

Supporting Information to Accompany

Uranium(IV)imidazolin-2-iminato Complexes: A New Class of Organo-actinides.

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Table of Contents

1. Materials and Methods.....	2
2. Experimental Procedures	3
2.1. General Procedure for the Synthesis of Uranium(IV) Imidazolin-2-iminato Complexes	3
2.2. ϵ -Caprolactone Polymerization	7
3. Crystallographic Data	9
3.1. Crystallographic Data for Complex 1	9
3.2. Crystallographic Data for Complex 2	18
3.3. Crystallographic Data for Complex 3	29
References	50

1. Materials and Methods

All manipulations of air sensitive materials were performed with the rigorous exclusion of oxygen and moisture in flamed Schlenk-type glassware on a high vacuum line (10^{-5} torr), or in nitrogen filled Vacuum Atmospheres glovebox with a medium capacity recirculator (1-2 ppm oxygen). Argon and nitrogen were purified by passage through a MnO oxygen removal column and a Davison 4 Å molecular sieve column. Analytically pure solvents were dried and stored with Na/K alloy and degassed by 3 freeze-pump-though cycles prior to use (THF, hexane, toluene, benzene- d_6 , toluene- d_8). $U(NMeEt)_4$ ¹, 1,3-di-tert-butyl-1H-imidazoli-2-imine, 1,3—dimesityl-1H-imidazol-2-imine and 1,3-bis(2,6-diisopropylphenyl)-1H-imidazol-2-imine,² were synthesized according to published literature procedures. ϵ -caprolactone (Sigma Aldrich) was distilled under reduced pressure from CaH_2 and stored in the glovebox prior to use. NMR spectra were recorded on DPX200, Avance 300 and Avance 500 Bruker spectrometers. Chemical shifts for 1H -NMR and ^{13}C -NMR are reported in ppm and referenced using residual proton or carbon signals of the deuterated solvent relative to tetramethylsilane. Crystal structures determination: Single crystals, immersed in Parathene-N oil were quickly fished with a glass rod and mounted on a KappaCCD diffractometer under a cold stream of nitrogen at 230 K. Data collection was carried out with monochromized MoK_α radiation using ω and π scans to cover the Ewald sphere. The structure was solved by direct methods and completed using successive Fourier difference maps. Refinement was performed anisotropically with respect to the non-hydrogen atoms. Hydrogens were placed at calculated positions and refined using the riding model until convergence was reached. Elemental analysis was carried out by the microanalysis laboratory at the Hebrew University of Jerusalem. GPC measurements were carried out on a Waters Breeze system with a styrogel RT column and with THF (HPLC grade, T.G. Baker) as mobile phase at 30 °C. Relative

calibration was done with polystyrene standards (Aldrich, 2000 – 1800000 range). M_n values were multiplied by a factor of 0.58 and correlated to actual PCL values.³

2. Experimental Procedures

2.1. General Procedure for the Synthesis of Uranium(IV) Imidazolin-2-iminato Complexes

A flame dried Schlenk flask, equipped with a magnetic stirring bar and a frit was charged with $U(NMeEt)_4$ (500 mg, 1.06 mmol) inside the glovebox. A second Schlenk flask was charged with the corresponding amount of ligand inside the glove box. THF (ca. 30 mL) was condensed into both flasks using a vacuum transfer. The reaction flask, containing $U(NMeEt)_4$ was cooled to -78°C (acetone/dry ice bath) and the THF solution of the imidazolin-2-iminato ligand was added slowly via syringe to the $U(NMeEt)_4$ solution under a constant stream of argon. Then, the reaction mixture was covered from light, warmed slowly to room temperature and stirred for 18 hours at room temperature. Then, the solvent was evaporated and the product was extracted with hexane (ca. 50 mL) by a Soxhlet type extraction under inert conditions. The product was purified by crystallization from a concentrated toluene solution at -60°C .

Tetrakis(1,3-di-tert-butyl-imidazolin-2-iminato)uranium(IV) (1): yield: 78 % (839 mg, 0.83 mmol); $^1\text{H-NMR}$ (C_6D_6 , 300 MHz) δ -0.61 (s, 72 H, $\text{C}(\text{CH}_3)_3$), 11.9 (s, 8 H, CH). $^{13}\text{C-NMR}$ (C_6D_6 , 50MHz) δ -8.98 ($\text{C}(\text{CH}_3)_3$), 32.1 ($\text{C}(\text{CH}_3)_3$), 58.3 (CH), 117.1 ($\text{C}_{\text{ipso}}=\text{N}$). Elemental analysis calculated: C:52.06, H: 7.94, N: 16.56. Found: C: 52.17, H: 7.98, N: 17.22.

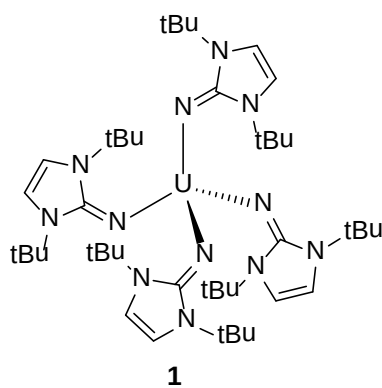


Figure 1: Structure of complex 1.

Variable temperature ^1H -NMR studies of 1:

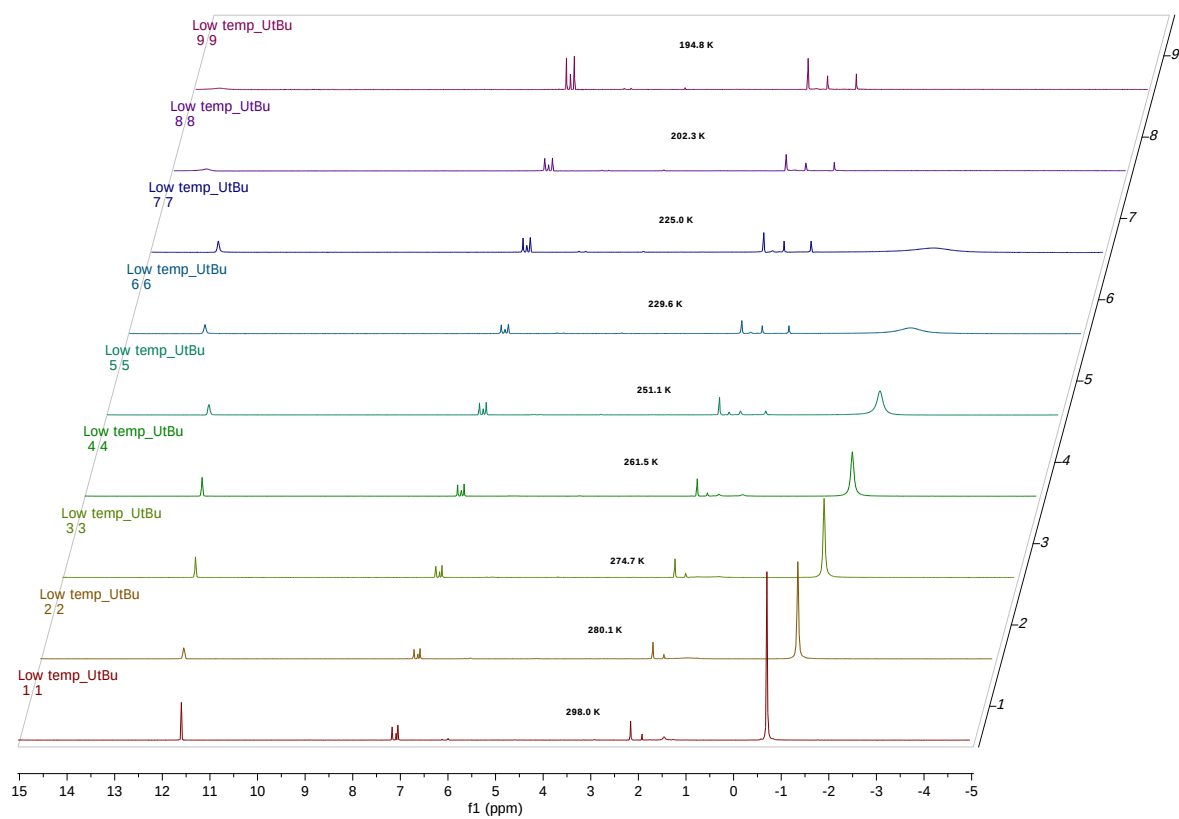


Figure 2: Low temperature NMR-studies for Complex 1.

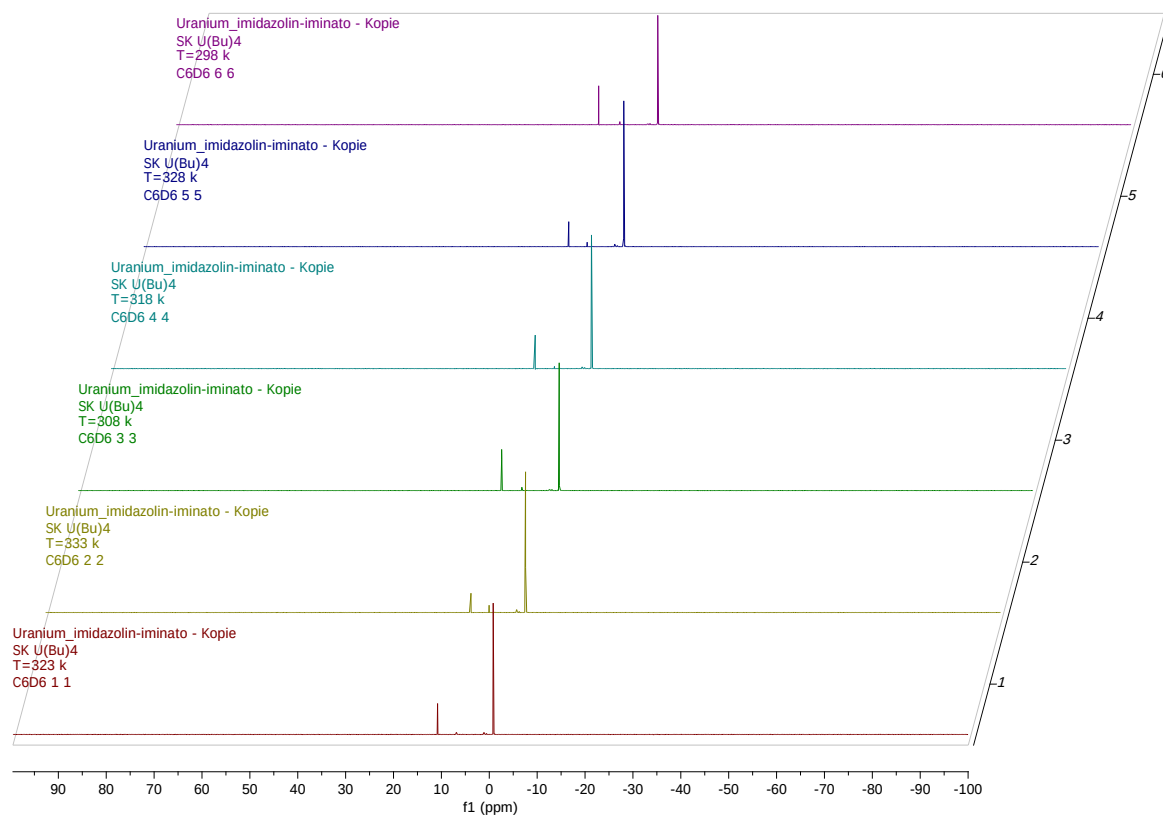


Figure 3: High Temperature NMR studies for complex 1.

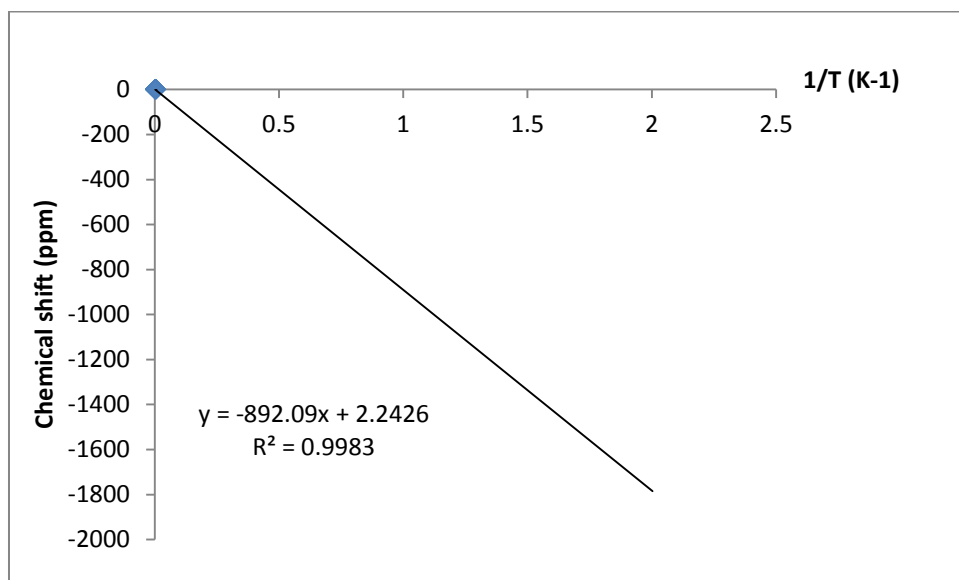


Figure 4: Curie Weiß Plot for the tert-butyl protons of the imidazolin-2-iminato ligand. (Signal B)

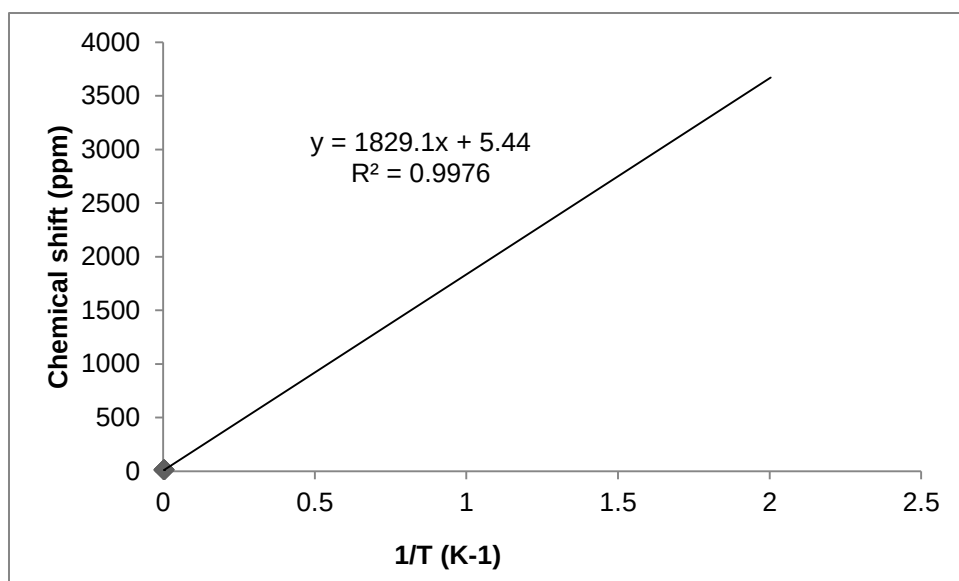
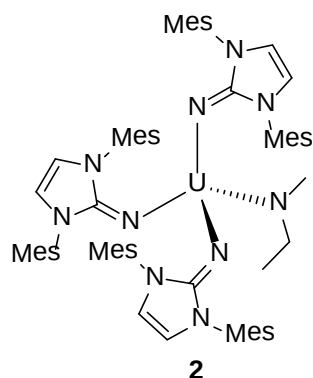
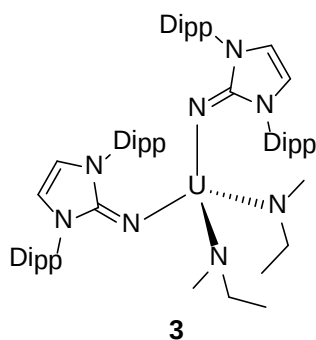


Figure 5: Curie Weiß Plot for the backbone protons of the imidazolin-2-iminato ligand. (Signal A.)

Tris(1,3-dimesityl-imidazolin-2-iminato)((*N*-ethyl(methyl)amido)uranium(IV) (2): yield: 67 % (889 mg, 0.71 mmol); ^1H -NMR (C_6D_6 , 200 MHz) δ 1.60-2.03 (s, 3H, brs, $\text{N}(\text{CH}_2\text{CH}_3)$), 2.33-2.89 (5H, m, $\text{CH}_3\text{-C}_6\text{H}_3$), 4.93 (s, 2H, brs, NCH_2CH_3), 6.37 (s, 3H, N-CH_3), 7.48 (s, 6H, CH), 7.83 (m, 12H, Ar-H). ^{13}C -NMR (C_6D_6 , 50MHz) δ 18.3 ($\text{N-CH}_2\text{CH}_3$), 21.3 ($\text{CH}_3\text{-C}_{\text{ar}}$), 24.9 (N-CH_3), 25.2 ($\text{N-CH}_2\text{-CH}_3$), 121.5 (CH), 132.5 ($\text{C}_{\text{ar-H}}$), 145.8 (*ipso*- C_{ar}), 154.2 ($\text{C}_{\text{ipso=N}}$). Elemental Analysis Calculated: C: 63.54, H: 6.44, N: 11.19, Found: C: 63.92, H: 6.46, N: 11.09.



Bis(1,3-bis(2,6-diisopropylphenyl)-imidazoline-2-iminato-bis(*N*-ethyl(methyl)amido)-uranium(IV) (3): yield: 81 % (995 mg, 0.86 mmol). $^1\text{H-NMR}$ (C_6D_6 , 200 MHz) δ -23.66 (s, 3H, $\text{N-CH}_2\text{CH}_3$), -13.54 (s, 3H, N-CH_3), -4.61 (s, 2H, $\text{N-CH}_2\text{CH}_3$), -1.41 (d, 24H, $^3J_{\text{CH}_3\text{-CH}} = 5.25$ Hz, $\text{CH}_3(^i\text{Pr})$), 1.62-1.71 (m, 8H, $\text{CH}(^i\text{Pr})$), 3.95 (d, 24H, $^3J_{\text{CH}_3\text{-CH}} = 5.25$ Hz, $\text{CH}_3(^i\text{Pr})$), 7.18-7.54 (m, 8H, Ar-H), 15.16 (s, 4H, CH), 16.56 (s, 4H, $\text{C}_{\text{ar-H}}$). $^{13}\text{C-NMR}$ (C_6D_6 , 50MHz) δ 7.3 ($\text{N-CH}_2\text{-CH}_3$), 23.9 (N-CH_3), 26.4 ($\text{N-CH}_2\text{-CH}_3$), 31.7 ($\text{CH}(\text{CH}_3)_2$) 32.2 ($\text{CH}(\text{CH}_3)_2$), 124.9 (CH), 129.7 ($\text{C}_{\text{ar-H}}$), 131.2 ($\text{C}_{\text{ar-H}}$), 148.4 ($\text{ipso-C}_{\text{ar}}$), 153.7 ($\text{C}_{\text{ipso=N}}$). Elemental Analysis Calculated: C: 62.16, H: 7.65, N: 9.66. Found: C: 63.57, H: 7.69, N: 9.71.



2.2. ϵ -Caprolactone Polymerization

A sealable glass tube, equipped with a magnetic stirring bar, was loaded with 2.5 mg of the uranium complex from a stock solution, the required amount of ϵ -caprolactone and 3 mL of dry toluene inside the glove box. The polymerization was carried out under strong stirring for the required amount of time and temperature. Then, the reaction was quenched by the addition of methanol. After removing the solvent under reduced pressure, the polymer was precipitated from cold methanol, isolated by filtration, washed with three portions of cold methanol and dried overnight under vacuum. The activity was determined as $\text{PCL (g)} / \text{mol}(\text{cat}) \cdot \text{time}(\text{h})$. A sample of the obtained PCL (40 mg) was dissolved in THF and used for determination of M_n , M_w and PDI.

^1H -NMR (CDCl_3 , 400 MHz) δ 1.37 (m, 2H, $-\text{OCH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CO}-$), 1.65 (m, 4H, $-\text{OCH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CO}-$), 2.30 (t, 2H, $^3J = 6.63 \text{ Hz}$, 7.46 Hz , $-\text{OCH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CO}-$) 4.05 (t, 2H, $^3J = 6.63 \text{ Hz}$, 7.46 Hz , $-\text{OCH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CO}-$). ^{13}C -NMR (CDCl_3 , 100MHz) δ 24.7 ($-\text{OCH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CO}-$), 25.6 ($-\text{OCH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CO}-$), 28.5 ($-\text{OCH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CO}-$), 34.2 ($-\text{OCH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CO}-$), 64.3 ($-\text{OCH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CO}-$), 173.5 ($-\text{OCH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CO}-$).

3. Crystallographic Data

3.1. Crystallographic Data for Complex 1

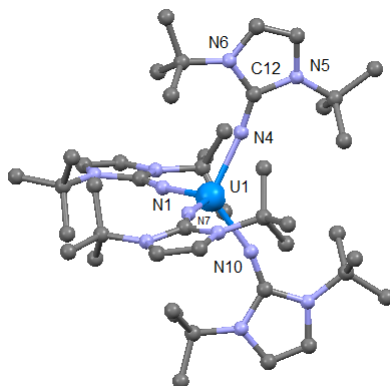


Figure 6: Molecular structure of 1. U: green, N: blue, C: grey. Hydrogen atoms are omitted for clarity.

Table 1: Crystal data and structure refinement for Complex 1.

Identification code	Complex 1
Empirical formula	C ₄₄ H ₈₀ N ₁₂ U
Formula weight	1015.23
Temperature	250(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P 2 ₁ /n
Unit cell dimensions	a = 11.8477(9) Å α = 90 deg. b = 20.4016(17) Å β = 92.457(3) deg. c = 20.8037(16) Å γ = 90 deg.
Volume	5023.9(7) Å ³
Z, Calculated density	4, 1.342 Mg/m ³
Absorption coefficient	3.272 mm ⁻¹
F(000)	2080
Crystal size	0.31 x 0.09 x 0.03 mm
Theta range for data collection	1.40 to 25.73 deg.
Limiting indices	-14 ≤ h ≤ 14, -24 ≤ k ≤ 23, -25 ≤ l ≤ 23
Reflections collected / unique	65510 / 9514 [R(int) = 0.1007]
Completeness to theta = 25.73	99.2 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9054 and 0.4323
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	9514 / 0 / 514
Goodness-of-fit on F ²	1.144
Final R indices [I > 2σ(I)]	R ₁ = 0.0406, wR ₂ = 0.0983
R indices (all data)	R ₁ = 0.0603, wR ₂ = 0.1103
Largest diff. peak and hole	1.476 and -1.556 e.Å ⁻³

Table 2: Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for complex 1.
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

U(eq)	x	y	z
U(1)	4545(1)	3946(1)	2501(1)
N(1)	6143(3)	4465(2)	2681(2)
N(2)	7638(3)	5024(2)	2145(2)
N(3)	7960(3)	4771(2)	3178(2)
N(4)	4927(3)	3256(2)	1729(2)
N(5)	6043(4)	2278(2)	1544(2)
N(6)	4789(4)	2575(2)	779(2)
N(7)	3833(3)	3360(2)	3267(2)
N(8)	3405(4)	2791(3)	4254(2)
N(9)	2172(4)	2690(2)	3429(2)
N(10)	3296(3)	4716(2)	2306(2)
N(11)	2033(3)	5488(2)	1754(2)
N(12)	2355(4)	5622(2)	2820(2)
C(1)	7131(4)	4730(2)	2661(2)
C(2)	8923(4)	5070(3)	2934(3)
C(3)	8728(4)	5204(3)	2334(3)
C(4)	7103(5)	5157(3)	1512(2)
C(5)	5999(6)	5530(4)	1570(3)
C(6)	7862(6)	5564(3)	1127(3)
C(7)	6876(8)	4521(4)	1167(3)
C(8)	7819(5)	4539(3)	3842(2)
C(9)	6842(6)	4916(3)	4127(3)
C(10)	7599(7)	3831(3)	3841(3)
C(11)	8895(6)	4694(4)	4242(3)
C(12)	5220(4)	2769(2)	1394(2)
C(13)	6084(6)	1844(3)	1058(3)
C(14)	5356(6)	2013(3)	588(3)
C(15)	4081(5)	2984(3)	348(2)
C(16)	2967(5)	3109(3)	671(3)
C(17)	3809(6)	2643(4)	-292(3)
C(18)	4703(6)	3634(3)	223(3)
C(19)	6836(5)	2298(2)	2118(3)
C(20)	7669(5)	1747(3)	2089(3)
C(21)	7509(5)	2943(3)	2118(4)
C(22)	6176(6)	2229(3)	2722(3)
C(23)	3202(4)	2995(2)	3607(2)
C(24)	2537(6)	2388(4)	4436(3)
C(25)	1797(6)	2331(4)	3945(4)
C(26)	4411(5)	2963(3)	4654(3)
C(27)	5437(5)	2651(4)	4365(3)
C(28)	4305(7)	2645(4)	5328(3)
C(29)	4520(8)	3676(4)	4722(4)
C(30)	1460(4)	2841(3)	2848(3)
C(31)	2136(6)	2822(5)	2263(3)
C(32)	561(7)	2300(4)	2772(4)
C(33)	922(8)	3471(4)	2888(4)
C(34)	2649(4)	5213(3)	2299(2)
C(35)	1412(5)	6029(2)	1959(3)

C(36)	1603(5)	6097(2)	2586(3)	66(2)
C(37)	1941(5)	5200(3)	1126(2)	59(1)
C(38)	1383(6)	4559(4)	1159(4)	92(2)
C(39)	1230(6)	5638(4)	693(3)	88(2)
C(40)	3124(6)	5136(4)	870(3)	90(2)
C(41)	2841(5)	5578(3)	3470(3)	67(
C(42)	2502(7)	4890(3)	3766(3)	93(2)
C(43)	4115(6)	5662(4)	3455(3)	95(2)
C(44)	2337(8)	6120(3)	3911(3)	93(2)

Table 3: Bond lengths [Å] and angles [deg] for shelxl.

U(1)-N(10)	2.185(4)
U(1)-N(7)	2.188(4)
U(1)-N(1)	2.188(4)
U(1)-N(4)	2.197(4)
N(1)-C(1)	1.292(6)
N(2)-C(3)	1.383(6)
N(2)-C(1)	1.387(6)
N(2)-C(4)	1.464(6)
N(3)-C(2)	1.408(7)
N(3)-C(1)	1.428(6)
N(3)-C(8)	1.476(6)
N(4)-C(12)	1.270(6)
N(5)-C(13)	1.347(7)
N(5)-C(12)	1.422(6)
N(5)-C(19)	1.487(7)
N(6)-C(14)	1.396(7)
N(6)-C(12)	1.414(6)
N(6)-C(15)	1.462(7)
N(7)-C(23)	1.289(6)
N(8)-C(24)	1.381(8)
N(8)-C(23)	1.420(6)
N(8)-C(26)	1.467(7)
N(9)-C(25)	1.388(7)
N(9)-C(23)	1.405(6)
N(9)-C(30)	1.476(7)
N(10)-C(34)	1.270(6)
N(11)-C(35)	1.402(6)
N(11)-C(34)	1.436(6)
N(11)-C(37)	1.432(6)
N(12)-C(36)	1.390(7)
N(12)-C(34)	1.424(6)
N(12)-C(41)	1.449(7)
C(2)-C(3)	1.290(7)
C(4)-C(7)	1.501(9)
C(4)-C(6)	1.483(8)
C(4)-C(5)	1.523(9)
C(8)-C(10)	1.469(8)
C(8)-C(9)	1.530(8)
C(8)-C(11)	1.525(8)
C(13)-C(14)	1.320(8)

C(15)-C(16)	1.527(8)
C(15)-C(18)	1.545(8)
C(15)-C(17)	1.525(7)
C(19)-C(22)	1.516(8)
C(19)-C(20)	1.499(7)
C(19)-C(21)	1.538(8)
C(24)-C(25)	1.323(9)
C(26)-C(29)	1.466(10)
C(26)-C(27)	1.519(9)
C(26)-C(28)	1.556(8)
C(30)-C(33)	1.439(9)
C(30)-C(31)	1.487(8)
C(30)-C(32)	1.537(8)
C(35)-C(36)	1.322(9)
C(37)-C(38)	1.469(9)
C(37)-C(39)	1.501(8)
C(37)-C(40)	1.527(8)
C(41)-C(43)	1.521(9)
C(41)-C(42)	1.591(9)
C(41)-C(44)	1.571(8)

N(10)-U(1)-N(7)	104.42(15)
N(10)-U(1)-N(1)	104.94(15)
N(7)-U(1)-N(1)	119.80(15)
N(10)-U(1)-N(4)	118.98(14)
N(7)-U(1)-N(4)	106.25(16)
N(1)-U(1)-N(4)	103.38(15)
C(1)-N(1)-U(1)	167.4(3)
C(3)-N(2)-C(1)	109.0(4)
C(3)-N(2)-C(4)	124.7(4)
C(1)-N(2)-C(4)	126.2(4)
C(2)-N(3)-C(1)	107.1(4)
C(2)-N(3)-C(8)	127.0(4)
C(1)-N(3)-C(8)	125.8(4)
C(12)-N(4)-U(1)	166.3(4)
C(13)-N(5)-C(12)	110.1(5)
C(13)-N(5)-C(19)	125.3(5)
C(12)-N(5)-C(19)	124.1(4)
C(14)-N(6)-C(12)	109.1(5)
C(14)-N(6)-C(15)	124.5(5)
C(12)-N(6)-C(15)	124.8(4)
C(23)-N(7)-U(1)	165.0(4)
C(24)-N(8)-C(23)	109.6(5)
C(24)-N(8)-C(26)	125.7(5)
C(23)-N(8)-C(26)	124.6(4)
C(25)-N(9)-C(23)	109.5(5)
C(25)-N(9)-C(30)	123.5(5)
C(23)-N(9)-C(30)	125.6(4)
C(34)-N(10)-U(1)	168.4(4)
C(35)-N(11)-C(34)	108.9(5)
C(35)-N(11)-C(37)	125.4(5)
C(34)-N(11)-C(37)	125.1(4)
C(36)-N(12)-C(34)	108.4(4)
C(36)-N(12)-C(41)	126.4(4)
C(34)-N(12)-C(41)	125.0(4)
N(1)-C(1)-N(3)	126.4(4)

N(1)-C(1)-N(2)	129.0(4)
N(3)-C(1)-N(2)	104.6(4)
C(3)-C(2)-N(3)	109.1(5)
C(2)-C(3)-N(2)	110.2(5)
N(2)-C(4)-C(7)	109.4(5)
N(2)-C(4)-C(6)	109.9(4)
C(7)-C(4)-C(6)	109.0(5)
N(2)-C(4)-C(5)	111.2(5)
C(7)-C(4)-C(5)	109.5(6)
C(6)-C(4)-C(5)	107.8(5)
N(3)-C(8)-C(10)	109.9(5)
N(3)-C(8)-C(9)	108.6(4)
C(10)-C(8)-C(9)	111.0(5)
N(3)-C(8)-C(11)	108.6(5)
C(10)-C(8)-C(11)	110.4(5)
C(9)-C(8)-C(11)	108.3(5)
N(4)-C(12)-N(5)	129.1(4)
N(4)-C(12)-N(6)	128.2(5)
N(5)-C(12)-N(6)	102.7(4)
C(14)-C(13)-N(5)	109.9(5)
C(13)-C(14)-N(6)	108.2(5)
N(6)-C(15)-C(16)	108.0(5)
N(6)-C(15)-C(18)	109.1(5)
C(16)-C(15)-C(18)	111.0(5)
N(6)-C(15)-C(17)	111.6(5)
C(16)-C(15)-C(17)	107.9(5)
C(18)-C(15)-C(17)	109.3(5)
N(5)-C(19)-C(22)	109.4(5)
N(5)-C(19)-C(20)	110.0(5)
C(22)-C(19)-C(20)	109.1(5)
N(5)-C(19)-C(21)	109.5(5)
C(22)-C(19)-C(21)	111.4(5)
C(20)-C(19)-C(21)	107.4(5)
N(7)-C(23)-N(9)	129.0(5)
N(7)-C(23)-N(8)	127.7(5)
N(9)-C(23)-N(8)	103.3(4)
C(25)-C(24)-N(8)	108.5(6)
C(24)-C(25)-N(9)	109.0(6)
N(8)-C(26)-C(29)	111.0(6)
N(8)-C(26)-C(27)	108.6(5)
C(29)-C(26)-C(27)	112.7(6)
N(8)-C(26)-C(28)	108.4(5)
C(29)-C(26)-C(28)	109.7(6)
C(27)-C(26)-C(28)	106.2(6)
C(33)-C(30)-N(9)	112.2(5)
C(33)-C(30)-C(31)	109.0(6)
N(9)-C(30)-C(31)	110.9(5)
C(33)-C(30)-C(32)	110.0(6)
N(9)-C(30)-C(32)	107.7(5)
C(31)-C(30)-C(32)	107.0(6)
N(10)-C(34)-N(11)	127.4(5)
N(10)-C(34)-N(12)	128.7(4)
N(11)-C(34)-N(12)	103.8(4)
C(36)-C(35)-N(11)	108.2(5)
C(35)-C(36)-N(12)	110.7(5)
N(11)-C(37)-C(38)	109.9(5)

N(11)-C(37)-C(39)	108.9(5)
C(38)-C(37)-C(39)	108.4(5)
N(11)-C(37)-C(40)	108.6(5)
C(38)-C(37)-C(40)	111.2(6)
C(39)-C(37)-C(40)	109.9(5)
N(12)-C(41)-C(43)	109.2(5)
N(12)-C(41)-C(42)	108.6(5)
C(43)-C(41)-C(42)	112.0(6)
N(12)-C(41)-C(44)	110.8(5)
C(43)-C(41)-C(44)	109.6(6)
C(42)-C(41)-C(44)	106.7(5)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Complex 1.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
U(1)	31(1)	47(1)	40(1)	-2(1)	2(1)	0(1)
N(1)	29(2)	66(3)	53(2)	-4(2)	-3(2)	-5(2)
N(2)	38(2)	56(2)	49(2)	10(2)	1(2)	11(2)
N(3)	33(2)	72(3)	59(3)	8(2)	-7(2)	-1(2)
N(4)	42(2)	50(2)	49(2)	-7(2)	2(2)	-1(2)
N(5)	50(3)	48(2)	68(3)	-11(2)	5(2)	2(2)
N(6)	53(3)	66(3)	51(3)	-18(2)	1(2)	-5(2)
N(7)	44(3)	61(3)	52(3)	10(2)	6(2)	-5(2)
N(8)	47(3)	111(4)	54(3)	18(3)	13(2)	-3(3)
N(9)	39(3)	84(3)	60(3)	6(2)	11(2)	11(2)
N(10)	43(2)	56(2)	46(2)	1(2)	1(2)	15(2)
N(11)	34(2)	69(3)	66(3)	-5(2)	-3(2)	6(2)
N(12)	51(3)	54(2)	49(2)	-5(2)	0(2)	12(2)
C(1)	39(3)	49(3)	49(3)	-3(2)	1(2)	1(2)
C(2)	31(3)	68(3)	78(4)	3(3)	-5(3)	-7(2)
C(3)	34(3)	69(3)	73(4)	21(3)	2(3)	-7(2)
C(4)	62(4)	77(4)	44(3)	-2(3)	-5(3)	21(3)
C(5)	64(5)	149(7)	76(4)	38(4)	-18(4)	12(5)
C(6)	87(5)	89(4)	56(3)	18(3)	-6(3)	38(4)
C(7)	184(9)	143(7)	64(4)	-16(4)	7(5)	107(7)
C(8)	54(3)	72(4)	44(3)	11(3)	-6(2)	-1(3)
C(9)	73(5)	107(5)	63(4)	13(3)	7(3)	13(4)
C(10)	94(5)	77(4)	75(4)	25(3)	-5(4)	5(4)
C(11)	74(5)	146(7)	79(5)	47(5)	-24(4)	11(4)
C(12)	45(3)	52(3)	47(3)	-5(2)	8(2)	11(2)
C(13)	77(4)	55(3)	83(4)	-15(3)	7(4)	12(3)
C(14)	78(5)	76(4)	76(4)	-37(3)	5(4)	2(3)
C(15)	52(3)	73(4)	51(3)	-11(3)	0(3)	-9(3)
C(16)	55(4)	95(4)	66(4)	-12(3)	0(3)	3(3)

C(17)	88(5)	120(6)	65(4)	-30(4)	-11(4)	-3(4)
C(18)	80(5)	100(5)	65(4)	12(4)	-3(3)	26(4)
C(19)	49(3)	51(3)	72(4)	3(3)	-1(3)	-2(2)
C(20)	61(4)	63(4)	114(5)	-1(3)	-1(4)	8(3)
C(21)	49(4)	58(4)	143(6)	-14(4)	-15(4)	-4(3)
C(22)	84(5)	101(5)	63(4)	17(3)	-2(3)	23(4)
C(23)	42(3)	62(3)	52(3)	-2(2)	9(2)	4(2)
C(24)	73(5)	158(7)	63(4)	23(4)	22(4)	27(5)
C(25)	62(4)	132(6)	91(5)	18(5)	21(4)	34(4)
C(26)	72(4)	100(5)	40(3)	4(3)	-3(3)	-2(3)
C(27)	49(4)	158(7)	84(5)	21(5)	5(3)	9(4)
C(28)	102(6)	191(9)	56(4)	33(5)	0(4)	-2(6)
C(29)	144(8)	112(6)	85(5)	-20(5)	-32(5)	2(6)
C(30)	34(3)	72(3)	65(3)	-3(3)	1(3)	0(3)
C(31)	66(5)	184(8)	54(4)	4(4)	2(3)	19(5)
C(32)	109(7)	134(7)	114(6)	23(5)	-23(5)	69(6)
C(33)	129(7)	127(7)	133(7)	-21(6)	-15(6)	77(6)
C(34)	35(3)	62(3)	55(3)	7(3)	0(2)	-6(2)
C(35)	53(4)	53(3)	86(5)	-2(3)	-4(3)	11(3)
C(36)	55(4)	57(3)	86(5)	-16(3)	-2(3)	15(3)
C(37)	48(3)	83(4)	45(3)	2(3)	-6(2)	5(3)
C(38)	69(5)	102(5)	103(5)	-16(4)	-20(4)	5(4)
C(39)	71(5)	117(6)	75(4)	6(4)	-17(3)	16(4)
C(40)	64(4)	149(7)	59(4)	25(4)	8(3)	14(4)
C(41)	64(4)	61(3)	75(4)	-11(3)	4(3)	13(3)
C(42)	120(6)	99(5)	59(4)	5(4)	16(4)	18(4)
C(43)	73(5)	106(5)	103(5)	-30(4)	-22(4)	10(4)
C(44)	109(6)	92(5)	76(5)	-24(4)	5(4)	26(4)

Table 5: Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) Complex 1.

	x	y	z	U(eq)
H(2)	9600	5157	3170	71
H(3)	9251	5396	2063	70
H(5A)	5512	5293	1853	146
H(5B)	5625	5573	1148	146
H(5C)	6156	5962	1747	146
H(6A)	8022	5973	1351	116
H(6B)	7497	5656	710	116
H(6C)	8562	5329	1069	116
H(7A)	7579	4282	1133	196
H(7B)	6552	4609	740	196
H(7C)	6351	4261	1406	196
H(9A)	7025	5379	4145	121
H(9B)	6721	4757	4558	121

H(9C)	6161	4851	3858	121
H(10A)	6939	3737	3565	123
H(10B)	7466	3686	4276	123
H(10C)	8247	3601	3683	123
H(11A)	9539	4506	4036	150
H(11B)	8842	4508	4669	150
H(11C)	8988	5165	4275	150
H(13)	6560	1476	1053	86
H(14)	5239	1792	194	92
H(16A)	2580	2696	731	109
H(16B)	2496	3395	402	109
H(16C)	3119	3315	1086	109
H(17A)	4505	2554	-505	137
H(17B)	3330	2923	-563	137
H(17C)	3421	2233	-215	137
H(18A)	4838	3865	627	123
H(18B)	4242	3904	-68	123
H(18C)	5418	3542	32	123
H(20A)	7267	1334	2043	119
H(20B)	8141	1740	2481	119
H(20C)	8138	1809	1723	119
H(21A)	8033	2934	1772	126
H(21B)	7927	2992	2527	126
H(21C)	6993	3308	2055	126
H(22A)	5623	2579	2738	124
H(22B)	6690	2255	3097	124
H(22C)	5792	1809	2719	124
H(24)	2482	2189	4841	117
H(25)	1125	2085	3945	114
H(27A)	5368	2177	4383	145
H(27B)	6115	2787	4606	145
H(27C)	5481	2788	3920	145
H(28A)	3607	2788	5512	175
H(28B)	4940	2778	5608	175
H(28C)	4301	2172	5286	175
H(29A)	4634	3870	4304	172
H(29B)	5161	3777	5011	172
H(29C)	3837	3853	4896	172
H(31A)	2529	3235	2218	153
H(31B)	1638	2749	1887	153
H(31C)	2682	2468	2301	153
H(32A)	920	1874	2821	180
H(32B)	190	2330	2348	180
H(32C)	7	2353	3097	180
H(33A)	521	3498	3284	196
H(33B)	393	3527	2523	196
H(33C)	1491	3813	2883	196
H(35)	941	6297	1695	77
H(36)	1276	6422	2838	79
H(38A)	1788	4285	1473	138
H(38B)	1381	4350	741	138
H(38C)	611	4618	1286	138
H(39A)	484	5681	861	132
H(39B)	1167	5448	265	132
H(39C)	1581	6066	671	132
H(40A)	3450	5568	821	136

H(40B)	3079	4917	456	136
H(40C)	3596	4881	1170	136
H(42A)	1686	4845	3743	139
H(42B)	2774	4867	4211	139
H(42C)	2837	4540	3523	139
H(43A)	4427	5321	3192	142
H(43B)	4443	5633	3889	142
H(43C)	4286	6088	3275	142
H(44A)	2537	6550	3752	139
H(44B)	2640	6067	4348	139
H(44C)	1521	6079	3904	139

3.2. Crystallographic Data for Complex 2

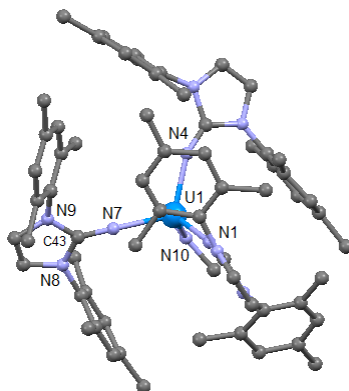


Figure 7: Molecular structure of 2. U: green, N:blue, C: grey. Hydrogen atoms are omitted for clarity.

Table 6: Crystal data and structure refinement for Complex 2

Identification code	Complex 2
Empirical formula	C ₆₅ H ₇₈ N ₁₀ U
Formula weight	1237.40
Temperature	240(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 11.8330(6)Å alpha = 81.532(2) deg. b = 12.4840(6)Å beta = 83.630(2) deg. c = 23.687(1)Å gamma = 65.465(2) deg.
Volume	3143.6(3) Å ³
Z, Calculated density	2, 1.307 Mg/m ³
Absorption coefficient	2.627 mm ⁻¹
F(000)	1260
Crystal size	0.28 x 0.13 x 0.12 mm
Theta range for data collection	1.74 to 25.50 deg.
Limiting indices	-14 ≤ h ≤ 13, -15 ≤ k ≤ 15, -28 ≤ l ≤ 18
Reflections collected / unique	16162 / 11586 [R(int) = 0.0438]
Completeness to theta = 25.50	99.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.75 and 0.63
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	11586 / 0 / 673
Goodness-of-fit on F ²	1.020
Final R indices [I > 2σ(I)]	R1 = 0.0669, wR2 = 0.1689
R indices (all data)	R1 = 0.0996, wR2 = 0.2198
Largest diff. peak and hole	2.278 and -2.440 e.Å ⁻³

Table 7. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Complex 2.
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
U(1)	4228(1)	2060(1)	2698(1)	40(1)
N(1)	5824(11)	2524(9)	2566(5)	74(3)
N(2)	7258(12)	3313(10)	2776(5)	74(3)
N(3)	6867(7)	3534(8)	1880(4)	50(2)
N(4)	4531(9)	511(7)	2247(4)	50(2)
N(5)	4589(9)	-1068(8)	1774(5)	60(3)
N(6)	5895(10)	-1525(8)	2472(5)	62(3)
N(7)	2532(7)	3696(7)	2466(4)	48(2)
N(8)	741(9)	5078(9)	2881(4)	60(3)
N(9)	707(8)	5012(7)	1968(4)	49(2)
N(10)	3965(17)	1473(11)	3596(5)	93(4)
C(1)	6624(9)	3006(9)	2426(5)	44(2)
C(2)	7940(14)	3920(13)	2485(6)	75(4)
C(3)	7638(12)	4075(10)	1906(6)	61(2)
C(4)	6450(12)	3381(10)	1360(6)	61(2)
C(5)	7280(12)	2564(11)	1015(6)	61(3)
C(6)	6903(11)	2425(11)	486(6)	62(3)
C(7)	5667(10)	3150(10)	334(5)	52(3)
C(8)	4852(10)	3962(11)	686(7)	70(4)
C(9)	5249(10)	4033(9)	1164(6)	53(3)
C(10)	8608(13)	1757(14)	1197(7)	84(4)
C(11)	5271(14)	2988(12)	-215(6)	74(4)
C(12)	4348(10)	4986(10)	1563(6)	68(4)
C(13)	7497(14)	2804(13)	3377(6)	67(4)
C(14)	8546(18)	1846(15)	3516(7)	84(5)
C(15)	8731(16)	1436(17)	4065(9)	102(6)
C(16)	7890(19)	1953(18)	4499(8)	97(5)
C(17)	6769(18)	2955(17)	4368(7)	96(5)
C(18)	6567(14)	3390(15)	3767(7)	81(4)
C(19)	9481(17)	1314(18)	3067(9)	112(6)
C(20)	8000(20)	1484(19)	5154(8)	126(7)
C(21)	5390(16)	4423(17)	3599(9)	108(6)
C(22)	4967(10)	-566(9)	2175(5)	50(3)
C(23)	5291(12)	-2266(10)	1832(7)	68(4)
C(24)	6051(14)	-2556(11)	2251(7)	73(4)
C(25)	3744(11)	-470(9)	1348(5)	47(3)
C(26)	2671(12)	-645(11)	1372(7)	73(4)
C(27)	1913(11)	-165(11)	913(6)	65(4)
C(28)	2235(11)	463(11)	434(6)	62(3)
C(29)	3315(13)	606(12)	417(6)	75(4)
C(30)	4084(11)	208(10)	880(5)	53(3)
C(31)	2281(17)	-1271(15)	1914(8)	101(6)
C(32)	1340(14)	989(14)	-57(7)	90(5)
C(33)	5237(16)	421(17)	880(7)	97(6)

C(34)	6597(12)	-1510(10)	2904(6)	63(3)
C(35)	7459(14)	-1046(12)	2797(7)	75(4)
C(36)	8195(18)	-1106(14)	3234(9)	102(6)
C(37)	8050(20)	-1563(15)	3781(9)	108(6)
C(38)	7050(20)	-1911(15)	3896(8)	107(6)
C(39)	6380(18)	-1965(15)	3472(8)	101(6)
C(40)	7780(17)	-638(15)	2194(8)	97(5)
C(41)	8780(30)	-1550(20)	4289(10)	199(16)
C(42)	5330(30)	-2400(20)	3604(10)	161(11)
C(43)	1435(11)	4514(9)	2444(5)	47(3)
C(44)	-401(10)	5892(10)	2687(6)	59(3)
C(45)	-403(10)	5882(9)	2150(6)	54(3)
C(46)	1111(13)	5041(11)	3438(5)	61(3)
C(47)	782(17)	4339(15)	3877(6)	87(5)
C(48)	1184(17)	4308(14)	4420(6)	89(5)
C(49)	1867(16)	4915(16)	4530(6)	86(5)
C(50)	2129(14)	5607(14)	4080(7)	79(4)
C(51)	1782(13)	5692(12)	3541(6)	70(4)
C(52)	180(20)	3560(20)	3771(8)	129(8)
C(53)	2420(20)	4835(18)	5120(8)	127(8)
C(54)	2060(20)	6470(20)	3037(8)	134(9)
C(55)	1121(10)	4816(9)	1389(5)	47(3)
C(56)	1141(11)	5777(10)	1010(6)	58(3)
C(57)	1373(11)	5624(12)	424(6)	62(3)
C(58)	1595(11)	4589(12)	219(5)	61(3)
C(59)	1535(10)	3673(11)	610(5)	57(3)
C(60)	1328(10)	3731(9)	1184(5)	49(3)
C(61)	997(15)	6923(11)	1215(6)	76(4)
C(62)	1852(14)	4363(19)	-431(6)	106(6)
C(63)	1299(12)	2699(10)	1601(5)	60(3)
C(64)	3000(20)	890(20)	3726(14)	207(13)
C(65)	4730(20)	1440(20)	4082(14)	207(13)

Table 8: Bond lengths [Å] and angles [deg] for Complex 2.

U(1)-N(1)	2.174(11)
U(1)-N(10)	2.177(11)
U(1)-N(4)	2.226(8)
U(1)-N(7)	2.239(7)
N(1)-C(1)	1.309(14)
N(2)-C(1)	1.366(14)
N(2)-C(2)	1.389(15)
N(2)-C(13)	1.478(16)
N(3)-C(3)	1.351(13)
N(3)-C(1)	1.420(14)
N(3)-C(4)	1.442(16)
N(4)-C(22)	1.255(13)
N(5)-C(23)	1.371(14)
N(5)-C(25)	1.399(14)
N(5)-C(22)	1.414(15)
N(6)-C(24)	1.394(16)
N(6)-C(22)	1.402(14)
N(6)-C(34)	1.395(16)

N(7)-C(43)	1.276(13)
N(8)-C(43)	1.338(15)
N(8)-C(44)	1.390(14)
N(8)-C(46)	1.424(16)
N(9)-C(45)	1.386(14)
N(9)-C(43)	1.401(13)
N(9)-C(55)	1.426(14)
N(10)-C(65)	1.52(4)
N(10)-C(64)	1.57(3)
C(2)-C(3)	1.421(18)
C(4)-C(5)	1.382(18)
C(4)-C(9)	1.404(18)
C(5)-C(6)	1.433(18)
C(5)-C(10)	1.542(19)
C(6)-C(7)	1.418(16)
C(7)-C(8)	1.382(18)
C(7)-C(11)	1.498(17)
C(8)-C(9)	1.301(19)
C(9)-C(12)	1.582(16)
C(13)-C(14)	1.35(2)
C(13)-C(18)	1.38(2)
C(14)-C(15)	1.33(2)
C(14)-C(19)	1.46(2)
C(15)-C(16)	1.38(3)
C(16)-C(17)	1.42(2)
C(16)-C(20)	1.58(2)
C(17)-C(18)	1.46(2)
C(18)-C(21)	1.50(2)
C(23)-C(24)	1.323(19)
C(25)-C(26)	1.369(17)
C(25)-C(30)	1.419(16)
C(26)-C(27)	1.387(19)
C(26)-C(31)	1.532(19)
C(27)-C(28)	1.391(19)
C(28)-C(29)	1.357(18)
C(28)-C(32)	1.542(17)
C(29)-C(30)	1.401(18)
C(30)-C(33)	1.495(18)
C(34)-C(35)	1.354(19)
C(34)-C(39)	1.42(2)
C(35)-C(36)	1.40(2)
C(35)-C(40)	1.51(2)
C(36)-C(37)	1.36(3)
C(37)-C(38)	1.42(3)
C(37)-C(41)	1.56(3)
C(38)-C(39)	1.37(2)
C(39)-C(42)	1.54(3)
C(44)-C(45)	1.274(17)
C(46)-C(47)	1.388(19)
C(46)-C(51)	1.410(18)
C(47)-C(48)	1.41(2)
C(47)-C(52)	1.49(2)
C(48)-C(49)	1.38(2)
C(49)-C(50)	1.36(2)
C(49)-C(53)	1.579(19)
C(50)-C(51)	1.360(19)

C(51)-C(54)	1.52(2)
C(55)-C(56)	1.395(15)
C(55)-C(60)	1.421(15)
C(56)-C(57)	1.411(18)
C(56)-C(61)	1.515(16)
C(57)-C(58)	1.360(18)
C(58)-C(59)	1.382(17)
C(58)-C(62)	1.58(2)
C(59)-C(60)	1.363(16)
C(60)-C(63)	1.514(15)

N(1)-U(1)-N(10)	110.5(6)
N(1)-U(1)-N(4)	111.5(4)
N(10)-U(1)-N(4)	104.3(4)
N(1)-U(1)-N(7)	108.0(4)
N(10)-U(1)-N(7)	107.3(5)
N(4)-U(1)-N(7)	115.1(3)
C(1)-N(1)-U(1)	167.9(9)
C(1)-N(2)-C(2)	113.7(10)
C(1)-N(2)-C(13)	124.4(9)
C(2)-N(2)-C(13)	120.1(11)
C(3)-N(3)-C(1)	111.6(10)
C(3)-N(3)-C(4)	125.0(9)
C(1)-N(3)-C(4)	123.0(8)
C(22)-N(4)-U(1)	155.6(8)
C(23)-N(5)-C(25)	124.1(10)
C(23)-N(5)-C(22)	108.0(10)
C(25)-N(5)-C(22)	127.5(9)
C(24)-N(6)-C(22)	108.1(11)
C(24)-N(6)-C(34)	123.4(10)
C(22)-N(6)-C(34)	128.4(9)
C(43)-N(7)-U(1)	165.0(8)
C(43)-N(8)-C(44)	108.8(10)
C(43)-N(8)-C(46)	128.2(10)
C(44)-N(8)-C(46)	122.2(11)
C(45)-N(9)-C(43)	107.2(9)
C(45)-N(9)-C(55)	125.9(9)
C(43)-N(9)-C(55)	126.0(9)
C(65)-N(10)-C(64)	118.4(17)
C(65)-N(10)-U(1)	126.3(14)
C(64)-N(10)-U(1)	114.9(15)
N(1)-C(1)-N(2)	128.8(11)
N(1)-C(1)-N(3)	127.6(10)
N(2)-C(1)-N(3)	102.7(9)
N(2)-C(2)-C(3)	104.3(11)
N(3)-C(3)-C(2)	107.7(10)
C(5)-C(4)-C(9)	116.3(12)
C(5)-C(4)-N(3)	119.0(12)
C(9)-C(4)-N(3)	124.6(11)
C(4)-C(5)-C(6)	120.2(12)
C(4)-C(5)-C(10)	121.1(12)
C(6)-C(5)-C(10)	118.6(12)
C(7)-C(6)-C(5)	117.8(12)
C(8)-C(7)-C(6)	121.1(11)
C(8)-C(7)-C(11)	121.3(11)
C(6)-C(7)-C(11)	117.6(11)

C(9)-C(8)-C(7)	118.0(10)
C(8)-C(9)-C(4)	126.6(11)
C(8)-C(9)-C(12)	118.9(11)
C(4)-C(9)-C(12)	114.4(12)
C(14)-C(13)-C(18)	124.4(15)
C(14)-C(13)-N(2)	121.3(14)
C(18)-C(13)-N(2)	114.3(13)
C(15)-C(14)-C(13)	119.0(19)
C(15)-C(14)-C(19)	121.3(18)
C(13)-C(14)-C(19)	119.7(14)
C(14)-C(15)-C(16)	122.5(18)
C(15)-C(16)-C(17)	120.1(16)
C(15)-C(16)-C(20)	125.8(18)
C(17)-C(16)-C(20)	114.0(19)
C(16)-C(17)-C(18)	117.1(17)
C(13)-C(18)-C(17)	116.8(15)
C(13)-C(18)-C(21)	123.3(15)
C(17)-C(18)-C(21)	119.9(17)
N(4)-C(22)-N(6)	128.6(11)
N(4)-C(22)-N(5)	126.2(10)
N(6)-C(22)-N(5)	105.2(9)
C(24)-C(23)-N(5)	110.0(11)
C(23)-C(24)-N(6)	108.6(11)
C(26)-C(25)-N(5)	118.7(11)
C(26)-C(25)-C(30)	122.4(11)
N(5)-C(25)-C(30)	118.7(10)
C(25)-C(26)-C(27)	118.2(12)
C(25)-C(26)-C(31)	120.1(14)
C(27)-C(26)-C(31)	121.5(13)
C(26)-C(27)-C(28)	121.4(11)
C(29)-C(28)-C(27)	119.1(12)
C(29)-C(28)-C(32)	122.1(14)
C(27)-C(28)-C(32)	118.7(12)
C(28)-C(29)-C(30)	122.4(13)
C(29)-C(30)-C(25)	116.2(11)
C(29)-C(30)-C(33)	122.9(12)
C(25)-C(30)-C(33)	120.8(11)
C(35)-C(34)-N(6)	121.4(13)
C(35)-C(34)-C(39)	119.3(14)
N(6)-C(34)-C(39)	119.3(13)
C(34)-C(35)-C(36)	119.8(16)
C(34)-C(35)-C(40)	120.7(14)
C(36)-C(35)-C(40)	118.8(16)
C(37)-C(36)-C(35)	123.3(19)
C(36)-C(37)-C(38)	115.5(18)
C(36)-C(37)-C(41)	125(2)
C(38)-C(37)-C(41)	119(2)
C(39)-C(38)-C(37)	122.5(19)
C(38)-C(39)-C(34)	118.8(17)
C(38)-C(39)-C(42)	121.6(19)
C(34)-C(39)-C(42)	119.4(15)
N(7)-C(43)-N(8)	126.2(10)
N(7)-C(43)-N(9)	128.1(11)
N(8)-C(43)-N(9)	105.7(9)
C(45)-C(44)-N(8)	109.3(11)
C(44)-C(45)-N(9)	108.9(10)

C(47)-C(46)-C(51)	121.3(12)
C(47)-C(46)-N(8)	117.3(11)
C(51)-C(46)-N(8)	121.5(12)
C(46)-C(47)-C(48)	115.6(14)
C(46)-C(47)-C(52)	122.2(14)
C(48)-C(47)-C(52)	121.8(14)
C(49)-C(48)-C(47)	124.4(15)
C(50)-C(49)-C(48)	116.6(13)
C(50)-C(49)-C(53)	117.3(15)
C(48)-C(49)-C(53)	126.1(16)
C(49)-C(50)-C(51)	123.3(14)
C(50)-C(51)-C(46)	118.9(13)
C(50)-C(51)-C(54)	123.7(15)
C(46)-C(51)-C(54)	117.3(14)
C(56)-C(55)-N(9)	117.8(10)
C(56)-C(55)-C(60)	120.5(11)
N(9)-C(55)-C(60)	121.0(9)
C(55)-C(56)-C(57)	117.5(11)
C(55)-C(56)-C(61)	122.0(12)
C(57)-C(56)-C(61)	120.4(11)
C(58)-C(57)-C(56)	123.0(11)
C(57)-C(58)-C(59)	117.3(12)
C(57)-C(58)-C(62)	125.5(13)
C(59)-C(58)-C(62)	117.2(13)
C(60)-C(59)-C(58)	124.0(12)
C(59)-C(60)-C(55)	117.7(10)
C(59)-C(60)-C(63)	122.5(10)
C(55)-C(60)-C(63)	119.8(10)

Symmetry transformations used to generate equivalent atoms:

Table 9: Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Complex 2.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2hka^*b^*U_{12}]$$

	U11	U22	U33	U23	U13	U12
U(1)	44(1)	32(1)	46(1)	-2(1)	-3(1)	18(1)
N(1)	103(9)	62(6)	74(7)	-5(6)	28(6)	58(6)
N(2)	105(9)	88(8)	57(6)	20(6)	-14(6)	74(7)
N(3)	34(4)	43(5)	77(7)	-6(5)	7(4)	23(4)
N(4)	80(6)	30(4)	44(5)	-15(4)	-6(5)	24(4)
N(5)	63(6)	38(5)	85(7)	1(5)	-20(5)	26(5)
N(6)	73(7)	32(5)	75(7)	-14(5)	-14(6)	10(5)
N(7)	25(4)	38(5)	71(6)	-2(4)	-13(4)	-1(4)
N(8)	51(6)	68(6)	59(6)	-4(5)	-13(5)	21(5)
N(9)	56(5)	35(4)	52(6)	-10(4)	-7(4)	12(4)

N(10)	164(14)	78(8)	39(6)	-10(6)	-8(7)	51(9)
C(1)	40(5)	37(5)	60(7)	-19(5)	-6(5)	13(4)
C(2)	98(10)	85(10)	73(9)	3(8)	-19(8)	67(9)
C(3)	80(6)	44(4)	81(6)	-12(4)	20(5)	51(5)
C(4)	80(6)	44(4)	81(6)	-12(4)	20(5)	51(5)
C(5)	65(7)	69(8)	68(8)	1(6)	-5(6)	48(7)
C(6)	57(7)	65(8)	74(8)	-13(6)	-8(6)	31(6)
C(7)	44(6)	46(6)	68(8)	-8(5)	-17(5)	15(5)
C(8)	22(5)	49(7)	115(12)	18(7)	-13(6)	2(5)
C(9)	43(6)	37(6)	66(8)	-7(5)	10(6)	-6(5)
C(10)	64(8)	94(11)	99(11)	-38(9)	-1(8)	30(8)
C(11)	91(10)	60(8)	74(9)	-25(7)	-5(8)	28(7)
C(12)	26(5)	51(7)	100(10)	-3(7)	2(6)	10(5)
C(13)	81(9)	77(9)	72(9)	-7(7)	-22(8)	56(8)
C(14)	117(13)	86(11)	69(10)	26(9)	39(10)	66(11)
C(15)	67(10)	102(13)	133(17)	9(12)	-28(11)	32(9)
C(16)	99(13)	108(14)	101(13)	24(11)	41(11)	62(12)
C(17)	112(14)	112(14)	80(11)	-18(10)	9(10)	63(12)
C(18)	72(9)	105(12)	86(11)	-10(9)	-23(8)	53(9)
C(19)	90(12)	117(15)	130(17)	-3(13)	30(12)	40(11)
C(20)	124(16)	142(18)	114(15)	-28(13)	54(13)	41(14)
C(21)	84(12)	113(14)	129(16)	-28(12)	8(11)	39(11)
C(22)	56(6)	39(6)	56(7)	0(5)	-12(5)	20(5)
C(23)	60(7)	31(6)	108(11)	-21(6)	-19(7)	-4(5)
C(24)	85(9)	26(5)	107(11)	-21(6)	-32(8)	12(6)
C(25)	69(7)	33(5)	51(6)	-18(5)	-14(5)	26(5)
C(26)	61(8)	44(7)	108(12)	2(7)	17(8)	22(6)
C(27)	44(6)	52(7)	100(11)	-34(7)	-17(7)	10(6)
C(28)	49(7)	53(7)	74(9)	-13(6)	-20(6)	-6(6)
C(29)	68(9)	69(9)	78(10)	14(7)	-8(7)	24(7)
C(30)	65(7)	50(6)	59(7)	-29(6)	-5(6)	28(6)
C(31)	113(13)	94(11)	117(13)	15(10)	9(10)	75(11)
C(32)	80(10)	93(11)	100(12)	-19(9)	-53(9)	24(9)
C(33)	112(13)	142(15)	71(10)	20(10)	-5(9)	95(12)
C(34)	57(7)	36(6)	87(10)	-12(6)	-22(7)	-5(5)
C(35)	80(9)	49(7)	101(12)	1(7)	-30(8)	28(7)
C(36)	117(14)	59(9)	132(17)	-5(10)	-48(12)	30(9)
C(37)	146(18)	66(10)	113(16)	-10(10)	54(14)	32(11)
C(38)	140(17)	77(11)	86(12)	-1(9)	49(12)	19(11)
C(39)	115(13)	86(11)	104(13)	31(10)	52(11)	45(10)
C(40)	113(13)	76(10)	116(14)	-14(10)	4(11)	51(10)
C(41)	380(50)	127(19)	150(20)	27(16)	160(30)	130(30)
C(42)	240(30)	190(30)	116(17)	36(17)	48(18)	160(30)
C(43)	60(7)	45(6)	47(6)	-5(5)	-14(5)	30(5)
C(44)	32(5)	53(7)	81(9)	-21(6)	1(5)	-4(5)
C(45)	45(6)	38(6)	69(8)	-17(5)	-11(5)	0(5)
C(46)	78(8)	60(7)	54(7)	-12(6)	-6(6)	35(7)
C(47)	133(14)	101(11)	58(9)	-20(8)	5(9)	77(11)
C(48)	142(15)	86(10)	56(8)	-31(8)	8(9)	58(11)
C(49)	109(12)	108(12)	63(9)	-31(9)	-19(8)	55(10)
C(50)	92(10)	90(10)	79(10)	-27(8)	-13(8)	51(9)
C(51)	78(9)	60(8)	70(9)	-20(7)	-1(7)	23(7)
C(52)	200(20)	160(19)	93(13)	-2(13)	4(14)	139(19)
C(53)	165(19)	126(15)	100(13)	-55(11)	59(13)	41(14)
C(54)	210(30)	155(19)	89(13)	16(13)	9(14)	140(20)
C(55)	55(6)	38(5)	48(6)	-1(5)	-15(5)	17(5)

C(56)	70(8)	41(6)	76(9)	3(6)	-32(6)	33(6)
C(57)	50(7)	66(8)	61(8)	16(7)	-23(6)	17(6)
C(58)	46(6)	68(8)	54(7)	-11(6)	-8(5)	-6(6)
C(59)	50(6)	55(7)	65(8)	-16(6)	-13(6)	15(5)
C(60)	52(6)	39(6)	57(7)	-3(5)	-12(5)	19(5)
C(61)	113(11)	46(7)	79(9)	3(6)	-28(8)	40(8)
C(62)	64(9)	163(18)	71(10)	8(11)	-10(8)	30(11)
C(63)	70(8)	42(6)	78(8)	-26(6)	4(6)	28(6)
C(64)	80(10)	157(17)	280(30)	62(18)	57(14)	8(10)
C(65)	80(10)	157(17)	280(30)	62(18)	57(14)	8(10)

Table 10: Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Complex 2.

	x	y	z	U(eq)
H(2)	8463	4185	2640	90
H(3)	7941	4465	1597	73
H(6)	7457	1871	247	75
H(8)	4035	4448	583	84
H(10A)	9053	1245	903	126
H(10B)	8564	1276	1553	126
H(10C)	9043	2241	1250	126
H(11A)	5965	2387	-403	111
H(11B)	5004	3731	-462	111
H(11C)	4587	2742	-135	111
H(12A)	4767	4928	1903	103
H(12B)	3605	4842	1673	103
H(12C)	4119	5773	1359	103
H(15)	9463	769	4160	122
H(17)	6182	3321	4658	115
H(19A)	10167	632	3236	168
H(19B)	9786	1891	2874	168
H(19C)	9112	1066	2794	168
H(20A)	7269	1988	5368	189
H(20B)	8738	1497	5287	189
H(20C)	8051	679	5211	189
H(21A)	4867	4690	3940	162
H(21B)	4953	4186	3353	162
H(21C)	5589	5063	3397	162
H(23)	5239	-2802	1606	82
H(24)	6603	-3328	2379	87
H(27)	1166	-266	926	78
H(29)	3555	985	83	90
H(31A)	2928	-1548	2185	152
H(31B)	2154	-1940	1818	152
H(31C)	1512	-720	2084	152
H(32A)	621	799	39	135
H(32B)	1764	656	-405	135
H(32C)	1072	1842	-114	135
H(33A)	5626	77	1240	146
H(33B)	5023	1267	830	146
H(33C)	5811	57	569	146
H(36)	8819	-817	3144	122
H(38)	6826	-2113	4278	128
H(40A)	8405	-326	2197	146
H(40B)	7039	-23	2028	146
H(40C)	8102	-1302	1968	146
H(41A)	8522	-1924	4636	299
H(41B)	8606	-735	4338	299
H(41C)	9667	-1976	4208	299
H(42A)	4982	-2395	3250	242
H(42B)	4681	-1887	3850	242
H(42C)	5659	-3205	3797	242
H(44)	-1067	6373	2916	70

H(45)	-1053	6384	1916	65
H(48)	974	3843	4727	107
H(50)	2573	6047	4145	95
H(52A)	23	3147	4131	193
H(52B)	723	2986	3519	193
H(52C)	-603	4036	3594	193
H(53A)	2168	4320	5404	191
H(53B)	2109	5619	5243	191
H(53C)	3320	4515	5074	191
H(54A)	1694	6419	2700	200
H(54B)	2948	6211	2967	200
H(54C)	1698	7289	3123	200
H(57)	1375	6268	162	74
H(59)	1644	2967	471	68
H(61A)	1025	7481	888	114
H(61B)	1668	6766	1458	114
H(61C)	206	7255	1429	114
H(62A)	2004	3549	-464	160
H(62B)	2576	4510	-586	160
H(62C)	1135	4893	-643	160
H(63A)	1164	2915	1987	90
H(63B)	2085	2019	1566	90
H(63C)	629	2503	1516	90
H(64A)	2632	925	3375	310
H(64B)	2355	1323	3998	310
H(64C)	3421	74	3885	310
H(65A)	5302	1802	3938	310
H(65B)	5186	628	4237	310
H(65C)	4171	1881	4380	310

3.3. Crystallographic Data for Complex 3

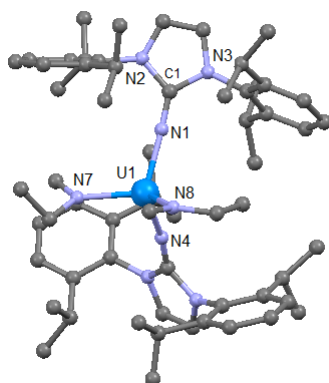


Figure 8: Molecular structure of 3. U: green, N: blue, C: grey. Only one of the two molecules in the unit cell is shown. Hydrogen atoms are omitted for clarity.

Table 11: Crystal data and structure refinement for Complex 3.

Identification code	Complex 3
Empirical formula	60 H88 N8 U
Formula weight	1159.41
Temperature	240(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, C 2/c
Unit cell dimensions	a = 45.543(4) Å alpha = 90 deg. b = 12.563(1) Å beta = 112.469(2)deg. c = 34.112(3) Å gamma = 90 deg.
Volume	18036(3) Å ³
Z, Calculated density	12, 1.281 Mg/m ³
Absorption coefficient	2.741 mm ⁻¹
F(000)	7152
Crystal size	0.60 x 0.24 x 0.20 mm
Theta range for data collection	1.29 to 24.95 deg.
Limiting indices	-33<=h<=52, -7<=k<=14, -39<=l<=40
Reflections collected / unique	23834 / 15309 [R(int) = 0.0192]
Completeness to theta = 24.95	97.1 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.6088 and 0.2887
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	15309 / 1 / 933
Goodness-of-fit on F ²	1.068
Final R indices [I>2sigma(I)]	R1 = 0.0372, wR2 = 0.1221
R indices (all data)	R1 = 0.0475, wR2 = 0.1343
Largest diff. peak and hole	1.128 and -1.282 e.Å ⁻³

Table 12: Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Complex 3.
 $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
U(1)	1803(1)	8716(1)	809(1)	34(1)
N(1)	1898(1)	10248(3)	1135(1)	42(1)
N(2)	1836(1)	11542(3)	1615(2)	49(1)
N(3)	2261(1)	11683(4)	1460(1)	47(1)
N(4)	1392(1)	8728(3)	207(1)	39(1)
N(5)	1117(1)	9106(3)	-534(1)	39(1)
N(6)	898(1)	7949(3)	-246(1)	39(1)
N(7)	1709(1)	7624(4)	1257(2)	61(1)
N(8)	2209(1)	8126(4)	664(2)	57(1)
C(1)	1984(1)	11050(4)	1377(2)	42(1)
C(2)	2015(2)	12383(5)	1846(2)	67(2)
C(3)	2272(2)	12480(5)	1756(2)	67(2)
C(4)	1576(2)	11080(4)	1701(2)	47(1)
C(5)	1268(2)	11198(4)	1408(2)	49(1)
C(6)	1027(2)	10788(5)	1514(2)	62(2)
C(7)	1084(2)	10310(5)	1895(2)	65(2)
C(8)	1387(2)	10191(5)	2175(2)	70(2)
C(9)	1652(2)	10571(5)	2096(2)	58(2)
C(10)	1199(2)	11754(6)	988(2)	69(2)
C(11)	1188(4)	12956(7)	1056(4)	184(8)
C(12)	907(2)	11355(11)	644(3)	132(5)
C(13)	1980(2)	10358(7)	2399(2)	84(2)
C(14)	2041(3)	10655(13)	2861(3)	156(5)
C(15)	2079(2)	9215(8)	2369(3)	109(3)
C(16)	2505(1)	11445(4)	1310(2)	47(1)
C(17)	2718(2)	10614(5)	1489(2)	62(2)
C(18)	2953(2)	10412(6)	1341(2)	72(2)
C(19)	2978(2)	10998(6)	1027(3)	76(2)
C(20)	2770(1)	11807(6)	840(2)	64(2)
C(21)	2526(1)	12046(5)	978(2)	53(1)
C(22)	2696(2)	9982(6)	1872(2)	76(2)
C(23)	2769(3)	8823(7)	1861(3)	127(4)
C(24)	2905(3)	10474(9)	2293(3)	123(4)
C(25)	2289(2)	12931(6)	762(2)	67(2)
C(26)	2214(2)	13063(7)	299(3)	81(2)
C(27)	2395(2)	14013(6)	984(3)	92(3)
C(28)	1164(1)	8607(3)	-151(2)	31(1)
C(29)	836(1)	8731(4)	-852(2)	50(1)
C(30)	703(1)	8027(4)	-680(2)	47(1)
C(31)	1353(1)	9689(4)	-629(2)	40(1)
C(32)	1397(1)	10776(4)	-516(2)	45(1)
C(33)	1608(2)	11338(5)	-646(2)	56(2)
C(34)	1771(2)	10840(5)	-860(2)	62(2)
C(35)	1727(2)	9769(5)	-957(2)	61(2)
C(36)	1521(1)	9176(4)	-835(2)	42(1)
C(37)	1214(2)	11314(4)	-290(2)	52(1)
C(38)	1403(2)	12136(6)	24(3)	86(2)
C(39)	904(2)	11765(9)	-604(3)	116(4)

C(40)	1496(1)	7975(5)	-920(2)	61(2)
C(41)	1790(2)	7421(6)	-571(3)	75(2)
C(42)	1460(3)	7687(7)	-1354(3)	105(3)
C(43)	857(1)	7163(4)	30(2)	40(1)
C(44)	652(2)	7352(5)	231(2)	53(1)
C(45)	598(2)	6530(5)	475(2)	66(2)
C(46)	753(2)	5577(5)	522(2)	69(2)
C(47)	963(2)	5420(5)	326(2)	62(2)
C(48)	1028(1)	6204(4)	76(2)	47(1)
C(49)	484(2)	8430(5)	201(2)	68(2)
C(50)	152(3)	8370(9)	-101(4)	179(8)
C(51)	480(2)	8766(7)	641(3)	95(3)
C(52)	1255(1)	5996(5)	-135(2)	54(1)
C(53)	1572(2)	5535(7)	180(3)	85(2)
C(54)	1120(2)	5311(8)	-499(3)	94(3)
C(55)	1406(2)	7836(9)	1296(3)	113(3)
C(56)	1900(3)	6815(7)	1554(3)	105(3)
C(57)	1754(4)	5709(9)	1468(4)	181(7)
C(58)	2352(2)	7072(6)	805(4)	102(3)
C(59)	2379(2)	8666(5)	452(2)	60(2)
C(60)	2220(2)	9697(6)	273(3)	74(2)
U(1A)	0	5287(1)	2500	38(1)
N(1A)	298(1)	6114(3)	2227(1)	42(1)
N(2A)	644(1)	7360(3)	2076(1)	40(1)
N(3A)	558(1)	5846(3)	1740(1)	39(1)
N(4A)	-361(1)	4323(4)	2007(2)	59(1)
C(1A)	473(1)	6402(4)	2032(2)	34(1)
C(2A)	811(1)	7350(4)	1815(2)	48(1)
C(3A)	760(1)	6427(4)	1608(2)	49(1)
C(4A)	641(1)	8246(4)	2332(2)	44(1)
C(5A)	877(1)	8352(5)	2730(2)	51(1)
C(6A)	905(2)	9312(5)	2951(2)	64(2)
C(7A)	688(2)	10102(5)	2780(2)	68(2)
C(8A)	441(2)	9990(6)	2388(2)	67(2)
C(9A)	409(1)	9031(5)	2153(2)	52(1)
C(10A)	1112(2)	7470(5)	2927(2)	63(2)
C(11A)	1450(2)	7732(8)	2935(3)	100(3)
C(12A)	1133(2)	7202(7)	3371(2)	98(3)
C(13A)	140(2)	8898(6)	1735(2)	68(2)
C(14A)	115(3)	9792(8)	1432(3)	115(3)
C(15A)	-167(2)	8699(9)	1796(4)	111(4)
C(16A)	443(1)	4809(4)	1563(2)	39(1)
C(17A)	178(1)	4751(5)	1164(2)	47(1)
C(18A)	97(2)	3738(5)	997(2)	61(2)
C(19A)	245(2)	2846(6)	1189(3)	74(2)
C(20A)	499(2)	2923(5)	1590(2)	66(2)
C(21A)	604(1)	3906(4)	1780(2)	49(1)
C(22A)	0(1)	5742(5)	957(2)	52(1)
C(23A)	-166(2)	5631(8)	471(2)	88(2)
C(24A)	-245(2)	6031(6)	1142(2)	67(2)
C(25A)	885(2)	3970(6)	2203(2)	69(2)
C(26A)	901(2)	3073(7)	2497(3)	92(2)
C(27A)	1192(2)	4039(10)	2140(3)	121(4)
C(28A)	-699(2)	4755(11)	1773(3)	126(4)
C(29A)	-215(3)	3510(6)	1815(4)	152(5)
C(30A)	-307(4)	2400(8)	1882(4)	161(6)

Table 13: Bond lengths [Å] and angles [deg] for Complex 3.

U(1)-N(1)	2.182(4)
U(1)-N(4)	2.186(4)
U(1)-N(7)	2.214(5)
U(1)-N(8)	2.216(5)
N(1)-C(1)	1.266(6)
N(2)-C(2)	1.381(7)
N(2)-C(1)	1.383(7)
N(2)-C(4)	1.446(7)
N(3)-C(3)	1.407(7)
N(3)-C(16)	1.423(7)
N(3)-C(1)	1.425(7)
N(4)-C(28)	1.276(6)
N(5)-C(28)	1.389(6)
N(5)-C(29)	1.405(6)
N(5)-C(31)	1.438(6)
N(6)-C(28)	1.396(6)
N(6)-C(30)	1.409(6)
N(6)-C(43)	1.426(6)
N(7)-C(56)	1.463(9)
N(7)-C(55)	1.460(11)
N(8)-C(59)	1.417(8)
N(8)-C(58)	1.475(9)
C(2)-C(3)	1.328(10)
C(2)-H(2)	0.9400
C(3)-H(3)	0.9400
C(4)-C(5)	1.384(9)
C(4)-C(9)	1.410(8)
C(5)-C(6)	1.377(8)
C(5)-C(10)	1.516(9)
C(6)-C(7)	1.364(9)
C(6)-H(6)	0.9400
C(7)-C(8)	1.353(10)
C(7)-H(7)	0.9400
C(8)-C(9)	1.415(9)
C(8)-H(8)	0.9400
C(9)-C(13)	1.482(10)
C(10)-C(12)	1.483(12)
C(10)-C(11)	1.532(12)
C(10)-H(10)	0.9900
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(11)-H(11C)	0.9700
C(12)-H(12A)	0.9700
C(12)-H(12B)	0.9700
C(12)-H(12C)	0.9700
C(13)-C(15)	1.520(13)
C(13)-C(14)	1.537(13)
C(13)-H(13)	0.9900

C(14)-H(14A)	0.9700
C(14)-H(14B)	0.9700
C(14)-H(14C)	0.9700
C(15)-H(15A)	0.9700
C(15)-H(15B)	0.9700
C(15)-H(15C)	0.9700
C(16)-C(17)	1.396(9)
C(16)-C(21)	1.394(8)
C(17)-C(18)	1.367(10)
C(17)-C(22)	1.566(10)
C(18)-C(19)	1.342(11)
C(18)-H(18)	0.9400
C(19)-C(20)	1.371(10)
C(19)-H(19)	0.9400
C(20)-C(21)	1.395(8)
C(20)-H(20)	0.9400
C(21)-C(25)	1.528(9)
C(22)-C(23)	1.498(11)
C(22)-C(24)	1.518(11)
C(22)-H(22)	0.9900
C(23)-H(23A)	0.9700
C(23)-H(23B)	0.9700
C(23)-H(23C)	0.9700
C(24)-H(24A)	0.9700
C(24)-H(24B)	0.9700
C(24)-H(24C)	0.9700
C(25)-C(26)	1.493(10)
C(25)-C(27)	1.541(10)
C(25)-H(25)	0.9900
C(26)-H(26A)	0.9700
C(26)-H(26B)	0.9700
C(26)-H(26C)	0.9700
C(27)-H(27A)	0.9700
C(27)-H(27B)	0.9700
C(27)-H(27C)	0.9700
C(29)-C(30)	1.330(8)
C(29)-H(29)	0.9400
C(30)-H(30)	0.9400
C(31)-C(36)	1.381(7)
C(31)-C(32)	1.413(8)
C(32)-C(33)	1.391(8)
C(32)-C(37)	1.499(8)
C(33)-C(34)	1.374(9)
C(33)-H(33)	0.9400
C(34)-C(35)	1.381(9)
C(34)-H(34)	0.9400
C(35)-C(36)	1.378(8)
C(35)-H(35)	0.9400
C(36)-C(40)	1.532(8)
C(37)-C(38)	1.501(10)
C(37)-C(39)	1.517(9)
C(37)-H(37)	0.9900
C(38)-H(38A)	0.9700
C(38)-H(38B)	0.9700
C(38)-H(38C)	0.9700
C(39)-H(39A)	0.9700

C(39)-H(39B)	0.9700
C(39)-H(39C)	0.9700
C(40)-C(42)	1.468(10)
C(40)-C(41)	1.573(10)
C(40)-H(40)	0.9900
C(41)-H(41A)	0.9700
C(41)-H(41B)	0.9700
C(41)-H(41C)	0.9700
C(42)-H(42A)	0.9700
C(42)-H(42B)	0.9700
C(42)-H(42C)	0.9700
C(43)-C(44)	1.374(8)
C(43)-C(48)	1.410(7)
C(44)-C(45)	1.404(8)
C(44)-C(49)	1.539(9)
C(45)-C(46)	1.367(10)
C(45)-H(45)	0.9400
C(46)-C(47)	1.375(10)
C(46)-H(46)	0.9400
C(47)-C(48)	1.408(8)
C(47)-H(47)	0.9400
C(48)-C(52)	1.491(9)
C(49)-C(50)	1.469(13)
C(49)-C(51)	1.566(10)
C(49)-H(49)	0.9900
C(50)-H(50A)	0.9700
C(50)-H(50B)	0.9700
C(50)-H(50C)	0.9700
C(51)-H(51A)	0.9700
C(51)-H(51B)	0.9700
C(51)-H(51C)	0.9700
C(52)-C(54)	1.441(10)
C(52)-C(53)	1.544(10)
C(52)-H(52)	0.9900
C(53)-H(53A)	0.9700
C(53)-H(53B)	0.9700
C(53)-H(53C)	0.9700
C(54)-H(54A)	0.9700
C(54)-H(54B)	0.9700
C(54)-H(54C)	0.9700
C(55)-H(55A)	0.9700
C(55)-H(55B)	0.9700
C(55)-H(55C)	0.9700
C(56)-C(57)	1.520(15)
C(56)-H(56A)	0.9800
C(56)-H(56B)	0.9800
C(57)-H(57A)	0.9700
C(57)-H(57B)	0.9700
C(57)-H(57C)	0.9700
C(58)-H(58A)	0.9700
C(58)-H(58B)	0.9700
C(58)-H(58C)	0.9700
C(59)-C(60)	1.495(9)
C(59)-H(59A)	0.9800
C(59)-H(59B)	0.9800
C(60)-H(60A)	0.9700

C(60)-H(60B)	0.9700
C(60)-H(60C)	0.9700
U(1A)-N(1A)	2.180(4)
U(1A)-N(1A)#1	2.180(4)
U(1A)-N(4A)	2.212(5)
U(1A)-N(4A)#1	2.212(5)
N(1A)-C(1A)	1.271(6)
N(2A)-C(2A)	1.373(6)
N(2A)-C(1A)	1.410(6)
N(2A)-C(4A)	1.419(6)
N(3A)-C(3A)	1.377(6)
N(3A)-C(1A)	1.390(6)
N(3A)-C(16A)	1.447(6)
N(4A)-C(29A)	1.4992(10)
N(4A)-C(28A)	1.535(11)
C(2A)-C(3A)	1.332(7)
C(2A)-H(2A)	0.9400
C(3A)-H(3A)	0.9400
C(4A)-C(5A)	1.378(8)
C(4A)-C(9A)	1.404(8)
C(5A)-C(6A)	1.403(8)
C(5A)-C(10A)	1.508(9)
C(6A)-C(7A)	1.365(10)
C(6A)-H(6A)	0.9400
C(7A)-C(8A)	1.385(10)
C(7A)-H(7A)	0.9400
C(8A)-C(9A)	1.423(9)
C(8A)-H(8A)	0.9400
C(9A)-C(13A)	1.492(10)
C(10A)-C(12A)	1.521(10)
C(10A)-C(11A)	1.565(11)
C(10A)-H(10A)	0.9900
C(11A)-H(11D)	0.9700
C(11A)-H(11E)	0.9700
C(11A)-H(11F)	0.9700
C(12A)-H(12D)	0.9700
C(12A)-H(12E)	0.9700
C(12A)-H(12F)	0.9700
C(13A)-C(14A)	1.500(11)
C(13A)-C(15A)	1.512(11)
C(13A)-H(13A)	0.9900
C(14A)-H(14D)	0.9700
C(14A)-H(14E)	0.9700
C(14A)-H(14F)	0.9700
C(15A)-H(15D)	0.9700
C(15A)-H(15E)	0.9700
C(15A)-H(15F)	0.9700
C(16A)-C(21A)	1.400(8)
C(16A)-C(17A)	1.433(7)
C(17A)-C(18A)	1.386(8)
C(17A)-C(22A)	1.507(8)
C(18A)-C(19A)	1.344(10)
C(18A)-H(18A)	0.9400
C(19A)-C(20A)	1.415(10)
C(19A)-H(19A)	0.9400
C(20A)-C(21A)	1.391(8)

C(20A)-H(20A)	0.9400
C(21A)-C(25A)	1.522(9)
C(22A)-C(24A)	1.519(9)
C(22A)-C(23A)	1.543(8)
C(22A)-H(22A)	0.9900
C(23A)-H(23D)	0.9700
C(23A)-H(23E)	0.9700
C(23A)-H(23F)	0.9700
C(24A)-H(24D)	0.9700
C(24A)-H(24E)	0.9700
C(24A)-H(24F)	0.9700
C(25A)-C(26A)	1.491(11)
C(25A)-C(27A)	1.498(12)
C(25A)-H(25A)	0.9900
C(26A)-H(26D)	0.9700
C(26A)-H(26E)	0.9700
C(26A)-H(26F)	0.9700
C(27A)-H(27D)	0.9700
C(27A)-H(27E)	0.9700
C(27A)-H(27F)	0.9700
C(28A)-H(28A)	0.9700
C(28A)-H(28B)	0.9700
C(28A)-H(28C)	0.9700
C(29A)-C(30A)	1.4989(10)
C(29A)-H(29A)	0.9800
C(29A)-H(29B)	0.9800
C(30A)-H(30A)	0.9700
C(30A)-H(30B)	0.9700
C(30A)-H(30C)	0.9700
N(1)-U(1)-N(4)	113.90(15)
N(1)-U(1)-N(7)	104.28(18)
N(4)-U(1)-N(7)	109.39(18)
N(1)-U(1)-N(8)	112.91(17)
N(4)-U(1)-N(8)	106.22(19)
N(7)-U(1)-N(8)	110.1(2)
C(1)-N(1)-U(1)	170.4(4)
C(2)-N(2)-C(1)	111.2(5)
C(2)-N(2)-C(4)	122.8(5)
C(1)-N(2)-C(4)	124.1(4)
C(3)-N(3)-C(16)	126.0(5)
C(3)-N(3)-C(1)	109.1(5)
C(16)-N(3)-C(1)	124.4(4)
C(28)-N(4)-U(1)	172.3(4)
C(28)-N(5)-C(29)	110.0(4)
C(28)-N(5)-C(31)	125.6(4)
C(29)-N(5)-C(31)	122.3(4)
C(28)-N(6)-C(30)	110.2(4)
C(28)-N(6)-C(43)	125.4(4)
C(30)-N(6)-C(43)	123.5(4)
C(56)-N(7)-C(55)	113.3(7)
C(56)-N(7)-U(1)	133.5(6)
C(55)-N(7)-U(1)	112.8(5)
C(59)-N(8)-C(58)	109.6(5)
C(59)-N(8)-U(1)	128.2(4)
C(58)-N(8)-U(1)	122.2(5)

N(1)-C(1)-N(2)	129.7(5)
N(1)-C(1)-N(3)	127.1(5)
N(2)-C(1)-N(3)	103.1(4)
C(3)-C(2)-N(2)	108.6(5)
C(3)-C(2)-H(2)	125.7
N(2)-C(2)-H(2)	125.7
C(2)-C(3)-N(3)	107.8(5)
C(2)-C(3)-H(3)	126.1
N(3)-C(3)-H(3)	126.1
C(5)-C(4)-C(9)	123.3(5)
C(5)-C(4)-N(2)	119.7(5)
C(9)-C(4)-N(2)	117.0(6)
C(6)-C(5)-C(4)	117.3(6)
C(6)-C(5)-C(10)	121.6(6)
C(4)-C(5)-C(10)	121.1(5)
C(7)-C(6)-C(5)	122.4(7)
C(7)-C(6)-H(6)	118.8
C(5)-C(6)-H(6)	118.8
C(8)-C(7)-C(6)	119.3(6)
C(8)-C(7)-H(7)	120.3
C(6)-C(7)-H(7)	120.3
C(7)-C(8)-C(9)	122.9(6)
C(7)-C(8)-H(8)	118.6
C(9)-C(8)-H(8)	118.6
C(4)-C(9)-C(8)	114.8(6)
C(4)-C(9)-C(13)	124.3(6)
C(8)-C(9)-C(13)	120.7(6)
C(12)-C(10)-C(5)	113.0(6)
C(12)-C(10)-C(11)	112.5(10)
C(5)-C(10)-C(11)	108.4(6)
C(12)-C(10)-H(10)	107.6
C(5)-C(10)-H(10)	107.6
C(11)-C(10)-H(10)	107.6
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(9)-C(13)-C(15)	111.7(7)
C(9)-C(13)-C(14)	114.2(9)
C(15)-C(13)-C(14)	111.0(9)
C(9)-C(13)-H(13)	106.5
C(15)-C(13)-H(13)	106.5
C(14)-C(13)-H(13)	106.5
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5

H(14B)-C(14)-H(14C)	109.5
C(13)-C(15)-H(15A)	109.5
C(13)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(13)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(17)-C(16)-C(21)	120.6(6)
C(17)-C(16)-N(3)	120.5(5)
C(21)-C(16)-N(3)	118.9(5)
C(18)-C(17)-C(16)	119.2(6)
C(18)-C(17)-C(22)	121.5(6)
C(16)-C(17)-C(22)	119.2(6)
C(19)-C(18)-C(17)	120.7(7)
C(19)-C(18)-H(18)	119.6
C(17)-C(18)-H(18)	119.6
C(18)-C(19)-C(20)	121.4(7)
C(18)-C(19)-H(19)	119.3
C(20)-C(19)-H(19)	119.3
C(19)-C(20)-C(21)	120.3(7)
C(19)-C(20)-H(20)	119.9
C(21)-C(20)-H(20)	119.9
C(20)-C(21)-C(16)	117.8(6)
C(20)-C(21)-C(25)	120.2(6)
C(16)-C(21)-C(25)	122.1(5)
C(23)-C(22)-C(24)	110.8(8)
C(23)-C(22)-C(17)	112.7(8)
C(24)-C(22)-C(17)	111.4(7)
C(23)-C(22)-H(22)	107.2
C(24)-C(22)-H(22)	107.2
C(17)-C(22)-H(22)	107.2
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(22)-C(24)-H(24A)	109.5
C(22)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(22)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(26)-C(25)-C(21)	115.0(6)
C(26)-C(25)-C(27)	108.8(6)
C(21)-C(25)-C(27)	111.9(6)
C(26)-C(25)-H(25)	106.9
C(21)-C(25)-H(25)	106.9
C(27)-C(25)-H(25)	106.9
C(25)-C(26)-H(26A)	109.5
C(25)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(25)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(25)-C(27)-H(27A)	109.5

C(25)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(25)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
N(4)-C(28)-N(5)	128.5(4)
N(4)-C(28)-N(6)	127.6(4)
N(5)-C(28)-N(6)	104.0(4)
C(30)-C(29)-N(5)	108.4(5)
C(30)-C(29)-H(29)	125.8
N(5)-C(29)-H(29)	125.8
C(29)-C(30)-N(6)	107.4(4)
C(29)-C(30)-H(30)	126.3
N(6)-C(30)-H(30)	126.3
C(36)-C(31)-C(32)	122.7(5)
C(36)-C(31)-N(5)	119.1(5)
C(32)-C(31)-N(5)	118.1(5)
C(33)-C(32)-C(31)	116.5(5)
C(33)-C(32)-C(37)	121.6(5)
C(31)-C(32)-C(37)	121.8(5)
C(34)-C(33)-C(32)	121.0(6)
C(34)-C(33)-H(33)	119.5
C(32)-C(33)-H(33)	119.5
C(33)-C(34)-C(35)	120.8(6)
C(33)-C(34)-H(34)	119.6
C(35)-C(34)-H(34)	119.6
C(36)-C(35)-C(34)	120.5(6)
C(36)-C(35)-H(35)	119.7
C(34)-C(35)-H(35)	119.7
C(35)-C(36)-C(31)	118.2(5)
C(35)-C(36)-C(40)	119.1(5)
C(31)-C(36)-C(40)	122.7(5)
C(32)-C(37)-C(38)	113.2(5)
C(32)-C(37)-C(39)	110.8(6)
C(38)-C(37)-C(39)	111.9(7)
C(32)-C(37)-H(37)	106.8
C(38)-C(37)-H(37)	106.8
C(39)-C(37)-H(37)	106.8
C(37)-C(38)-H(38A)	109.5
C(37)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(37)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(37)-C(39)-H(39A)	109.5
C(37)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(37)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(42)-C(40)-C(36)	113.9(6)
C(42)-C(40)-C(41)	112.9(6)
C(36)-C(40)-C(41)	108.2(5)
C(42)-C(40)-H(40)	107.2
C(36)-C(40)-H(40)	107.2
C(41)-C(40)-H(40)	107.2

C(40)-C(41)-H(41A)	109.5
C(40)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
C(40)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
C(40)-C(42)-H(42A)	109.5
C(40)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(40)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(44)-C(43)-C(48)	123.0(5)
C(44)-C(43)-N(6)	119.8(5)
C(48)-C(43)-N(6)	117.1(5)
C(43)-C(44)-C(45)	118.2(6)
C(43)-C(44)-C(49)	122.3(5)
C(45)-C(44)-C(49)	119.5(5)
C(46)-C(45)-C(44)	121.0(6)
C(46)-C(45)-H(45)	119.5
C(44)-C(45)-H(45)	119.5
C(45)-C(46)-C(47)	119.5(6)
C(45)-C(46)-H(46)	120.2
C(47)-C(46)-H(46)	120.2
C(46)-C(47)-C(48)	122.7(6)
C(46)-C(47)-H(47)	118.7
C(48)-C(47)-H(47)	118.7
C(47)-C(48)-C(43)	115.5(6)
C(47)-C(48)-C(52)	120.9(5)
C(43)-C(48)-C(52)	123.6(5)
C(50)-C(49)-C(44)	110.7(6)
C(50)-C(49)-C(51)	107.7(8)
C(44)-C(49)-C(51)	111.1(6)
C(50)-C(49)-H(49)	109.1
C(44)-C(49)-H(49)	109.1
C(51)-C(49)-H(49)	109.1
C(49)-C(50)-H(50A)	109.5
C(49)-C(50)-H(50B)	109.5
H(50A)-C(50)-H(50B)	109.5
C(49)-C(50)-H(50C)	109.5
H(50A)-C(50)-H(50C)	109.5
H(50B)-C(50)-H(50C)	109.5
C(49)-C(51)-H(51A)	109.5
C(49)-C(51)-H(51B)	109.5
H(51A)-C(51)-H(51B)	109.5
C(49)-C(51)-H(51C)	109.5
H(51A)-C(51)-H(51C)	109.5
H(51B)-C(51)-H(51C)	109.5
C(54)-C(52)-C(48)	111.9(5)
C(54)-C(52)-C(53)	110.7(6)
C(48)-C(52)-C(53)	111.6(6)
C(54)-C(52)-H(52)	107.5
C(48)-C(52)-H(52)	107.5
C(53)-C(52)-H(52)	107.5
C(52)-C(53)-H(53A)	109.5
C(52)-C(53)-H(53B)	109.5

H(53A)-C(53)-H(53B)	109.5
C(52)-C(53)-H(53C)	109.5
H(53A)-C(53)-H(53C)	109.5
H(53B)-C(53)-H(53C)	109.5
C(52)-C(54)-H(54A)	109.5
C(52)-C(54)-H(54B)	109.5
H(54A)-C(54)-H(54B)	109.5
C(52)-C(54)-H(54C)	109.5
H(54A)-C(54)-H(54C)	109.5
H(54B)-C(54)-H(54C)	109.5
N(7)-C(55)-H(55A)	109.5
N(7)-C(55)-H(55B)	109.5
H(55A)-C(55)-H(55B)	109.5
N(7)-C(55)-H(55C)	109.5
H(55A)-C(55)-H(55C)	109.5
H(55B)-C(55)-H(55C)	109.5
N(7)-C(56)-C(57)	113.6(9)
N(7)-C(56)-H(56A)	108.8
C(57)-C(56)-H(56A)	108.8
N(7)-C(56)-H(56B)	108.8
C(57)-C(56)-H(56B)	108.8
H(56A)-C(56)-H(56B)	107.7
C(56)-C(57)-H(57A)	109.5
C(56)-C(57)-H(57B)	109.5
H(57A)-C(57)-H(57B)	109.5
C(56)-C(57)-H(57C)	109.5
H(57A)-C(57)-H(57C)	109.5
H(57B)-C(57)-H(57C)	109.5
N(8)-C(58)-H(58A)	109.5
N(8)-C(58)-H(58B)	109.5
H(58A)-C(58)-H(58B)	109.5
N(8)-C(58)-H(58C)	109.5
H(58A)-C(58)-H(58C)	109.5
H(58B)-C(58)-H(58C)	109.5
N(8)-C(59)-C(60)	110.6(5)
N(8)-C(59)-H(59A)	109.5
C(60)-C(59)-H(59A)	109.5
N(8)-C(59)-H(59B)	109.5
C(60)-C(59)-H(59B)	109.5
H(59A)-C(59)-H(59B)	108.1
C(59)-C(60)-H(60A)	109.5
C(59)-C(60)-H(60B)	109.5
H(60A)-C(60)-H(60B)	109.5
C(59)-C(60)-H(60C)	109.5
H(60A)-C(60)-H(60C)	109.5
H(60B)-C(60)-H(60C)	109.5
N(1A)-U(1A)-N(1A)#1	123.1(2)
N(1A)-U(1A)-N(4A)	109.83(17)
N(1A)#1-U(1A)-N(4A)	100.54(18)
N(1A)-U(1A)-N(4A)#1	100.55(18)
N(1A)#1-U(1A)-N(4A)#1	109.83(17)
N(4A)-U(1A)-N(4A)#1	113.6(3)
C(1A)-N(1A)-U(1A)	167.7(4)
C(2A)-N(2A)-C(1A)	110.1(4)
C(2A)-N(2A)-C(4A)	123.0(4)
C(1A)-N(2A)-C(4A)	126.7(4)

C(3A)-N(3A)-C(1A)	111.9(4)
C(3A)-N(3A)-C(16A)	121.5(4)
C(1A)-N(3A)-C(16A)	126.6(4)
C(29A)-N(4A)-C(28A)	122.6(8)
C(29A)-N(4A)-U(1A)	112.2(6)
C(28A)-N(4A)-U(1A)	120.5(6)
N(1A)-C(1A)-N(3A)	129.5(4)
N(1A)-C(1A)-N(2A)	128.4(4)
N(3A)-C(1A)-N(2A)	102.1(4)
C(3A)-C(2A)-N(2A)	108.9(4)
C(3A)-C(2A)-H(2A)	125.5
N(2A)-C(2A)-H(2A)	125.5
C(2A)-C(3A)-N(3A)	106.9(5)
C(2A)-C(3A)-H(3A)	126.5
N(3A)-C(3A)-H(3A)	126.5
C(5A)-C(4A)-C(9A)	122.4(5)
C(5A)-C(4A)-N(2A)	119.6(5)
C(9A)-C(4A)-N(2A)	117.8(5)
C(4A)-C(5A)-C(6A)	119.3(6)
C(4A)-C(5A)-C(10A)	121.4(5)
C(6A)-C(5A)-C(10A)	119.3(5)
C(7A)-C(6A)-C(5A)	119.5(6)
C(7A)-C(6A)-H(6A)	120.2
C(5A)-C(6A)-H(6A)	120.2
C(6A)-C(7A)-C(8A)	121.8(6)
C(6A)-C(7A)-H(7A)	119.1
C(8A)-C(7A)-H(7A)	119.1
C(7A)-C(8A)-C(9A)	120.0(6)
C(7A)-C(8A)-H(8A)	120.0
C(9A)-C(8A)-H(8A)	120.0
C(4A)-C(9A)-C(8A)	116.8(6)
C(4A)-C(9A)-C(13A)	122.9(5)
C(8A)-C(9A)-C(13A)	120.3(6)
C(5A)-C(10A)-C(12A)	111.7(6)
C(5A)-C(10A)-C(11A)	112.3(6)
C(12A)-C(10A)-C(11A)	110.0(6)
C(5A)-C(10A)-H(10A)	107.5
C(12A)-C(10A)-H(10A)	107.5
C(11A)-C(10A)-H(10A)	107.5
C(10A)-C(11A)-H(11D)	109.5
C(10A)-C(11A)-H(11E)	109.5
H(11D)-C(11A)-H(11E)	109.5
C(10A)-C(11A)-H(11F)	109.5
H(11D)-C(11A)-H(11F)	109.5
H(11E)-C(11A)-H(11F)	109.5
C(10A)-C(12A)-H(12D)	109.5
C(10A)-C(12A)-H(12E)	109.5
H(12D)-C(12A)-H(12E)	109.5
C(10A)-C(12A)-H(12F)	109.5
H(12D)-C(12A)-H(12F)	109.5
H(12E)-C(12A)-H(12F)	109.5
C(9A)-C(13A)-C(14A)	113.2(7)
C(9A)-C(13A)-C(15A)	110.5(7)
C(14A)-C(13A)-C(15A)	112.7(8)
C(9A)-C(13A)-H(13A)	106.6
C(14A)-C(13A)-H(13A)	106.6

C(15A)-C(13A)-H(13A)	106.6
C(13A)-C(14A)-H(14D)	109.5
C(13A)-C(14A)-H(14E)	109.5
H(14D)-C(14A)-H(14E)	109.5
C(13A)-C(14A)-H(14F)	109.5
H(14D)-C(14A)-H(14F)	109.5
H(14E)-C(14A)-H(14F)	109.5
C(13A)-C(15A)-H(15D)	109.5
C(13A)-C(15A)-H(15E)	109.5
H(15D)-C(15A)-H(15E)	109.5
C(13A)-C(15A)-H(15F)	109.5
H(15D)-C(15A)-H(15F)	109.5
H(15E)-C(15A)-H(15F)	109.5
C(21A)-C(16A)-C(17A)	122.8(5)
C(21A)-C(16A)-N(3A)	118.4(4)
C(17A)-C(16A)-N(3A)	118.8(5)
C(18A)-C(17A)-C(16A)	115.7(5)
C(18A)-C(17A)-C(22A)	123.7(5)
C(16A)-C(17A)-C(22A)	120.6(5)
C(19A)-C(18A)-C(17A)	124.0(6)
C(19A)-C(18A)-H(18A)	118.0
C(17A)-C(18A)-H(18A)	118.0
C(18A)-C(19A)-C(20A)	119.1(6)
C(18A)-C(19A)-H(19A)	120.4
C(20A)-C(19A)-H(19A)	120.4
C(21A)-C(20A)-C(19A)	121.3(6)
C(21A)-C(20A)-H(20A)	119.4
C(19A)-C(20A)-H(20A)	119.4
C(20A)-C(21A)-C(16A)	117.1(6)
C(20A)-C(21A)-C(25A)	120.3(6)
C(16A)-C(21A)-C(25A)	122.6(5)
C(17A)-C(22A)-C(24A)	110.7(5)
C(17A)-C(22A)-C(23A)	112.5(6)
C(24A)-C(22A)-C(23A)	109.4(5)
C(17A)-C(22A)-H(22A)	108.0
C(24A)-C(22A)-H(22A)	108.0
C(23A)-C(22A)-H(22A)	108.0
C(22A)-C(23A)-H(23D)	109.5
C(22A)-C(23A)-H(23E)	109.5
H(23D)-C(23A)-H(23E)	109.5
C(22A)-C(23A)-H(23F)	109.5
H(23D)-C(23A)-H(23F)	109.5
H(23E)-C(23A)-H(23F)	109.5
C(22A)-C(24A)-H(24D)	109.5
C(22A)-C(24A)-H(24E)	109.5
H(24D)-C(24A)-H(24E)	109.5
C(22A)-C(24A)-H(24F)	109.5
H(24D)-C(24A)-H(24F)	109.5
H(24E)-C(24A)-H(24F)	109.5
C(26A)-C(25A)-C(27A)	109.3(7)
C(26A)-C(25A)-C(21A)	113.9(6)
C(27A)-C(25A)-C(21A)	111.1(6)
C(26A)-C(25A)-H(25A)	107.4
C(27A)-C(25A)-H(25A)	107.4
C(21A)-C(25A)-H(25A)	107.4
C(25A)-C(26A)-H(26D)	109.5

C(25A)-C(26A)-H(26E)	109.5
H(26D)-C(26A)-H(26E)	109.5
C(25A)-C(26A)-H(26F)	109.5
H(26D)-C(26A)-H(26F)	109.5
H(26E)-C(26A)-H(26F)	109.5
C(25A)-C(27A)-H(27D)	109.5
C(25A)-C(27A)-H(27E)	109.5
H(27D)-C(27A)-H(27E)	109.5
C(25A)-C(27A)-H(27F)	109.5
H(27D)-C(27A)-H(27F)	109.5
H(27E)-C(27A)-H(27F)	109.5
N(4A)-C(28A)-H(28A)	109.5
N(4A)-C(28A)-H(28B)	109.5
H(28A)-C(28A)-H(28B)	109.5
N(4A)-C(28A)-H(28C)	109.5
H(28A)-C(28A)-H(28C)	109.5
H(28B)-C(28A)-H(28C)	109.5
C(30A)-C(29A)-N(4A)	111.8(8)
C(30A)-C(29A)-H(29A)	109.3
N(4A)-C(29A)-H(29A)	109.3
C(30A)-C(29A)-H(29B)	109.3
N(4A)-C(29A)-H(29B)	109.3
H(29A)-C(29A)-H(29B)	107.9
C(29A)-C(30A)-H(30A)	109.5
C(29A)-C(30A)-H(30B)	109.5
H(30A)-C(30A)-H(30B)	109.5
C(29A)-C(30A)-H(30C)	109.5
H(30A)-C(30A)-H(30C)	109.5
H(30B)-C(30A)-H(30C)	109.5

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+1/2

Table 14: Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Complex 3.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2hka^*b^*U_{12}]$$

	U11	U22	U33	U23	U13	U12
U(1)	33(1)	34(1)	31(1)	-1(1)	7(1)	3(1)
N(1)	44(2)	41(2)	41(2)	-7(2)	16(2)	-5(2)
N(2)	65(3)	37(2)	53(3)	-5(2)	34(2)	9(2)
N(3)	48(2)	47(2)	40(2)	-12(2)	13(2)	21(2)
N(4)	40(2)	38(2)	35(2)	2(2)	9(2)	6(2)
N(5)	29(2)	46(2)	37(2)	9(2)	6(2)	5(2)

N(6)	43(2)	44(2)	29(2)	2(2)	11(2)	6(2)
N(7)	75(3)	54(3)	54(3)	14(2)	24(3)	2(3)
N(8)	43(2)	46(3)	81(4)	-1(2)	23(2)	4(2)
C(1)	53(3)	40(3)	34(3)	-2(2)	17(2)	8(2)
C(2)	102(5)	53(3)	59(4)	-22(3)	43(4)	27(4)
C(3)	84(5)	58(4)	63(4)	-26(3)	33(4)	31(3)
C(4)	69(4)	32(2)	56(3)	-3(2)	39(3)	1(2)
C(5)	66(4)	40(3)	50(3)	-2(2)	34(3)	2(2)
C(6)	69(4)	54(4)	76(4)	-2(3)	42(4)	6(3)
C(7)	80(5)	60(4)	73(4)	9(3)	50(4)	2(3)
C(8)	105(6)	52(4)	69(4)	13(3)	52(4)	6(4)
C(9)	81(4)	51(3)	54(3)	5(3)	36(3)	0(3)
C(10)	90(5)	66(4)	66(4)	9(3)	46(4)	4(4)
C(11)	370(20)	76(6)	194(13)	83(7)	210(16)	105(10)
C(12)	66(5)	244(15)	70(6)	36(7)	8(4)	21(7)
C(13)	86(5)	94(6)	65(4)	25(4)	22(4)	13(4)
C(14)	154(11)	230(15)	70(6)	-3(8)	27(7)	35(11)
C(15)	88(6)	104(7)	113(8)	38(6)	13(5)	12(5)
C(16)	41(3)	49(3)	44(3)	-11(2)	9(2)	14(2)
C(17)	53(3)	60(4)	63(4)	-5(3)	11(3)	14(3)
C(18)	50(4)	84(5)	71(5)	-6(4)	10(3)	2(3)
C(19)	52(4)	77(5)	101(6)	-20(4)	32(4)	11(4)
C(20)	50(3)	71(4)	76(4)	-14(3)	30(3)	19(3)
C(21)	49(3)	54(3)	56(3)	-13(3)	23(3)	25(3)
C(22)	65(4)	86(5)	62(4)	13(4)	7(3)	5(4)
C(23)	181(12)	75(6)	91(7)	16(5)	14(7)	9(6)
C(24)	149(9)	128(8)	60(5)	-2(5)	3(6)	23(7)
C(25)	59(4)	77(4)	77(4)	-4(4)	39(3)	18(3)
C(26)	78(5)	81(5)	91(6)	25(4)	40(4)	8(4)
C(27)	102(6)	62(4)	126(8)	-1(5)	60(6)	1(4)
C(28)	29(2)	31(2)	31(2)	0(2)	10(2)	1(2)
C(29)	43(3)	65(4)	33(3)	5(2)	3(2)	12(2)
C(30)	32(2)	57(3)	42(3)	2(2)	3(2)	12(2)
C(31)	32(2)	48(3)	36(2)	7(2)	9(2)	5(2)
C(32)	38(3)	48(3)	45(3)	13(2)	12(2)	1(2)
C(33)	58(4)	50(3)	59(4)	12(3)	22(3)	13(3)
C(34)	55(3)	70(4)	68(4)	10(3)	29(3)	15(3)
C(35)	52(3)	72(4)	63(4)	-1(3)	29(3)	4(3)
C(36)	32(2)	50(3)	43(3)	-1(2)	12(2)	5(2)
C(37)	58(3)	49(3)	49(3)	12(2)	22(3)	7(3)
C(38)	92(5)	79(5)	105(6)	-28(5)	57(5)	14(4)
C(39)	76(5)	169(9)	110(7)	42(7)	43(5)	76(6)
C(40)	49(3)	63(4)	76(4)	-16(3)	31(3)	13(3)
C(41)	68(4)	60(4)	98(6)	-2(4)	35(4)	3(3)
C(42)	136(8)	93(6)	74(5)	-32(5)	26(5)	19(6)
C(43)	39(2)	38(3)	40(3)	0(2)	11(2)	8(2)
C(44)	64(4)	50(3)	51(3)	-1(3)	29(3)	11(3)
C(45)	81(5)	67(4)	68(4)	1(3)	49(4)	11(4)
C(46)	96(5)	54(4)	62(4)	17(3)	34(4)	11(4)
C(47)	76(4)	44(3)	68(4)	11(3)	31(3)	8(3)
C(48)	45(3)	39(3)	47(3)	4(2)	8(2)	5(2)
C(49)	87(5)	58(4)	76(5)	2(3)	51(4)	4(3)
C(50)	181(12)	125(8)	120(9)	-61(7)	-65(8)	93(8)
C(51)	122(7)	90(6)	78(6)	-23(4)	43(5)	6(5)
C(52)	50(3)	48(3)	64(4)	-1(3)	23(3)	3(3)
C(53)	64(4)	94(6)	91(6)	-1(5)	22(4)	9(4)

C(54)	76(5)	120(7)	96(6)	-34(5)	44(5)	10(5)
C(55)	97(6)	176(11)	75(6)	7(6)	43(5)	31(7)
C(56)	155(9)	82(6)	65(5)	20(4)	26(6)	14(6)
C(57)	320(20)	91(7)	91(8)	28(6)	35(11)	9(10)
C(58)	95(6)	52(4)	180(10)	0(5)	76(7)	15(4)
C(59)	45(3)	75(4)	57(4)	-10(3)	17(3)	3(3)
C(60)	63(4)	71(4)	92(5)	-13(4)	36(4)	13(3)
U(1A)	41(1)	47(1)	34(1)	0	24(1)	0
N(1A)	47(2)	52(2)	34(2)	0(2)	24(2)	0(2)
N(2A)	43(2)	38(2)	44(2)	-3(2)	23(2)	6(2)
N(3A)	43(2)	44(2)	36(2)	-7(2)	23(2)	9(2)
N(4A)	67(3)	67(3)	41(3)	-6(2)	20(2)	16(3)
C(1A)	26(2)	43(3)	31(2)	-2(2)	9(2)	1(2)
C(2A)	51(3)	55(3)	48(3)	-9(2)	31(3)	22(3)
C(3A)	56(3)	60(3)	47(3)	-9(3)	37(3)	13(3)
C(4A)	56(3)	44(3)	39(3)	-6(2)	26(2)	8(2)
C(5A)	55(3)	53(3)	44(3)	-11(3)	20(3)	10(3)
C(6A)	67(4)	67(4)	58(4)	-25(3)	23(3)	25(3)
C(7A)	76(4)	54(4)	80(5)	-27(3)	38(4)	10(3)
C(8A)	72(4)	61(4)	76(5)	-8(3)	39(4)	2(3)
C(9A)	51(3)	49(3)	68(4)	2(3)	35(3)	3(3)
C(10A)	71(4)	60(4)	44(3)	0(3)	5(3)	3(3)
C(11A)	74(5)	112(7)	115(7)	38(6)	37(5)	22(5)
C(12A)	116(7)	106(6)	56(4)	6(4)	14(4)	22(5)
C(13A)	60(4)	71(4)	72(5)	5(3)	23(3)	17(3)
C(14A)	121(8)	123(8)	87(6)	25(6)	25(6)	1(6)
C(15A)	56(5)	168(11)	106(8)	-13(6)	27(5)	26(5)
C(16A)	41(3)	45(3)	34(2)	-10(2)	19(2)	7(2)
C(17A)	44(3)	61(3)	42(3)	-12(2)	25(2)	14(3)
C(18A)	56(4)	78(5)	47(3)	-24(3)	17(3)	14(3)
C(19A)	77(5)	58(4)	96(6)	-30(4)	42(4)	12(4)
C(20A)	77(4)	54(4)	68(4)	-11(3)	30(4)	4(3)
C(21A)	55(3)	48(3)	50(3)	-9(2)	30(3)	5(3)
C(22A)	46(3)	73(4)	33(3)	3(3)	10(2)	9(3)
C(23A)	87(5)	120(7)	49(4)	3(4)	18(4)	22(5)
C(24A)	53(4)	87(5)	52(4)	10(3)	11(3)	19(3)
C(25A)	68(4)	72(4)	55(4)	-6(3)	12(3)	12(3)
C(26A)	99(6)	92(6)	77(5)	1(4)	26(5)	13(5)
C(27A)	63(5)	174(10)	98(7)	18(7)	-1(5)	20(6)
C(28A)	106(7)	215(13)	53(5)	14(6)	26(5)	6(8)
C(29A)	221(16)	152(11)	107(9)	-39(8)	90(10)	36(11)
C(30A)	277(19)	93(8)	157(12)	5(8)	132(14)	13(10)

Table 15: Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Complex 3.

	x	y	z	U(eq)
H(2)	1963	12814	2035	81
H(3)	2434	12991	1869	80

H(6)	817	10840	1317	74
H(7)	914	10066	1963	78
H(8)	1423	9841	2433	83
H(10)	1380	11613	902	83
H(11A)	1144	13324	790	276
H(11B)	1390	13191	1263	276
H(11C)	1021	13113	1159	276
H(12A)	875	11736	383	198
H(12B)	726	11466	722	198
H(12C)	930	10600	602	198
H(13)	2122	10815	2312	101
H(14A)	2262	10522	3038	234
H(14B)	1905	10228	2960	234
H(14C)	1993	11403	2876	234
H(15A)	2298	9112	2563	164
H(15B)	2061	9070	2081	164
H(15C)	1942	8733	2444	164
H(18)	3098	9857	1461	87
H(19)	3143	10850	932	91
H(20)	2791	12202	618	76
H(22)	2474	10036	1851	91
H(23A)	2632	8522	1591	191
H(23B)	2734	8457	2090	191
H(23C)	2989	8739	1894	191
H(24A)	2846	11214	2299	185
H(24B)	3126	10432	2325	185
H(24C)	2877	10091	2523	185
H(25)	2087	12743	792	81
H(26A)	2062	13635	189	122
H(26B)	2125	12406	152	122
H(26C)	2407	13232	256	122
H(27A)	2237	14549	842	138
H(27B)	2597	14214	971	138
H(27C)	2419	13957	1278	138
H(29)	756	8942	-1138	60
H(30)	513	7651	-821	56
H(33)	1639	12069	-587	67
H(34)	1914	11232	-942	75
H(35)	1837	9443	-1107	73
H(37)	1157	10756	-126	62
H(38A)	1273	12451	162	130
H(38B)	1471	12686	-122	130
H(38C)	1588	11803	236	130
H(39A)	787	12096	-451	174
H(39B)	778	11196	-781	174
H(39C)	950	12292	-781	174
H(40)	1304	7723	-880	73
H(41A)	1800	7625	-292	112
H(41B)	1983	7641	-604	112
H(41C)	1767	6654	-602	112
H(42A)	1274	8041	-1555	157
H(42B)	1434	6923	-1390	157
H(42C)	1647	7909	-1402	157
H(45)	454	6637	608	79
H(46)	717	5034	688	83
H(47)	1068	4761	361	74

H(49)	597	8980	105	81
H(50A)	50	9054	-115	268
H(50B)	41	7829	-9	268
H(50C)	147	8187	-380	268
H(51A)	696	8768	852	143
H(51B)	353	8266	725	143
H(51C)	390	9474	620	143
H(52)	1303	6687	-237	64
H(53A)	1656	5994	427	128
H(53B)	1723	5494	43	128
H(53C)	1536	4829	267	128
H(54A)	1276	5178	-622	141
H(54B)	935	5651	-707	141
H(54C)	1057	4641	-412	141
H(55A)	1293	8385	1096	170
H(55B)	1445	8074	1582	170
H(55C)	1280	7190	1237	170
H(56A)	1929	7028	1843	127
H(56B)	2111	6788	1540	127
H(57A)	1896	5208	1668	272
H(57B)	1721	5497	1181	272
H(57C)	1551	5718	1501	272
H(58A)	2236	6704	951	153
H(58B)	2572	7159	996	153
H(58C)	2343	6658	560	153
H(59A)	2389	8218	223	72
H(59B)	2596	8803	652	72
H(60A)	2339	10055	128	110
H(60B)	2214	10146	501	110
H(60C)	2006	9561	73	110
H(2A)	940	7906	1787	57
H(3A)	846	6212	1410	59
H(6A)	1072	9412	3215	77
H(7A)	706	10739	2932	81
H(8A)	295	10547	2278	80
H(10A)	1034	6827	2749	76
H(11D)	1435	7889	2649	150
H(11E)	1589	7125	3045	150
H(11F)	1536	8345	3116	150
H(12D)	923	7029	3363	147
H(12E)	1217	7809	3556	147
H(12F)	1273	6596	3479	147
H(13A)	185	8246	1605	82
H(14D)	-60	9654	1165	172
H(14E)	311	9846	1385	172
H(14F)	77	10454	1551	172
H(15D)	-139	8107	1989	167
H(15E)	-334	8531	1524	167
H(15F)	-225	9332	1912	167
H(18A)	-73	3671	733	73
H(19A)	182	2179	1059	89
H(20A)	597	2299	1731	79
H(22A)	154	6335	1018	63
H(23D)	-10	5469	352	131
H(23E)	-273	6294	352	131
H(23F)	-322	5061	405	131

H(24D)	-354	6678	1010	100
H(24E)	-139	6142	1446	100
H(24F)	-398	5457	1090	100
H(25A)	862	4635	2344	82
H(26D)	1085	3164	2759	138
H(26E)	920	2405	2365	138
H(26F)	710	3065	2558	138
H(27D)	1367	4085	2413	182
H(27E)	1191	4668	1974	182
H(27F)	1218	3410	1991	182
H(28A)	-748	5267	1952	189
H(28B)	-850	4172	1707	189
H(28C)	-712	5099	1512	189
H(29A)	-283	3646	1511	182
H(29B)	17	3579	1943	182
H(30A)	-202	1896	1763	241
H(30B)	-535	2318	1743	241
H(30C)	-242	2266	2184	241

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