 |
| H   | 3.559320 | 5.240552 | 10.845357 |
| H   | 1.431778 | 5.669197 | 8.684939 |
| H   | 2.808340 | 6.725979 | 8.999796 |
| H   | 1.537270 | 6.531594 | 10.227097 |
| H   | 1.385454 | 4.371114 | 11.573178 |
| H   | 2.459854 | 3.012394 | 11.244763 |
| At | X      | Y      | Z      |
|----|--------|--------|--------|
| H  | 1.189324 | 3.438413 | 10.092150 |
| H  | 3.761546 | 1.905331 | 9.766122  |
| H  | 6.467181 | 2.326520 | 8.379487  |
| H  | 5.061785 | 1.546756 | 7.652257  |
| H  | 5.876124 | 0.786647 | 9.032444  |
| H  | 5.717690 | 1.789023 | 11.344318 |
| H  | 4.743325 | 3.230516 | 11.657372 |
| H  | 6.263391 | 3.371981 | 10.763566 |
| H  | 8.388798 | 6.842292 | 1.406139  |
| H  | 10.005379| 5.140480 | 2.274940  |
| H  | 8.519802 | 5.205488 | 3.248095  |
| H  | 10.002039| 5.959525 | 3.847720  |
| H  | 10.974496| 8.027069 | 2.572995  |
| H  | 10.045583| 8.756796 | 1.254753  |
| H  | 10.813492| 7.184391 | 1.033541  |
| H  | 8.620337 | 10.139246| 2.266842  |
| H  | 6.199597 | 8.722176 | 1.048070  |
| H  | 7.831342 | 8.809478 | 0.365439  |
| H  | 6.833295 | 10.264959| 0.449825  |
| H  | 6.563941 | 11.550421| 2.522933  |
| H  | 7.109302 | 10.925311| 4.093428  |
| H  | 5.733029 | 10.184386| 3.301822  |
| H  | 7.462389 | 5.314242 | 11.389771 |
| H  | 9.797953 | 5.433845 | 9.422684  |
| H  | 8.409788 | 4.338294 | 9.349215  |
| H  | 9.588071 | 4.195016 | 10.675669 |
| H  | 9.528932 | 5.881826 | 12.592330 |
| H  | 8.548129 | 7.343328 | 12.478361 |
| H  | 9.944776 | 7.124979 | 11.415409 |
| H  | 7.141748 | 8.743481 | 11.383018 |
| H  | 5.064619 | 8.094849 | 12.672347 |
| H  | 6.271820 | 6.804452 | 12.667553 |
| H  | 4.865590 | 6.705950 | 11.596009 |
| H  | 4.591517 | 8.519139 | 9.693604  |
| H  | 5.904433 | 9.647071 | 9.387965  |
| H  | 4.942341 | 9.800854 | 10.872332 |
| O  | 9.908230 | 6.092240 | 6.592199  |
| C  | 11.230308| 6.656191 | 6.579815  |
| C  | 12.116414| 5.587559 | 7.195410  |
| C  | 11.512825| 4.316635 | 6.592877  |
| C  | 10.019239| 4.644096 | 6.490964  |
| H  | 11.693631| 3.424897 | 7.198914  |
| H  | 11.935496| 4.134387 | 5.598933  |
| H  | 13.173019| 5.723979 | 6.947940  |
| Atom | X   | Y   | Z   |
|------|-----|-----|-----|
| H    | 12.015332 | 5.591563 | 8.285992 |
| H    | 11.529488 | 6.860087 | 5.541398 |
| H    | 11.192975 | 7.597709 | 7.126911 |
| H    | 9.434971  | 4.218637 | 7.307518 |
| H    | 9.576080  | 4.320757 | 5.548467 |
| O    | -1.812045 | 2.543108 | 5.253148 |
| C    | -2.375957 | 3.789368 | 5.662384 |
| C    | -3.503363 | 3.437277 | 6.626387 |
| C    | -4.033457 | 2.144437 | 6.000676 |
| C    | -4.274893 | 1.486995 | 5.489449 |
| H    | -1.582176 | 4.394462 | 6.111525 |
| H    | -2.766166 | 4.331085 | 4.786345 |
| H    | -3.102429 | 3.244647 | 7.627960 |
| H    | -4.257757 | 4.224756 | 6.706304 |
| H    | -4.579221 | 1.509650 | 6.704011 |
| H    | -4.705216 | 2.376838 | 5.166624 |
| H    | -2.900257 | 0.923416 | 4.561065 |
| H    | -2.325105 | 0.801062 | 6.236377 |

**Complex 5: 5-UNi**

SCF Energy: -1661.13486617,

| Atom | X   | Y   | Z   |
|------|-----|-----|-----|
| C    | 12.382946 | 8.856300 | 7.382619 |
| C    | 10.909635 | 9.239199 | 7.232094 |
| C    | 10.274981 | 9.581062 | 8.580435 |
| P    | 9.829641  | 7.961826 | 6.348993 |
| C    | 10.801041 | 7.586010 | 4.771127 |
| C    | 11.086824 | 8.858468 | 3.970376 |
| Ni   | 7.745802  | 8.909439 | 6.031209 |
| P    | 5.695602  | 7.818565 | 5.969520 |
| C    | 4.309535  | 9.040841 | 6.359811 |
| C    | 4.250425  | 10.166520 | 5.323929 |
| U    | 7.626634  | 6.664242 | 8.231532 |
| O    | 6.335767  | 4.472435 | 8.483491 |
| C    | 4.930889  | 4.784208 | 8.564496 |
| C    | 4.588925  | 5.566973 | 7.297289 |
| N    | 5.631435  | 6.549985 | 7.094163 |
| Cl   | 8.058111  | 11.050712 | 5.414579 |
| Cl   | 7.223481  | 7.198453 | 10.846011 |
| N    | 9.720768  | 6.528766 | 7.255316 |
| C    | 10.786275 | 5.671695 | 7.731410 |
| C    | 10.184166 | 4.305492 | 8.031570 |
| O    | 8.981284  | 4.507941 | 8.796134 |
|      |        |        |        |
|------|--------|--------|--------|
| C    | 8.279525 | 3.304756 | 9.097044 |
| C    | 6.874603 | 3.668792 | 9.532169 |
| C    | 5.274145 | 7.164611 | 4.242027 |
| C    | 6.162503 | 5.961817 | 3.923929 |
| C    | 10.069127 | 6.546851 | 3.925638 |
| C    | 3.795487 | 6.839943 | 4.012108 |
| C    | 4.508866 | 9.590939 | 7.772426 |
| H    | 11.259104 | 6.056155 | 8.649674 |
| H    | 11.597668 | 5.516107 | 7.002466 |
| H    | 9.915112 | 3.791530 | 7.098055 |
| H    | 10.875884 | 3.674050 | 8.605168 |
| H    | 8.792907 | 2.751078 | 9.894415 |
| H    | 8.237611 | 2.674457 | 8.197745 |
| H    | 6.279846 | 2.754032 | 9.657330 |
| H    | 6.876857 | 4.231220 | 10.475515 |
| H    | 4.754544 | 5.387527 | 9.465290 |
| H    | 4.356784 | 3.850807 | 8.633851 |
| H    | 4.513750 | 4.857621 | 6.457777 |
| H    | 3.586315 | 6.001238 | 7.438606 |
| H    | 10.821273 | 10.121527 | 6.585491 |
| H    | 12.938342 | 9.683953 | 7.840005 |
| H    | 12.865144 | 8.634095 | 6.425895 |
| H    | 12.508834 | 7.985925 | 8.034662 |
| H    | 10.255156 | 8.713957 | 9.252454 |
| H    | 9.251706 | 9.952581 | 8.458146 |
| H    | 10.847294 | 10.368685 | 9.084181 |
| H    | 11.750605 | 7.152527 | 5.115075 |
| H    | 9.173625 | 6.983827 | 3.472019 |
| H    | 9.763476 | 5.678682 | 4.517744 |
| H    | 10.713564 | 6.196224 | 3.110689 |
| H    | 11.583916 | 8.601293 | 3.027168 |
| H    | 11.739271 | 9.552866 | 4.506459 |
| H    | 10.162094 | 9.394727 | 3.732904 |
| H    | 5.560212 | 7.993107 | 3.580088 |
| H    | 3.647909 | 6.500514 | 2.979402 |
| H    | 3.143539 | 7.703778 | 4.164861 |
| H    | 3.448078 | 6.035801 | 4.668405 |
| H    | 5.902254 | 5.100428 | 4.547584 |
| H    | 7.218728 | 6.183473 | 4.092371 |
| H    | 6.039994 | 5.664480 | 2.875753 |
| H    | 3.376067 | 8.462039 | 6.330687 |
| H    | 5.413042 | 10.208102 | 7.827285 |
| H    | 4.594911 | 8.793150 | 8.516947 |
| H    | 3.660475 | 10.225228 | 8.054822 |
|     |    X    |    Y    |    Z    | SCF Energy: -3338.83668418, |
|-----|---------|---------|---------|----------------------------|
| H   | 3.454891| 10.873498| 5.587559|
| H   | 4.040517| 9.800358 | 4.314190|
| H   | 5.193961| 10.721771| 5.291382|

**Complex 7.7-U2Pt3**

SCF Energy: -3338.83668418,

|    |    X    |    Y    |    Z    | SCF Energy: -3338.83668418, |
|----|---------|---------|---------|----------------------------|
| C  | 10.057844| 6.775036| 14.726637| -0.395717 |
| P  | 7.328346 | 5.975917| 15.269862| 10.342971|
| C  | 8.163749 | 4.360423| 15.735874| -0.169855|
| C  | 7.169989 | 3.207417| 15.618710| -0.404013|
| C  | 8.724747 | 7.250405| 15.311981| -0.186958|
| C  | 8.263231 | 8.541837| 14.631102| -0.395638|
| C  | 8.792020 | 4.467587| 17.127735| -0.414455|
| N  | 6.758928 | 5.832364| 13.675118| -0.955588|
| U  | 4.556877 | 6.388614| 13.793777| 61.362183|
| Cl | 3.878487 | 3.797101| 13.466842| 9.467958 |
| C  | 7.571617 | 5.480420| 12.528480| -0.099006|
| C  | 6.641659 | 4.993588| 11.432853| -0.016173|
| O  | 5.570118 | 5.940608| 11.377246| -0.515758|
| C  | 4.675398 | 5.738087| 10.293346| 0.001694 |
| C  | 3.557983 | 6.738901| 10.457480| -0.014080|
| O  | 2.982363 | 6.475025| 11.726014| -0.522153|
| C  | 1.723591 | 7.089943| 11.988329| 0.007531 |
| C  | 1.289910 | 6.595518| 13.339833| -0.130995|
| N  | 2.328822 | 6.840848| 14.334725| -0.695723|
| P  | 1.828158 | 7.244725| 15.905795| 10.315453|
| C  | 0.601477 | 5.928005| 16.434941| 60.084808|
| C  | 0.074575 | 5.210043| 17.849102| -0.417259|
| Cl | 4.856863 | 8.959374| 13.039440| 9.461571 |
| Pt | 5.475542 | 6.572406| 16.434941| 60.084808|
| Pt | 3.430899 | 7.960628| 17.451507| 59.419757|
| P  | 4.575903 | 9.363874| 18.938706| 10.340112|
| N  | 5.159467 | 8.848304| 20.456315| -0.707775|
| C  | 5.648502 | 9.896732| 21.355731| -0.121710|
| C  | 6.742536 | 9.358995| 22.253761| -0.007325|
| O  | 6.190324 | 8.212805| 22.900817| -0.521293|
| C  | 7.004769 | 7.636717| 23.912981| -0.010199|
| C  | 6.190458 | 6.529894| 24.534159| -0.004639|
| O  | 5.868882 | 5.618573| 23.493416| -0.513086|
| C  | 5.065304 | 4.514535| 23.917211| -0.010336|
| C  | 4.927826 | 3.609158| 22.707470| -0.105984|
| N  | 4.618439 | 4.444711| 21.565408| -0.700778|
| Symbol | X          | Y          | Z          | Endgame (E)  |
|--------|------------|------------|------------|--------------|
| P      | 3.897306   | 3.86967    | 20.135508  | 10.288058    |
| C      | 2.233737   | 3.124935   | 20.627514  | -0.167798    |
| C      | 1.294482   | 2.829561   | 19.498632  | -0.401520    |
| Pt     | 3.884067   | 5.694565   | 18.790626  | 59.680921    |
| C      | 4.921610   | 2.366755   | 19.627514  | -0.167798    |
| C      | 4.421035   | 1.673611   | 18.35214   | -0.413389    |
| C      | 3.185204   | 10.644965  | 19.193831  | -0.196682    |
| C      | 2.098929   | 10.033098  | 20.081962  | -0.400274    |
| C      | 5.965897   | 10.333792  | 18.119675  | -0.402385    |
| C      | 7.223812   | 9.472635   | 18.052224  | -0.404350    |
| C      | 3.604193   | 12.033584  | 19.683635  | -0.397334    |
| C      | 0.810697   | 8.863044   | 15.874803  | -0.193268    |
| C      | -0.621377  | 8.811694   | 15.33035   | -0.397261    |
| C      | 1.629685   | 9.951781   | 15.177614  | -0.393389    |
| C      | 1.244504   | 4.548944   | 16.315236  | -0.412906    |
| C      | 5.535661   | 10.847916  | 16.744989  | -0.417477    |
| C      | 6.382569   | 2.783019   | 19.491095  | -0.402385    |
| C      | 1.540696   | 4.031096   | 21.682736  | -0.395267    |
| H      | 8.295488   | 4.679141   | 12.742318  | 0.122993     |
| H      | 8.142542   | 6.344574   | 12.155198  | 0.137107     |
| H      | 7.151181   | 4.956503   | 10.459962  | 0.121174     |
| H      | 6.224365   | 4.007677   | 11.675301  | 0.183261     |
| H      | 4.276843   | 4.714841   | 10.328121  | 0.178587     |
| H      | 5.196867   | 5.897610   | 9.339085   | 0.132901     |
| H      | 3.937216   | 7.768790   | 10.422875  | 0.191241     |
| H      | 2.808796   | 6.592865   | 9.664724   | 0.131463     |
| H      | 1.009475   | 6.805393   | 11.202287  | 0.121221     |
| H      | 1.845140   | 8.181314   | 12.003001  | 0.167936     |
| H      | 0.324094   | 7.017243   | 13.583703  | 0.116531     |
| H      | 1.119620   | 5.476153   | 13.24919   | 0.173574     |
| H      | 8.863609   | 7.445309   | 16.384325  | 0.172946     |
| H      | 9.975598   | 6.544161   | 13.660226  | 0.130405     |
| H      | 10.461048  | 5.895752   | 15.235213  | 0.135294     |
| H      | 10.802229  | 7.574647   | 14.824545  | 0.135568     |
| H      | 9.007781   | 9.332642   | 14.783103  | 0.125146     |
| H      | 7.304185   | 8.891613   | 15.017450  | 0.202134     |
| H      | 8.136766   | 8.400353   | 13.553672  | 0.154465     |
| H      | 8.960224   | 4.216673   | 14.992304  | 0.130418     |
| H      | 7.656260   | 2.264449   | 15.896556  | 0.123138     |
| H      | 6.774317   | 3.107198   | 14.604876  | 0.173326     |
| H      | 6.313167   | 3.361799   | 16.280481  | 0.178779     |
| H      | 8.063514   | 4.786801   | 17.878422  | 0.206369     |
| H      | 9.620696   | 5.181265   | 17.160429  | 0.134796     |
| H      | 9.187165   | 3.493006   | 17.437200  | 0.132756     |
|   |   |   |   |   |
|---|---|---|---|---|
| H | 0.748156 | 9.107277 | 16.945864 | 0.167571 |
| H | 1.767015 | 9.729731 | 14.115617 | 0.165119 |
| H | 2.634760 | 10.047870 | 15.672344 | 0.135915 |
| H | -1.125886 | 9.75817 | 15.769550 | 0.140722 |
| H | -1.217700 | 8.04037 | 15.766284 | 0.139842 |
| H | -0.641999 | 8.70509 | 15.306600 | 0.184127 |
| H | -0.226554 | 5.995891 | 15.723442 | 0.135915 |
| H | 2.096492 | 4.454119 | 17.000125 | 0.186460 |
| H | 1.616218 | 4.352725 | 15.306600 | 0.134639 |
| H | 0.516256 | 3.770626 | 16.571241 | 0.129799 |
| H | -0.644572 | 5.437311 | 18.145781 | 0.138058 |
| H | -0.436290 | 7.15703 | 17.922079 | 0.137740 |
| H | 0.898135 | 6.207980 | 18.54057 | 0.203798 |
| H | 6.158794 | 11.194737 | 18.773154 | 0.131411 |
| H | 8.041446 | 10.040492 | 17.592675 | 0.131069 |
| H | 7.544826 | 9.129463 | 19.038703 | 0.168840 |
| H | 7.039269 | 8.579097 | 17.441261 | 0.187933 |
| H | 6.356295 | 11.406998 | 16.280617 | 0.140606 |
| H | 5.278692 | 10.022250 | 16.072384 | 0.221445 |
| H | 4.674572 | 11.522510 | 16.800762 | 0.136619 |
| H | 2.778365 | 10.765047 | 18.178630 | 0.165979 |
| H | 1.248675 | 10.721057 | 20.165937 | 0.129280 |
| H | 1.731263 | 9.083989 | 19.677546 | 0.175097 |
| H | 2.469116 | 9.821213 | 21.089124 | 0.181340 |
| H | 2.733693 | 12.700598 | 19.665896 | 0.138743 |
| H | 3.964783 | 12.008665 | 20.717885 | 0.137039 |
| H | 4.377346 | 12.492026 | 19.062889 | 0.138049 |
| H | 2.509126 | 2.176732 | 21.152684 | 0.132914 |
| H | 0.402411 | 2.307654 | 19.866028 | 0.129597 |
| H | 0.967362 | 3.762112 | 19.034626 | 0.175403 |
| H | 1.742543 | 2.211197 | 16.718721 | 0.142575 |
| H | 0.594528 | 3.574587 | 21.998239 | 0.123551 |
| H | 2.147884 | 4.215499 | 22.570270 | 0.153332 |
| H | 1.317508 | 5.010521 | 21.248782 | 0.195784 |
| H | 4.819122 | 1.675598 | 20.477689 | 0.134017 |
| H | 7.005463 | 1.902257 | 19.294241 | 0.123419 |
| H | 6.499774 | 3.476555 | 18.655674 | 0.173173 |
| H | 6.764442 | 3.288223 | 20.381087 | 0.176417 |
| H | 5.144705 | 0.911702 | 18.046530 | 0.136307 |
| H | 3.464242 | 1.166741 | 18.505537 | 0.132929 |
| H | 4.313086 | 2.382288 | 17.531546 | 0.192213 |
| H | 4.146136 | 2.865125 | 22.925917 | 0.123463 |
| H | 5.868827 | 3.056677 | 22.558637 | 0.143667 |
| Symbol | X      | Y      | Z      | Energy   |
|--------|--------|--------|--------|----------|
| H      | 5.558995 | 3.999721 | 24.753248 | 0.121908 |
| H      | 4.087362 | 4.894317 | 24.242138 | 0.177266 |
| H      | 5.267734 | 6.932332 | 24.974260 | 0.132707 |
| H      | 6.776836 | 6.021845 | 25.312696 | 0.133505 |
| H      | 7.247510 | 8.393658 | 24.671644 | 0.132707 |
| H      | 7.931105 | 7.246284 | 23.471220 | 0.189538 |
| H      | 7.024657 | 10.103914 | 23.011396 | 0.122575 |
| H      | 7.627724 | 9.058187 | 21.678603 | 0.182033 |
| H      | 6.069909 | 10.757798 | 20.818924 | 0.121500 |
| H      | 4.837531 | 10.276224 | 21.995601 | 0.160316 |
| U      | 5.044236 | 6.639076 | 21.181107 | 61.393984 |
| Cl     | 2.957676 | 7.334890 | 22.737047 | 9.477328 |
| Cl     | 7.651254 | 6.279350 | 20.614980 | 9.456693 |

**Complex 6-UPd**

SCF Energy: -2319.36345369,

| Symbol | X      | Y      | Z      |
|--------|--------|--------|--------|
| C      | -1.816143 | -0.714730 | 2.732197 |
| C      | -2.883013 | -0.928328 | 1.849927 |
| C      | -3.975113 | -1.700660 | 2.265119 |
| C      | -4.001602 | -2.236472 | 3.551523 |
| C      | -2.948058 | -1.999369 | 4.435046 |
| C      | -1.853993 | -1.240033 | 4.023575 |
| P      | -2.797402 | -0.095405 | 0.197131 |
| C      | -3.728955 | 1.484468  | 0.501021 |
| C      | -3.952071 | 1.981800  | 1.789518 |
| C      | -4.634833 | 3.185338  | 1.969853 |
| C      | -5.102481 | 3.900938  | 0.869940 |
| C      | -4.886162 | 3.408652  | -0.418312 |
| C      | -4.200455 | 2.211317  | -0.602506 |
| Pd     | -0.582282 | -0.017274 | -0.673697 |
| U      | 2.190754  | 0.092821  | 0.307810 |
| Cl     | 3.439137 | 0.042196 | -2.257970 |
| P      | 0.116760 | 2.386238 | -0.676462 |
| N      | 1.728317 | 2.314119 | -0.184695 |
| C      | 2.727818 | 3.360414 | -0.072292 |
| C      | 4.127147 | 2.746833 | -0.201971 |
| O      | 4.224346 | 1.593245 | 0.664015 |
| C      | 5.463753 | 0.882126 | 0.580767 |
| C      | 5.316294 | -0.437427 | 1.322917 |
| O      | 4.325712 | -1.191887 | 0.629890 |
| C      | 4.009358 | -2.515736 | 1.096233 |
| C      | 2.993760 | -3.113907 | 0.113468 |
| Element | X      | Y      | Z      |
|---------|--------|--------|--------|
| N       | 1.887466 | -2.184756 | -0.040963 |
| P       | 0.345086  | -2.404369 | -0.689081 |
| C       | 0.374747  | -3.016480 | -2.494264 |
| C       | 1.512531  | -3.997579 | -2.779935 |
| C       | -0.811560 | 3.582672  | 0.463299  |
| C       | -0.443698 | 5.052462  | 0.238843  |
| C       | -0.563002 | 3.168766  | 1.912597  |
| C       | 0.007352  | 3.198909  | -2.381458 |
| C       | 0.820153  | 2.406920  | -3.401993 |
| C       | -1.444547 | 3.360341  | -2.829450 |
| C       | -0.365819 | -3.937970 | 0.187294  |
| Cl      | 1.939270  | -0.037267 | 3.059345  |
| C       | -3.995877 | -0.979266 | -0.914704 |
| C       | -5.384117 | -0.887740 | -0.730305 |
| C       | -6.253057 | -1.546188 | -1.597478 |
| C       | -5.749387 | -2.288570 | -2.665925 |
| C       | -4.373048 | -2.368510 | -2.866958 |
| C       | -3.501369 | -1.716174 | -1.995681 |
| C       | 0.410179  | -1.844002 | -3.473927 |
| H       | 2.656037  | 3.883679  | 0.895199  |
| H       | 2.662242  | 4.133114  | -0.856506 |
| H       | 4.296377  | 2.408186  | -1.230715 |
| H       | 4.895000  | 3.476843  | 0.090690  |
| H       | 6.266179  | 1.475490  | 1.040709  |
| H       | 5.695686  | 0.686846  | -0.473922 |
| H       | 6.277895  | -0.969272 | 1.306567  |
| H       | 5.006002  | -0.272993 | 2.364244  |
| H       | 3.587806  | -2.446053 | 2.107790  |
| H       | 4.927531  | -3.119056 | 1.117051  |
| H       | 3.513035  | -3.298759 | -0.836788 |
| H       | 2.701019  | -4.096477 | 0.520879  |
| H       | -1.873284 | 3.444016  | 0.229674  |
| H       | -0.986972 | 5.681552  | 0.954622  |
| H       | -0.702131 | 5.406086  | -0.763267 |
| H       | 0.624320  | 5.231738  | 0.396781  |
| H       | 0.495957  | 3.249521  | 2.175273  |
| H       | -0.858551 | 2.133010  | 2.099366  |
| H       | -1.137285 | 3.808525  | 2.592808  |
| H       | 0.462093  | 4.191206  | -2.257725 |
| H       | 0.357270  | 1.433004  | -3.596751 |
| H       | 1.841026  | 2.209601  | -3.066474 |
| H       | 0.860105  | 2.952099  | -4.353300 |
| Element | X     | Y     | Z     |
|---------|-------|-------|-------|
| H       | -1.48 | 3.84  | -3.82 |
| H       | -2.04 | 3.96  | -2.14 |
| H       | -1.92 | 2.38  | -2.91 |
| H       | -0.58 | -3.54 | -2.60 |
| H       | 1.38  | -4.44 | -3.77 |
| H       | 1.56  | -4.81 | -2.06 |
| H       | -1.52 | 2.38  | -2.92 |
| H       | 1.33  | -1.27 | -1.36 |
| H       | -0.43 | -1.16 | -3.32 |
| H       | 0.36  | -2.20 | -4.51 |
| H       | -0.26 | -4.75 | -0.20 |
| H       | -0.85 | -3.13 | 2.14  |
| H       | 0.85  | -3.53 | 1.96  |
| H       | -0.36 | -4.83 | 2.16  |
| H       | -2.14 | -5.18 | 0.34  |
| H       | -1.99 | -4.39 | -1.23 |
| H       | -2.49 | -3.45 | 0.18  |
| H       | -3.60 | 1.43  | 2.65  |
| H       | -4.81 | 3.56  | 2.97  |
| H       | -5.64 | 4.84  | 1.02  |
| H       | -5.25 | 3.96  | -1.28 |
| H       | -4.04 | 1.84  | -1.61 |
| H       | -5.79 | -0.29 | 0.08  |
| H       | -7.33 | -1.48 | -1.43 |
| H       | -6.43 | -2.79 | -3.35 |
| H       | -3.97 | -2.93 | -3.70 |
| H       | -2.43 | -1.76 | -2.15 |
| H       | -4.81 | -1.90 | 1.57  |
| H       | -4.85 | -2.84 | 3.86  |
| H       | -2.98 | -2.42 | 5.43  |
| H       | -1.09 | -1.07 | 4.69  |
| H       | -0.94 | -0.17 | 2.41  |
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