Application of Imidazolinium Salts and N-Heterocyclic Olefins for the Synthesis of Anionic and Neutral Tungsten Imido Alkylidene Complexes

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Experimental

General. All manipulations of moisture and air sensitive materials were performed under a nitrogen atmosphere with standard Schlenk techniques or in a N_2-filled glove box (Lab Master 130, MBraun, Garching, Germany). Methylene chloride, diethyl ether, toluene, pentane and tetrahydrofuran were dried by a solvent purification system (SPS, MBraun). 1,2-Dimethoxyethane (DME) and benzene were vacuum distilled from a dark purple solution of sodium benzophenone ketyl, and degassed three times by freeze-pump-thaw technique. Starting materials and all reagents were purchased from Sigma-Aldrich (Munich, Germany), Alfa Aesar (Karlsruhe, Germany), ABCR (Karlsruhe, Germany) and Acros Chemicals (Geel, Belgium), dried and, where appropriate, distilled prior to use. NMR measurements were recorded on a Bruker Avance III 400. Chemical shifts are reported in ppm relative to the solvent signal. GC-MS data were recorded on an Agilent Technologies device consisting of a 7693 autosampler, a 7890 A GC and a 5975C quadrupole MS. Dodecane was used as internal standard. An SPB-5 fused silica column (34.13 m x 0.25 mm x 0.25 mm film thickness) was used. The injection temperature was set to 150°C. The column temperature ramped from 45°C to 250°C within eight minutes and was then held for further five minutes. The column flow was 1.05 mL per minute. All substrates for HM, CM, RCM, and SM were either distilled from CaH_2 or recrystallized and stored under nitrogen.

[1,3-Bis-(2,4,6-trimethylphenyl)imidazolinium$^+$ W(2,6-$iPr_2C_6H_3$)(CHCMe$_2$Ph)(2,5-$Me_2Pyr)_2Cl^-$] (2). A suspension of 1,3-Bis-(2,4,6-trimethylphenyl)imidazolinium chloride (103 mg, 0.3 mmol) in 4 mL benzene was added to a stirred solution of W(2,6-$iPr_2C_6H_3$)(CHCMe$_2$Ph)(2,5-$Me_2NC_4H_4)_2$ (200 mg, 0.3 mmol) in 5 mL benzene. The reaction mixture was stirred for 1 h at room temperature. All volatiles were removed from the yellow solution *in vacuo*. The yellow solid was washed several times with pentane and crystallized from a mixture of methylene chloride and diethyl ether to get analytically pure product; yield 245 mg (80 %): 1H NMR (400 MHz, CD_2Cl_2) δ = 10.85 (s, 1H, W=CH), 7.42 (d, 2H, Ar, J = 7.35 Hz), 7.31 - 7.17 (m, 6H, Ar), 7.02 (s, 4H, Ar), 6.98 (s, 1H, NCHN), 5.49 (brs, 4H, NC_4H_2), 4.15 (s, 4H, NC_2H_4N), 3.01 (brs, 4H, iPr), 2.35 (s, 6H, Me), 2.32 (s, 6H, Me), 1.96 (brs, 12H,

Me), 1.75 (brs, 6H, Me), 1.59 (s, 6H, Me), 0.88 (brs, 12H, iPr); ^{13}C NMR (100 MHz, CD_2Cl_2) δ = 273.6 (W=*C*), 160.4 (N*C*N), 153.0 (C_{ipso}), 151.5 ($C_{ArImido}$), 149.3 (NC_{Mes}), 141.1 (C_{Ar}), 135.9 (C_{Ar}), 134.4 (C_{Ar}), 131.1 (C_{Ar}), 130.5 (C_{Ar}), 128.5 (C_{Ar}), 126.5 (C_{Ar}), 126.0 (C_{Ar}), 123.6 (C_{Ar}), 106.6 (C_{pyr}), 106.2 (C_{pyr}), 105.8 (C_{pyr}), 51.9 (*C*Me_2Ph), 33.7 (N*C*H_2), 27.7 (C*Me*$_2$Ph), 26.8 (C*Me*$_2$Ph), 25.8 (Me), 24.7 (Me), 21.4 (Me), 20.4 (Me), 18.6 (Me), 18.2 (Me); elemental analysis calcd. (%) for $C_{55}H_{73}ClN_3W$ $0.5CH_2Cl_2$: C = 62.59, H = 6.91, N = 6.58; found: C = 62.88, H = 6.89, N = 6.55.

[1,3-Bis-(2,4,6-trimethylphenyl)imidazolinium$^+$ W(2,6-i$Pr_2C_6H_3$)(CHCMe_2Ph)(2,5-Me_2Pyr)$_2$($OC_6F_5^-$)] (3). A suspension of lithium pentafluorophenoxide (10.6 mg, 0.056 mmol) in 2 mL of methylene chloride was added to a stirred solution of **2** (57.5 mg, 0.056 mmol) in 2 mL of the same solvent. The reaction mixture was stirred for 3 h, then filtered over celite and all volatiles were removed *in vacuo*. The yellow solid was washed several times with pentane and crystallized from a mixture of methylene chloride and pentane to get analytically pure product; yield 54.4 mg (83 %): ^{1}H NMR (400 MHz, C_6D_6) δ = 12.22 (s, 1H, W=CH) , 7.76 - 7.74 (m, 2H, Ar), 7.25 - 7.19 (m, 5H, Ar), 7.07 - 7.02 (m, 2H, Ar), 6.48 (s, 4H, Ar), 5.95 (m, 4H, NC_4H_2), 4.26 (s, 1H, NHN), 3.70 (sept., 2H, iPr, J = 6.73), 2.80 (s, 6H, Me), 2.33 (s, 6H, Me), 2.03 (s, 12H, Me), 1.71 (s, 12H, Me), 1.35 (d, 6H, iPr, J= 6.63 Hz), 1.28 (d, 6H, iPr, J = 6.63 Hz); ^{19}F (376 MHz, C_6D_6) δ = -159.08 (d, 2F, J = 30.1), -169.54 (m, 2F), -178.50 (m, 1F). ^{13}C NMR (100 MHz, CD_2Cl_2) δ = 271.5 (W=*C*), 159.1 (C_{ipso}), 158.9 ($C_{ArImido}$), 153.7 (NC_{Mes}), 151.9 (C_{Ar}), 149.2 (C_{Ar}), 141.9 (C_{Ar}), 135.3 (C_{Ar}), 134.2 (C_{Ar}), 130.7 (C_{Ar}), 130.2 (C_{Ar}), 128.3 (C_{Ar}), 126.5 (C_{Ar}), 125.8 (C_{Ar}), 125.1 (C_{Ar}), 123.4 (C_{Ar}), 106.6 (C_{pyr}), 106.2 (C_{pyr}), 105.2 (C_{pyr}), 66.2 (*C*Me_2), 54.1 (*C*Me_2Ph), 52.0 (N*C*H_2), 34.3 (C*Me*$_2$Ph), 26.5 (Me), 26.0 (Me), 24.5 (Me), 21.3 (Me), 20.1 (Me), 18.3 (Me), 17.9 (Me), 15.7 (Me); elemental analysis calcd. (%) for $C_{61}H_{72}F_5N_5OW$ 0.33 CH_2Cl_2: C = 61.47, H = 6.11, N = 5.84, found: C =61.81, H = 6.18, N = 5.70.

[1,3-Bis-(2,6-diisopropylphenyl)imidazolinium$^+$ W(2,6-i$Pr_2C_6H_3$)(CHCMe_2Ph)(2,5-Me_2Pyr)Cl_2^-] (4). A suspension of 1,3-bis-(2,6-diisopropylphenyl) imidazolinium chloride (119.3 mg, 0.28 mmol) in 2 mL of benzene was added to a stirred solution of W(2,6-i$Pr_2C_6H_3$)(CHCMe_2Ph)(2,5-$Me_2NC_4H_4$)$_2$ (95.8 mg, 0.14 mmol) in 2 mL of benzene. The reaction mixture was stirred for 16 h at 50 °C. All volatiles were removed from the yellow solution *in vacuo*. The yellow solid was extracted by toluene, filtered over Celite, washed with diethyl ether and all volatiles were removed. The compound was crystallized form a mixture of

methylene chloride and diethyl ether to get analytically pure product; yield: 57.1 mg (39 %): 1H NMR (400 MHz, CD_2Cl_2) δ = 10.52 (s, 1H, W=CH), 7.8 (s, 1H, NCHN), 7.46 (m, 4H, Ar), 7.33 (d, 4H, Ar, J = 8.18 Hz), 7.07 (m, 5H, Ar), 5.6 (m, 2H, NC_4H_2), 4.44 (s, 4H, NC_2H_4N),3.98 (brs, 2H, iPr), 2.99 (sept., 4H, iPr, J = 6.89 Hz), 2.10 (m, 6H, Me), 1.64 (s, 3H, Me), 1.57 (s, 3H, Me), 1.40 (d, 12H, iPr, j = 6.78), 1.25 (d, 12H, iPr, J = 6.77), 1.13 (brs, 6H, iPr), 0.89 (brs, 6H, iPr); ^{13}C NMR (100 MHz, CD_2Cl_2) δ = 271.7 (W=*C*), 158.9 (N*C*N), 153.5 (C_{ipso}), 151.1 ($C_{ArImido}$), 149.0 (NC_{Dipp}), 146.8 (C_{Ar}), 134.1 (C_{Ar}), 132.1 (C_{Ar}), 131.7 (C_{Ar}), 129.9 (C_{Ar}), 128.4 (C_{Ar}), 128.1 (C_{Ar}), 126.6 (C_{Ar}), 126.4 (C_{Ar}), 125.8 (C_{Ar}), 125.7 (C_{Ar}), 125.6 (C_{Ar}), 123.6 (C_{Ar}), 123.2 (C_{Ar}), 106.8 (C_{pyr}), 105.6 (C_{pyr}), 55.2 (*C*Me_2Ph), 33.7 (Me), 33.2, 30.8, 29.7, 27.8, 25.6, 24.7, 24.5, 24.2, 19.8, 18.5, 15.3; elemental analysis calcd. (%) for $C_{55}H_{76}Cl_2N_4W$ 0.33 CH_2Cl_2: C = 61.75, H = 7.18, N = 5.21, found: C = 61.74, H = 7.27, N = 5.32.

W(N-2,6-$iPr_2C_6H_3$)(=CHCMe_2Ph)(2-methylene-1,3,4,5-tetramethyl-imidazoline)$_2$(OTf)$_2$ (6). A solution of 2-methylene-1,3,4,5-tetramethyl-imidazoline (24.5 mg, 0.175 mmol) in 5 mL diethylether was added dropwise to a stirred solution of W(2,6-$iPr_2C_6H_3$)(CHCMe_2Ph)$(OTf)_2$(dme) (76.4 mg, 0.088 mmol) in 25 mL diethylether. The reaction mixture was stirred for 1 h at room temperature. All volatiles were removed from the yellow solution *in vacuo*. The yellow solid was crystallized form a mixture of diethylether and pentan to get analytically pure product; yield: 75.0 mg (80%): ^{1}H NMR (400 MHz, CD_2Cl_2) δ = 9.35 (s, 1H, W=CH) , 7.36 – 7.14 (m, 8H, Ar), 3.77 (sept., 2H, iPr, J = 6.7 Hz), 3.17 (s, 12H, Me), 3.33 (dd, 4H, CH2, J = 11.86, 175.04 Hz), 2.02 (s, 12H, Me), 1.41 (s, 6H, Me), 1.28 (d, 12H, iPr, J = 6.8 Hz); ^{19}F (376 MHz, CD_2Cl_2) δ = -78.4 (s, 6F) , ^{13}C NMR (100 MHz, CD_2Cl_2) δ = 264.9 (W=*C*), 156.6 (C_{ipso}), 152.3 ($C_{ArImido}$), 152.2 (C_{Ar}), 147.2 (C_{Ar}), 128.9 (C_{Ar}), 127.1 (C_{Ar}), 126.4 (C_{Ar}), 126.1 (C_{Ar}), 124.0 (C_{Ar}), 122.8 (C_{Ar}), 120.5 (OTf), 54.4, 53.5, 32.9, 32.7, 31.3, 28.9, 24.8, 8.8; elemental analysis calcd. (%) for $C_{40}H_{57}F_6N_5O_6S_2W$: C = 45.07, H = 5.38, N = 6.57, found: C = 45.01, H = 5.41, N = 6.57.

General procedure for metathesis reactions: Reactions were carried out in 1,2-dichloroethane (2 mL) using catalyst **2**-**4** and **6** and the corresponding substrates (Table S1) with catalyst/substrate ratio of 1:1000 at T = 80°C. TONs were determined by GC-MS with dodecane as internal standard.

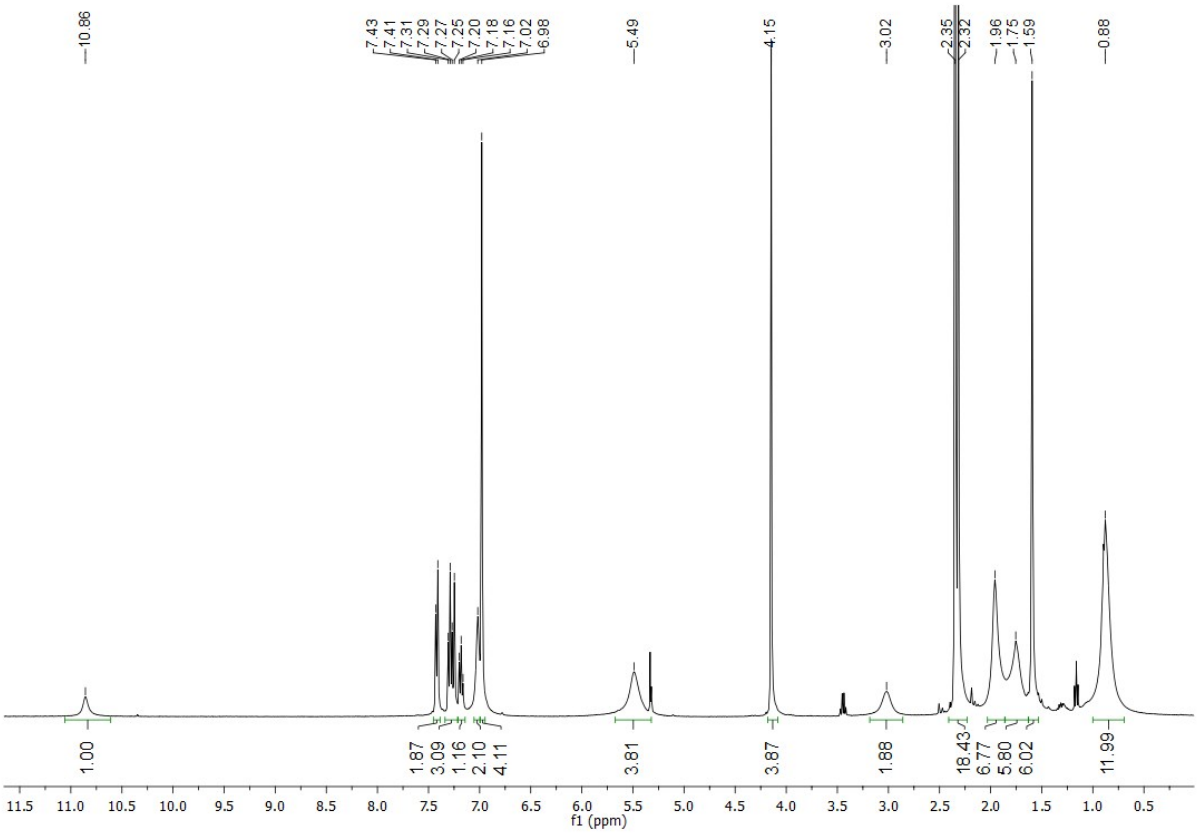


Figure S1: ^{1}H NMR spectrum (rt, 400 MHz, CD_2Cl_2) of 2.

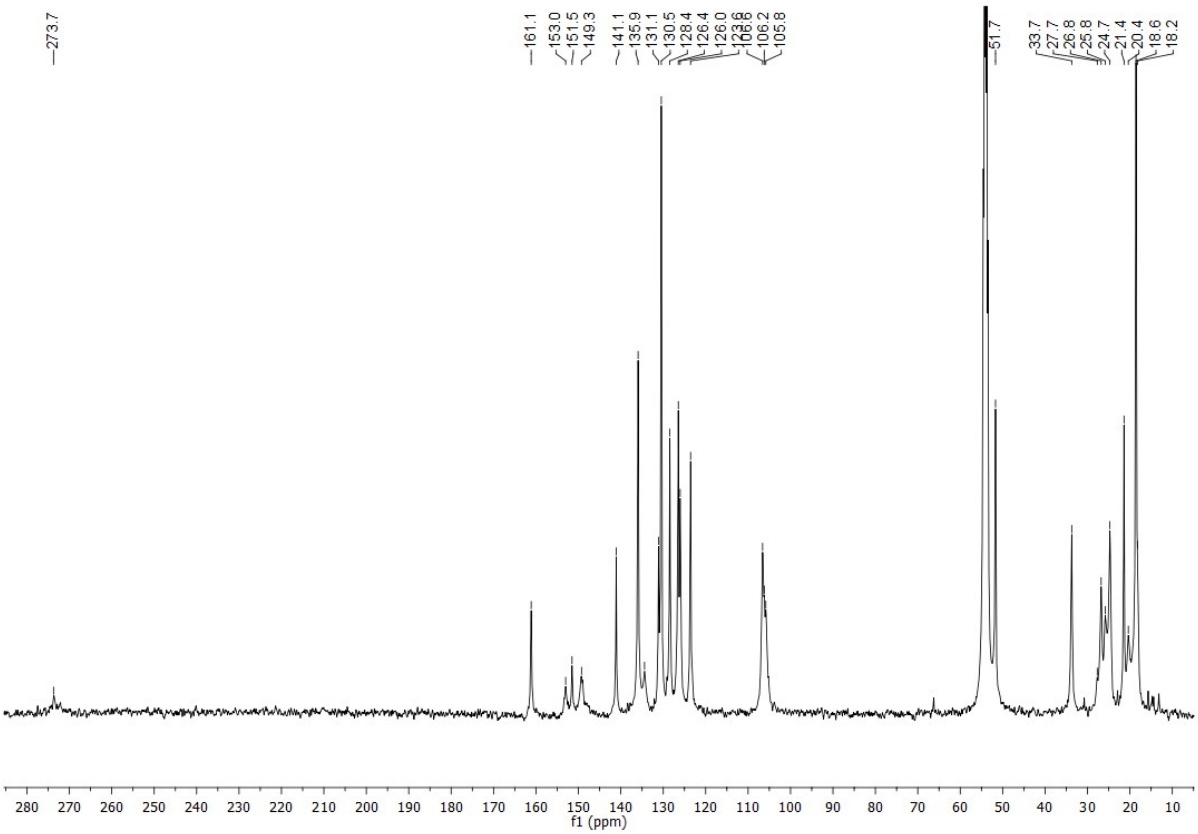


Figure S2: ^{13}C NMR spectrum (rt, 100 MHz, CD_2Cl_2) of 2.

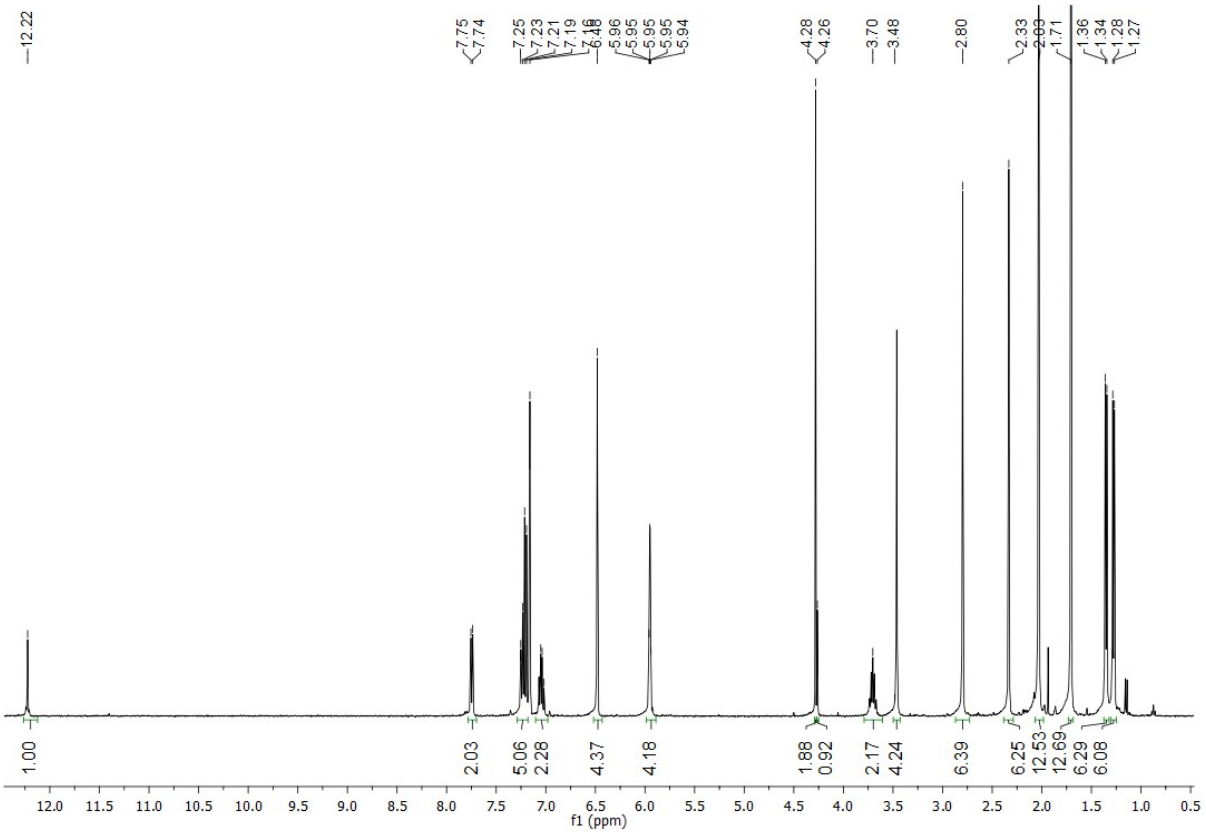


Figure S3: ^{1}H NMR spectrum (rt, 400 MHz, CD_2Cl_2) of 3.

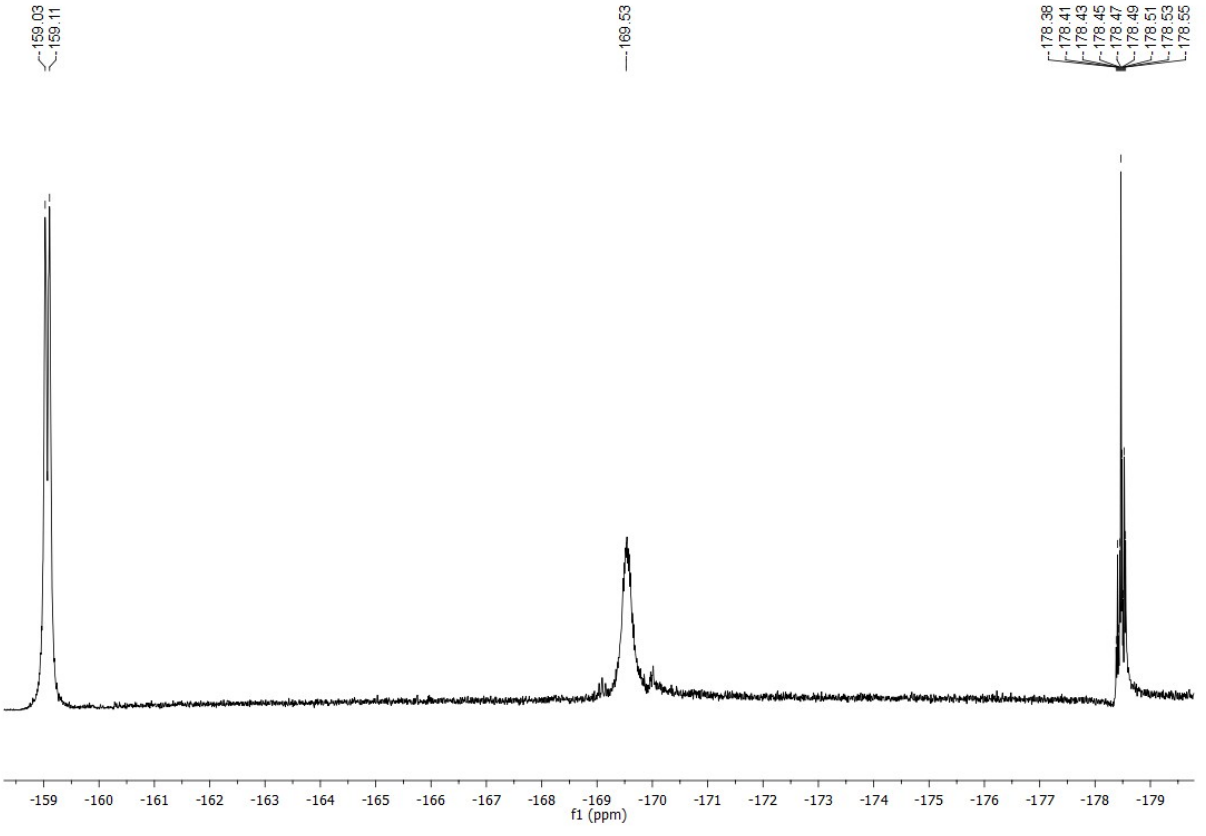


Figure S4: ^{19}F NMR spectrum (rt, 400 MHz, CD_2Cl_2) of 3.

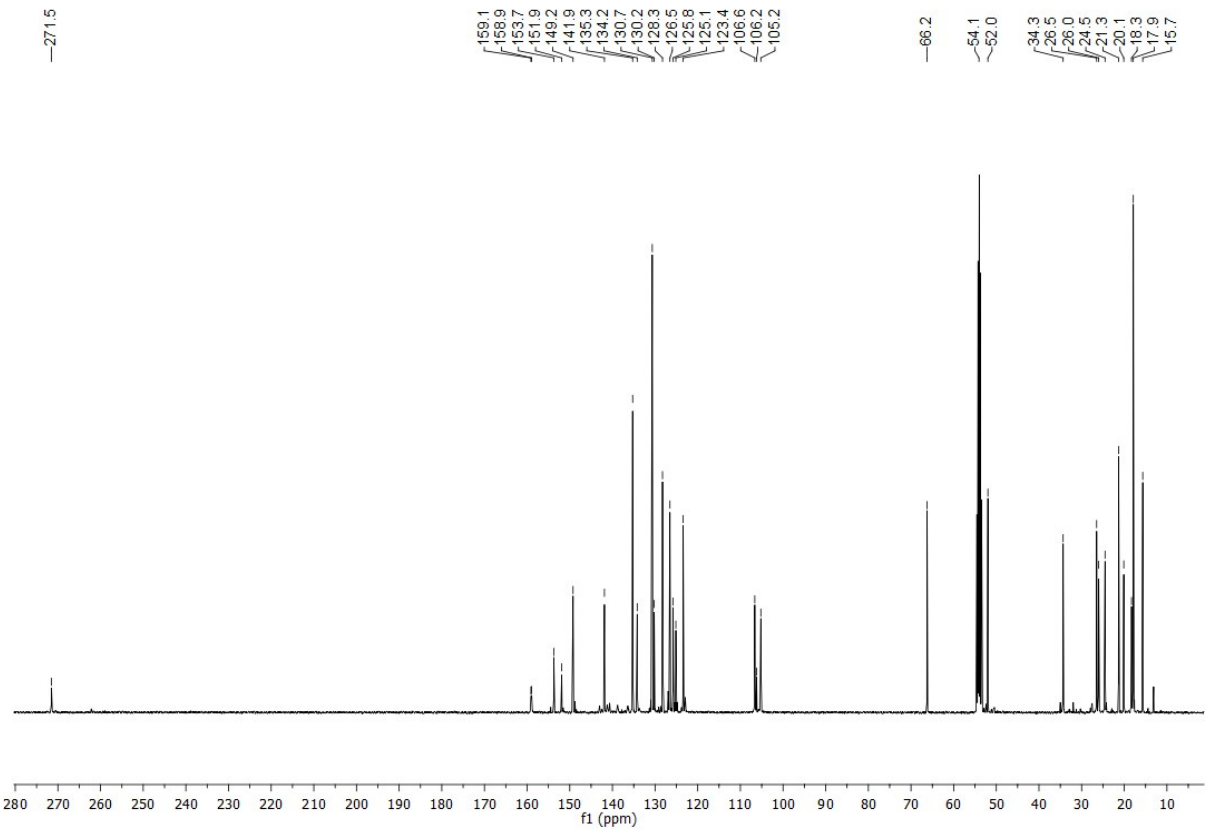


Figure S5: ^{13}C NMR spectrum (rt, 400 MHz, CD_2Cl_2) of 3.

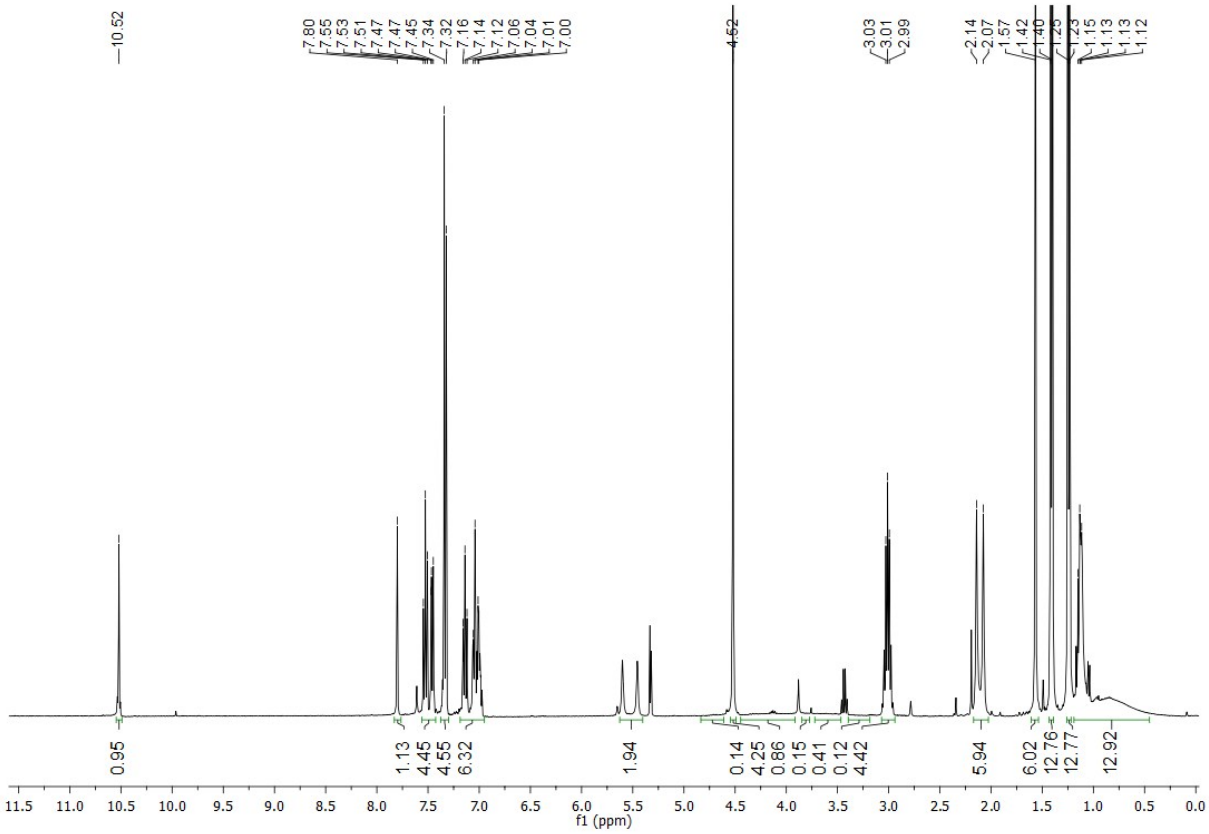


Figure S6: ^{1}H NMR spectrum (rt, 400 MHz, CD_2Cl_2) of 4.

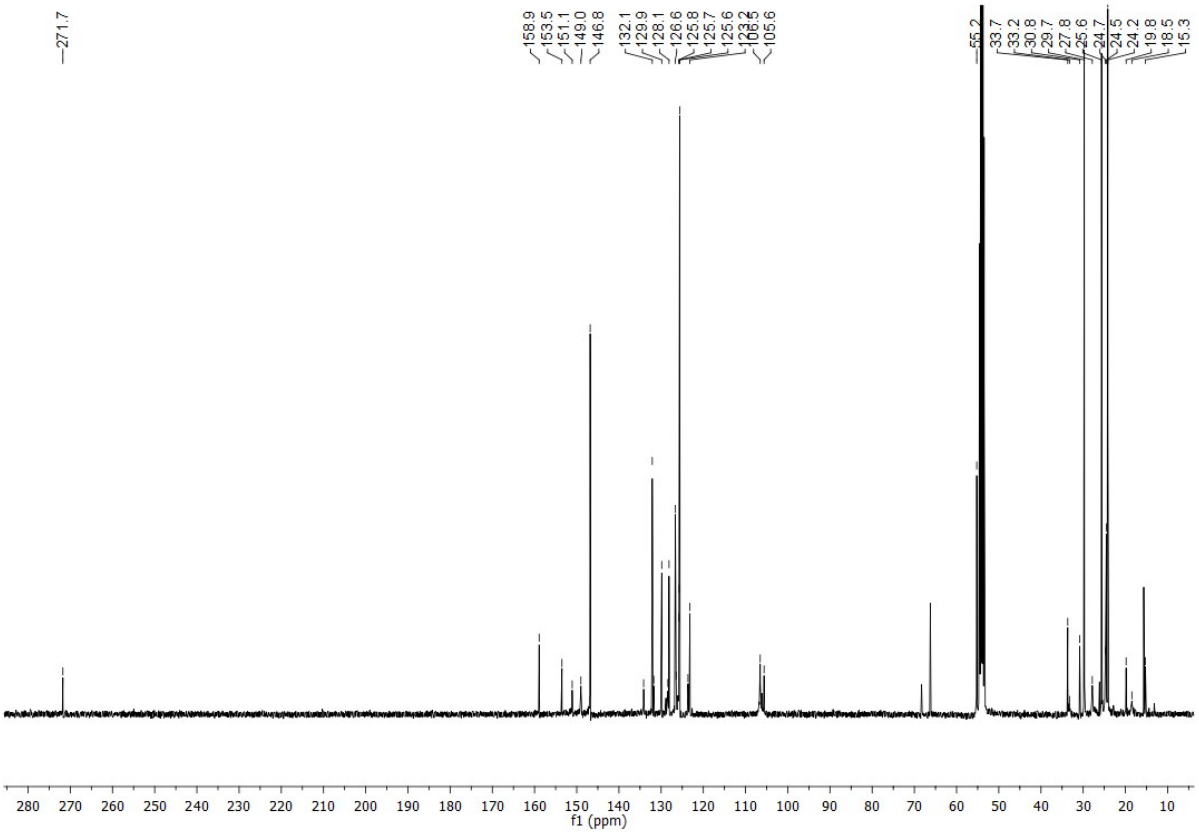


Figure S7: ^{13}C NMR spectrum (rt, 400 MHz, CD_2Cl_2) of 4.

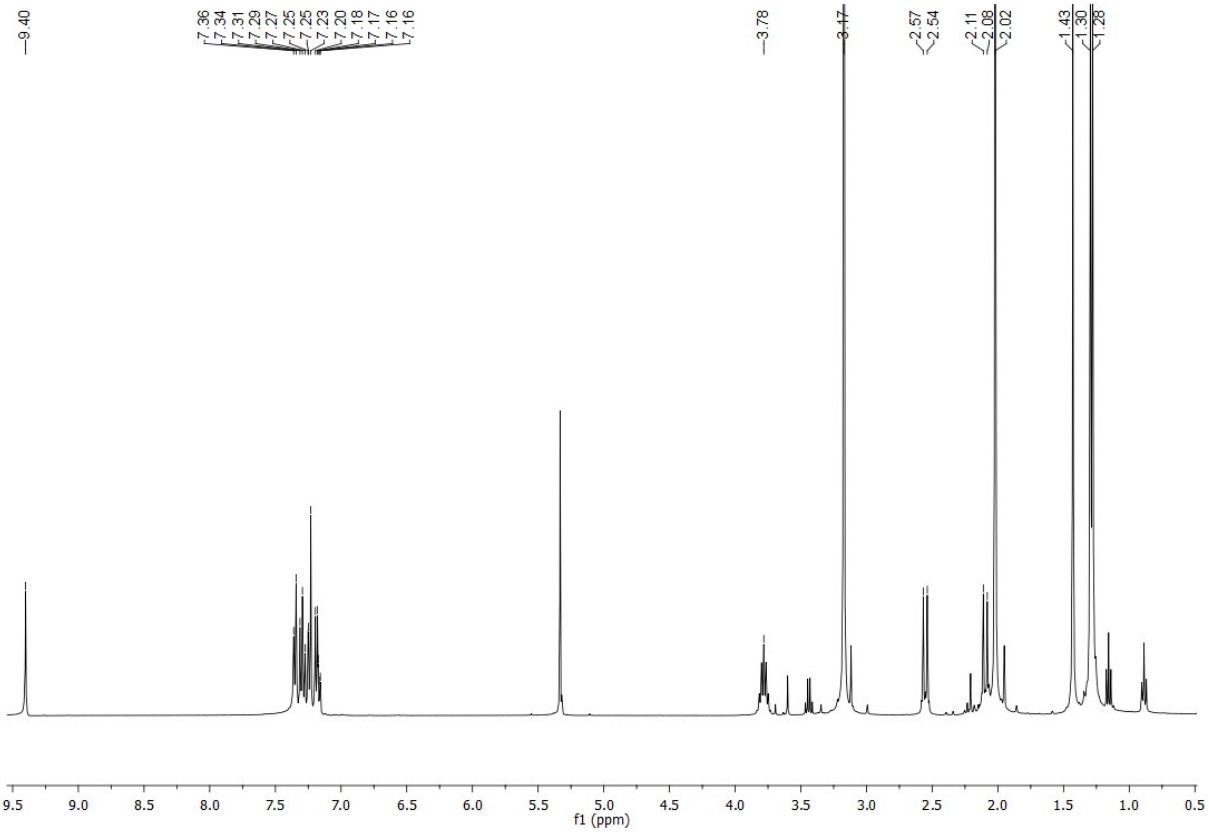


Figure S8: ^{1}H NMR spectrum (rt, 400 MHz, CD_2Cl_2) of 6.

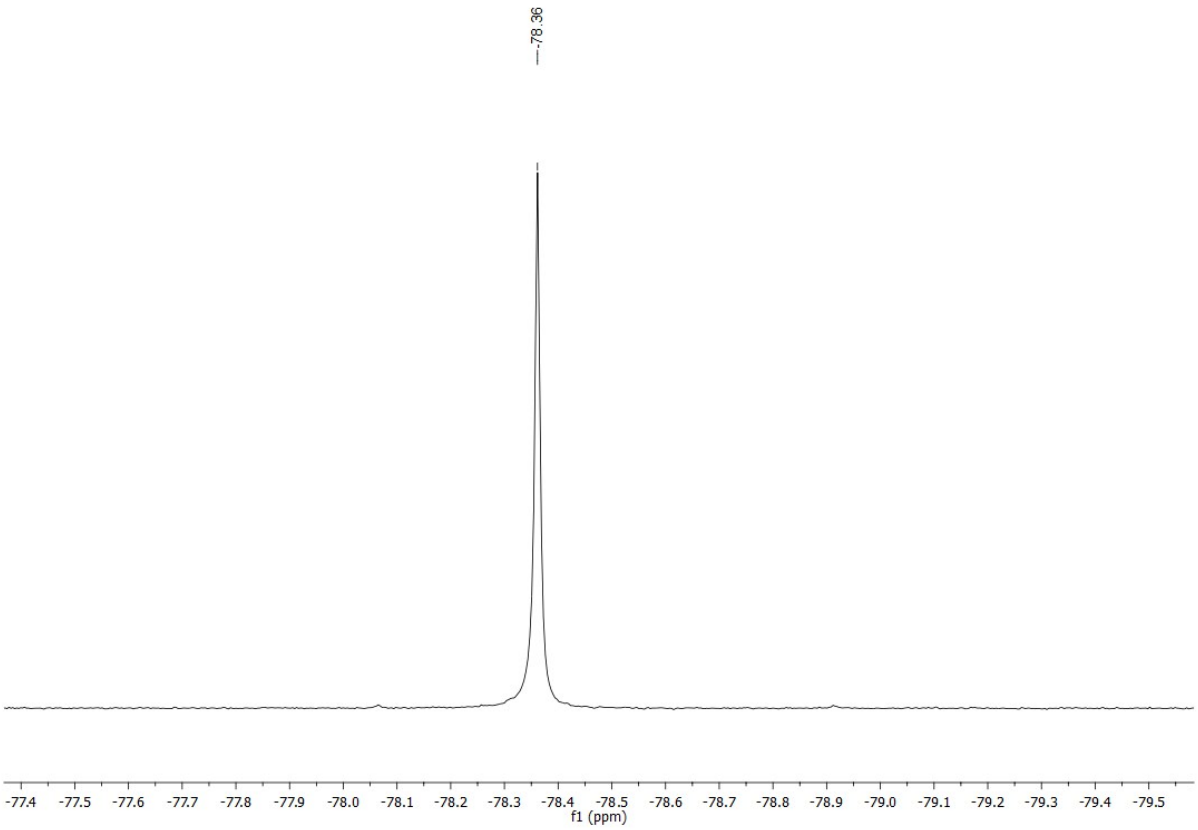


Figure S9: ^{19}F NMR spectrum (rt, 376 MHz, CD_2Cl_2) of 6.

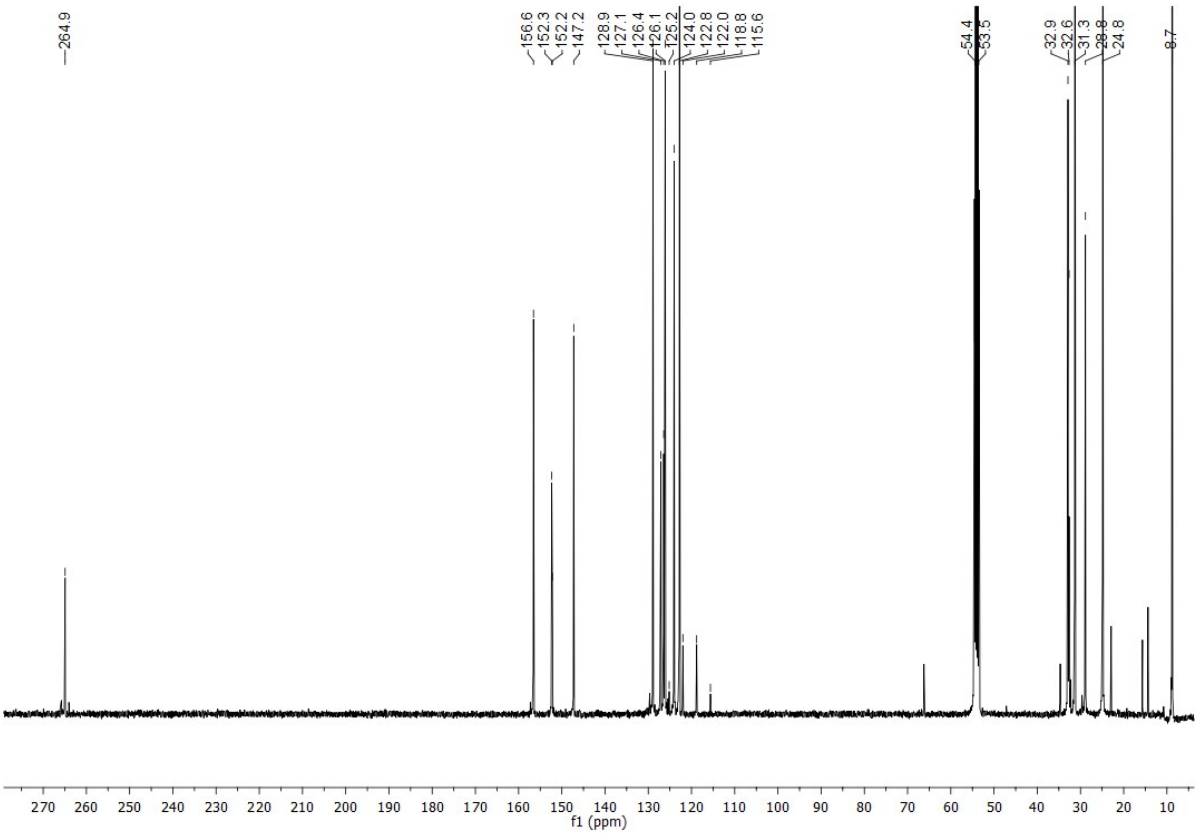


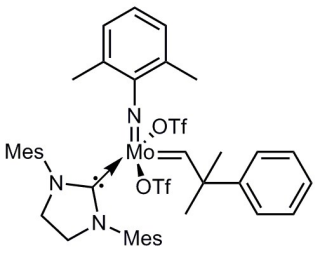
Figure S10: ^{13}C NMR spectrum (rt, 100 MHz, CD_2Cl_2) of 6.

Table S1: Reactivity (TON)[a)] in Olefin Metathesis Reactions Using Anionic Compounds 2-4 and NHO Alkylidene 6.

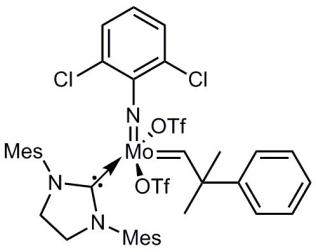
substrate/reaction type	**2**	**3**	**4**	**6**
RCM				
octa-1,7-diene	0	0	0	0
diallyl diphenylsilane	50	75	410	140
N,N-diallyl-*p*-toluolsulfonamide	0	0	0	0
diallyl ether	0	0	0	0
diallyl thioether	0	0	0	0
1,6-heptadien-3-ol	0	0	0	0
diallyl amine	0	0	0	0
1,3-diallylurea	0	0	0	0
HM				
1-hexene	0	150	0	250
1-octene	50	0	0	0
SM				
ethyl oleate	0	0	0	0

a) Reactions at T = 80°C in 1,2-dichloroethane using a catalyst/substrate ratio of 1:1000. TON determined *via* GC-MS using dodecane as internal standard. All reactions conducted under nitrogen.

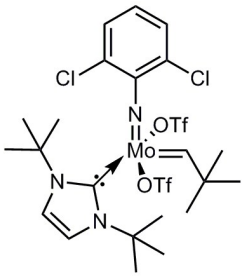
Table S2: Comparison of ^{19}F NMR [CD_2Cl_2] data and crystal data (bond lengths) of some bistriflate complexes with compound 6. Both indicators suggest that the triflate in 6 is only weakly bound. Free triflate shows at δ = -79.1 ppm.



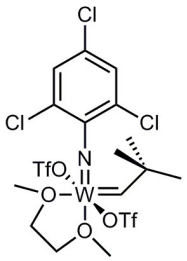
A



B



C



D

Compound/Reference	**^{19}F δ = [ppm]**	**W-OTf [pm]**
6	-78.4	227.0; 240.1
A / i)	-74.6; -76.5	-
B / i)	-74.7; -76.6	-
C / ii)	-77.7; -78.1	-
D / iii)	-77.4; -78.2	205.6; 217.3

i) *Chem. Eur. J.* **2015**, *21*, 13778 – 13787.

ii) *Angew. Chem. Int. Ed.* **2014**, *53*, 9384 –9388.

iii) *Organometallics* **2014**, *33*, 5342−5348.

Crystal data and structure refinement for complex 2.

Empirical formula	C58.50 H79 Cl8 N5 W
Formula weight	1319.72
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P 21/c
Unit cell dimensions	a = 21.6865(19) Å, α = 90°
	b = 18.8737(16) Å, β = 106.667(3)°
	c = 16.1005(13) Å, γ = 90°
Volume	6313.1(9) $Å^3$
Z, Calculated density	4, 1.388 Mg/m^3
Absorption coefficient	2.208 mm^{-1}
F(000)	2700
Crystal size	0.77 x 0.42 x 0.09 mm
Theta range for data collection	1.71 to 26.50°
Limiting indices	-18<=h<=27, -22<=k<=23, -20<=l<=19
Reflections collected / unique	55336 / 13040 [R(int) = 0.0310]
Completeness to theta = 26.50	99.7 %
Absorption correction	Numerical
Max. and min. transmission	0.7825 and 0.3395
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	13040 / 6 / 682
Goodness-of-fit on F^2	1.064
Final R indices [I>2sigma(I)]	R1 = 0.0566, wR2 = 0.1458
R indices (all data)	R1 = 0.0800, wR2 = 0.1608
Largest diff. peak and hole	5.305 and -2.142 e. $Å^{-3}$

Table S3: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) complex 2. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
W(1)	2881(1)	5143(1)	1141(1)	16(1)
Cl(1)	3034(1)	6391(1)	772(1)	22(1)
N(1)	2449(2)	4375(3)	1272(3)	18(1)
C(1)	2094(3)	3782(3)	1362(4)	19(1)
N(2)	2687(3)	5073(3)	-234(3)	22(1)
C(2)	1874(3)	3712(3)	2113(4)	24(1)
N(3)	2797(2)	5667(3)	2289(3)	20(1)
C(3)	1530(3)	3106(3)	2193(4)	29(1)
C(4)	1405(3)	2569(3)	1574(5)	32(2)
C(5)	1626(3)	2649(4)	846(5)	32(2)
C(6)	1969(3)	3246(3)	726(4)	24(1)
C(7)	2002(3)	4274(4)	2807(4)	26(1)
C(8)	2446(4)	3999(5)	3665(5)	46(2)
C(9)	1377(4)	4563(5)	2939(5)	41(2)
C(10)	2211(3)	3280(3)	-79(4)	26(1)
C(11)	2723(3)	2708(4)	-27(5)	32(2)
C(12)	1654(4)	3186(4)	-910(4)	35(2)
C(13)	3738(3)	4792(3)	1531(4)	16(1)
C(14)	4145(3)	4138(3)	1862(4)	18(1)
C(15)	3769(3)	3600(3)	2237(4)	27(1)
C(16)	4322(3)	3763(3)	1102(4)	26(1)
C(17)	4777(3)	4373(3)	2529(4)	20(1)
C(18)	4965(3)	4127(3)	3377(4)	25(1)
C(19)	5536(3)	4363(4)	3963(5)	33(2)
C(20)	5929(4)	4832(4)	3700(5)	35(2)
C(21)	5759(3)	5081(3)	2854(5)	29(2)
C(22)	5178(3)	4851(3)	2272(4)	24(1)
C(23)	2076(4)	4999(4)	-796(4)	29(1)
C(24)	2107(4)	4940(4)	-1631(4)	38(2)
C(25)	2761(4)	4992(4)	-1599(5)	40(2)
C(26)	3105(4)	5080(3)	-753(4)	29(2)
C(27)	1478(4)	5029(4)	-499(5)	33(2)
C(28)	3808(4)	5195(4)	-417(5)	32(2)
C(29)	2204(3)	5983(3)	2280(4)	23(1)
C(30)	2242(3)	6207(3)	3113(4)	27(1)
C(31)	2864(3)	6036(3)	3645(4)	26(1)
C(32)	3193(3)	5709(3)	3123(4)	21(1)
C(33)	1644(3)	6022(4)	1495(4)	29(1)
C(34)	3862(3)	5439(3)	3398(4)	26(1)
N(4)	6312(2)	2679(3)	2344(3)	21(1)
N(5)	7312(2)	2982(3)	3019(3)	21(1)
C(35)	6917(3)	2492(3)	2576(4)	20(1)
C(36)	6258(3)	3438(4)	2576(5)	37(2)
C(37)	6943(3)	3595(4)	3169(5)	33(2)

C(38)	5765(3)	2332(3)	1775(3)	18(1)
C(39)	5296(3)	2043(3)	2113(4)	21(1)
C(40)	4746(3)	1763(3)	1537(4)	22(1)
C(41)	4646(3)	1777(3)	638(4)	22(1)
C(42)	5125(3)	2075(3)	331(4)	23(1)
C(43)	5687(3)	2361(3)	873(4)	22(1)
C(44)	5380(3)	2035(4)	3076(4)	27(1)
C(45)	4045(3)	1466(4)	31(4)	28(1)
C(46)	6193(3)	2687(4)	513(4)	29(1)
C(47)	8009(3)	2991(3)	3233(4)	22(1)
C(48)	8372(3)	2930(3)	4090(4)	28(1)
C(49)	9043(3)	2970(4)	4272(5)	33(2)
C(50)	9339(3)	3062(4)	3622(5)	39(2)
C(51)	8951(4)	3135(4)	2775(5)	40(2)
C(52)	8282(3)	3103(3)	2553(4)	28(1)
C(53)	8083(4)	2844(4)	4832(4)	37(2)
C(54)	10066(4)	3081(6)	3822(7)	63(3)
C(55)	7878(3)	3200(4)	1630(4)	31(2)
C(1X)	1492(7)	5019(6)	5879(9)	79(4)
Cl(2)	2030(2)	5237(2)	5310(2)	88(1)
Cl(3)	921(3)	4445(3)	5343(4)	151(2)
C(2X)	2919(4)	3300(4)	7704(6)	49(2)
Cl(4)	3723(1)	3228(1)	8337(2)	53(1)
Cl(5)	2853(1)	3695(1)	6684(1)	56(1)
C(3X)	278(5)	3997(5)	10606(6)	53(2)
Cl(6)	24(1)	3989(2)	9484(2)	61(1)
Cl(7)	-200(1)	3451(2)	11057(2)	73(1)
C(4X)	-266(8)	4170(10)	6564(11)	50(4)
Cl(8)	215(2)	4816(3)	7175(3)	56(1)
Cl(9)	-285(4)	3390(3)	7048(4)	86(2)

Table S4: Bond lengths [A] and angles [°] for complex 2

W(1)-N(1)	1.770(5)
W(1)-C(13)	1.902(5)
W(1)-N(2)	2.136(5)
W(1)-N(3)	2.150(5)
W(1)-Cl(1)	2.4749(14)
N(1)-C(1)	1.391(7)
C(1)-C(6)	1.410(9)
C(1)-C(2)	1.427(8)
N(2)-C(23)	1.380(9)
N(2)-C(26)	1.398(8)
C(2)-C(3)	1.393(9)
C(2)-C(7)	1.507(9)
N(3)-C(32)	1.373(7)
N(3)-C(29)	1.413(8)
C(3)-C(4)	1.393(10)
C(3)-H(3)	0.9500
C(4)-C(5)	1.395(10)
C(4)-H(4)	0.9500
C(5)-C(6)	1.393(9)
C(5)-H(5)	0.9500
C(6)-C(10)	1.532(9)
C(7)-C(8)	1.530(10)
C(7)-C(9)	1.531(10)
C(7)-H(7)	10.000
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-C(11)	1.533(9)
C(10)-C(12)	1.534(9)
C(10)-H(10)	10.000
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(14)	1.523(8)
C(13)-H(13)	0.9500
C(14)-C(15)	1.529(8)
C(14)-C(17)	1.546(8)
C(14)-C(16)	1.554(8)
C(15)-H(15A)	0.9800

C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-C(18)	1.387(9)
C(17)-C(22)	1.395(9)
C(18)-C(19)	1.397(9)
C(18)-H(18)	0.9500
C(19)-C(20)	1.377(11)
C(19)-H(19)	0.9500
C(20)-C(21)	1.388(11)
C(20)-H(20)	0.9500
C(21)-C(22)	1.406(10)
C(21)-H(21)	0.9500
C(22)-H(22)	0.9500
C(23)-C(24)	1.370(10)
C(23)-C(27)	1.508(11)
C(24)-C(25)	1.407(13)
C(24)-H(24)	0.9500
C(25)-C(26)	1.363(10)
C(25)-H(25)	0.9500
C(26)-C(28)	1.481(11)
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-C(30)	1.386(9)
C(29)-C(33)	1.483(9)
C(30)-C(31)	1.411(10)
C(30)-H(30)	0.9500
C(31)-C(32)	1.392(8)
C(31)-H(31)	0.9500
C(32)-C(34)	1.483(9)
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
N(4)-C(35)	1.304(8)
N(4)-C(38)	1.432(8)
N(4)-C(36)	1.493(8)
N(5)-C(35)	1.321(8)
N(5)-C(47)	1.451(8)

N(5)-C(37)	1.468(8)
C(35)-H(35)	0.9500
C(36)-C(37)	1.545(10)
C(36)-H(36A)	0.9900
C(36)-H(36B)	0.9900
C(37)-H(37A)	0.9900
C(37)-H(37B)	0.9900
C(38)-C(39)	1.396(8)
C(38)-C(43)	1.413(8)
C(39)-C(40)	1.388(9)
C(39)-C(44)	1.509(8)
C(40)-C(41)	1.400(8)
C(40)-H(40)	0.9500
C(41)-C(42)	1.391(9)
C(41)-C(45)	1.506(9)
C(42)-C(43)	1.388(9)
C(42)-H(42)	0.9500
C(43)-C(46)	1.511(9)
C(44)-H(44A)	0.9800
C(44)-H(44B)	0.9800
C(44)-H(44C)	0.9800
C(45)-H(45A)	0.9800
C(45)-H(45B)	0.9800
C(45)-H(45C)	0.9800
C(46)-H(46A)	0.9800
C(46)-H(46B)	0.9800
C(46)-H(46C)	0.9800
C(47)-C(48)	1.384(9)
C(47)-C(52)	1.400(9)
C(48)-C(49)	1.402(10)
C(48)-C(53)	1.508(9)
C(49)-C(50)	1.387(11)
C(49)-H(49)	0.9500
C(50)-C(51)	1.390(11)
C(50)-C(54)	1.516(11)
C(51)-C(52)	1.393(10)
C(51)-H(51)	0.9500
C(52)-C(55)	1.505(9)
C(53)-H(53A)	0.9800
C(53)-H(53B)	0.9800
C(53)-H(53C)	0.9800
C(54)-H(54A)	0.9800
C(54)-H(54B)	0.9800
C(54)-H(54C)	0.9800
C(55)-H(55A)	0.9800
C(55)-H(55B)	0.9800
C(55)-H(55C)	0.9800

C(1X)-Cl(3)	1.685(14)
C(1X)-Cl(2)	1.729(12)
C(1X)-H(1X1)	0.9900
C(1X)-H(1X2)	0.9900
C(2X)-Cl(4)	1.754(9)
C(2X)-Cl(5)	1.772(9)
C(2X)-H(2X1)	0.9900
C(2X)-H(2X2)	0.9900
C(3X)-Cl(6)	1.731(9)
C(3X)-Cl(7)	1.759(9)
C(3X)-H(3X1)	0.9900
C(3X)-H(3X2)	0.9900
C(4X)-Cl(9)	1.671(19)
C(4X)-Cl(8)	1.721(19)
C(4X)-H(4X1)	0.9900
C(4X)-H(4X2)	0.9900

N(1)-W(1)-C(13)	100.2(2)
N(1)-W(1)-N(2)	96.8(2)
C(13)-W(1)-N(2)	101.8(2)
N(1)-W(1)-N(3)	95.5(2)
C(13)-W(1)-N(3)	101.1(2)
N(2)-W(1)-N(3)	151.56(19)
N(1)-W(1)-Cl(1)	156.81(16)
C(13)-W(1)-Cl(1)	103.00(17)
N(2)-W(1)-Cl(1)	79.08(14)
N(3)-W(1)-Cl(1)	79.51(13)
C(1)-N(1)-W(1)	178.4(4)
N(1)-C(1)-C(6)	119.9(5)
N(1)-C(1)-C(2)	119.5(5)
C(6)-C(1)-C(2)	120.6(5)
C(23)-N(2)-C(26)	106.0(6)
C(23)-N(2)-W(1)	123.6(4)
C(26)-N(2)-W(1)	130.5(5)
C(3)-C(2)-C(1)	118.2(6)
C(3)-C(2)-C(7)	119.9(6)
C(1)-C(2)-C(7)	121.9(5)
C(32)-N(3)-C(29)	107.3(5)
C(32)-N(3)-W(1)	133.1(4)
C(29)-N(3)-W(1)	119.1(4)
C(4)-C(3)-C(2)	122.0(6)
C(4)-C(3)-H(3)	119.0
C(2)-C(3)-H(3)	119.0
C(3)-C(4)-C(5)	118.6(6)
C(3)-C(4)-H(4)	120.7
C(5)-C(4)-H(4)	120.7
C(6)-C(5)-C(4)	122.0(6)

C(6)-C(5)-H(5)	119.0
C(4)-C(5)-H(5)	119.0
C(5)-C(6)-C(1)	118.5(6)
C(5)-C(6)-C(10)	118.6(6)
C(1)-C(6)-C(10)	122.9(5)
C(2)-C(7)-C(8)	111.4(6)
C(2)-C(7)-C(9)	111.8(6)
C(8)-C(7)-C(9)	110.4(6)
C(2)-C(7)-H(7)	107.7
C(8)-C(7)-H(7)	107.7
C(9)-C(7)-H(7)	107.7
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(6)-C(10)-C(11)	110.0(5)
C(6)-C(10)-C(12)	110.9(5)
C(11)-C(10)-C(12)	110.1(5)
C(6)-C(10)-H(10)	108.6
C(11)-C(10)-H(10)	108.6
C(12)-C(10)-H(10)	108.6
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(14)-C(13)-W(1)	144.2(4)
C(14)-C(13)-H(13)	107.9
W(1)-C(13)-H(13)	107.9
C(13)-C(14)-C(15)	110.8(5)
C(13)-C(14)-C(17)	108.6(5)
C(15)-C(14)-C(17)	112.6(5)

C(13)-C(14)-C(16)	110.0(5)
C(15)-C(14)-C(16)	106.9(5)
C(17)-C(14)-C(16)	107.9(5)
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(14)-C(16)-H(16A)	109.5
C(14)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(14)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(18)-C(17)-C(22)	118.4(6)
C(18)-C(17)-C(14)	122.6(5)
C(22)-C(17)-C(14)	118.9(5)
C(17)-C(18)-C(19)	120.7(6)
C(17)-C(18)-H(18)	119.6
C(19)-C(18)-H(18)	119.6
C(20)-C(19)-C(18)	120.2(7)
C(20)-C(19)-H(19)	119.9
C(18)-C(19)-H(19)	119.9
C(19)-C(20)-C(21)	120.4(7)
C(19)-C(20)-H(20)	119.8
C(21)-C(20)-H(20)	119.8
C(20)-C(21)-C(22)	119.0(6)
C(20)-C(21)-H(21)	120.5
C(22)-C(21)-H(21)	120.5
C(17)-C(22)-C(21)	121.2(6)
C(17)-C(22)-H(22)	119.4
C(21)-C(22)-H(22)	119.4
C(24)-C(23)-N(2)	110.1(7)
C(24)-C(23)-C(27)	127.1(7)
N(2)-C(23)-C(27)	122.7(6)
C(23)-C(24)-C(25)	106.9(7)
C(23)-C(24)-H(24)	126.6
C(25)-C(24)-H(24)	126.6
C(26)-C(25)-C(24)	107.6(6)
C(26)-C(25)-H(25)	126.2
C(24)-C(25)-H(25)	126.2
C(25)-C(26)-N(2)	109.4(7)
C(25)-C(26)-C(28)	126.5(7)
N(2)-C(26)-C(28)	124.1(6)
C(23)-C(27)-H(27A)	109.5
C(23)-C(27)-H(27B)	109.5

H(27A)-C(27)-H(27B)	109.5
C(23)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(26)-C(28)-H(28A)	109.5
C(26)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(26)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(30)-C(29)-N(3)	108.5(6)
C(30)-C(29)-C(33)	128.1(6)
N(3)-C(29)-C(33)	123.3(5)
C(29)-C(30)-C(31)	107.4(6)
C(29)-C(30)-H(30)	126.3
C(31)-C(30)-H(30)	126.3
C(32)-C(31)-C(30)	107.5(5)
C(32)-C(31)-H(31)	126.3
C(30)-C(31)-H(31)	126.3
N(3)-C(32)-C(31)	109.3(5)
N(3)-C(32)-C(34)	123.8(5)
C(31)-C(32)-C(34)	126.9(5)
C(29)-C(33)-H(33A)	109.5
C(29)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(29)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(32)-C(34)-H(34A)	109.5
C(32)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(32)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(35)-N(4)-C(38)	129.8(5)
C(35)-N(4)-C(36)	109.4(5)
C(38)-N(4)-C(36)	119.3(5)
C(35)-N(5)-C(47)	127.4(5)
C(35)-N(5)-C(37)	109.8(5)
C(47)-N(5)-C(37)	122.2(5)
N(4)-C(35)-N(5)	114.2(5)
N(4)-C(35)-H(35)	122.9
N(5)-C(35)-H(35)	122.9
N(4)-C(36)-C(37)	102.1(5)
N(4)-C(36)-H(36A)	111.4
C(37)-C(36)-H(36A)	111.4
N(4)-C(36)-H(36B)	111.4

C(37)-C(36)-H(36B)	111.4
H(36A)-C(36)-H(36B)	109.2
N(5)-C(37)-C(36)	102.7(5)
N(5)-C(37)-H(37A)	111.2
C(36)-C(37)-H(37A)	111.2
N(5)-C(37)-H(37B)	111.2
C(36)-C(37)-H(37B)	111.2
H(37A)-C(37)-H(37B)	109.1
C(39)-C(38)-C(43)	122.0(5)
C(39)-C(38)-N(4)	119.5(5)
C(43)-C(38)-N(4)	118.2(5)
C(40)-C(39)-C(38)	118.0(5)
C(40)-C(39)-C(44)	120.7(5)
C(38)-C(39)-C(44)	121.2(5)
C(39)-C(40)-C(41)	122.2(6)
C(39)-C(40)-H(40)	118.9
C(41)-C(40)-H(40)	118.9
C(42)-C(41)-C(40)	117.7(6)
C(42)-C(41)-C(45)	121.5(5)
C(40)-C(41)-C(45)	120.8(6)
C(43)-C(42)-C(41)	123.0(5)
C(43)-C(42)-H(42)	118.5
C(41)-C(42)-H(42)	118.5
C(42)-C(43)-C(38)	117.1(5)
C(42)-C(43)-C(46)	121.3(5)
C(38)-C(43)-C(46)	121.6(5)
C(39)-C(44)-H(44A)	109.5
C(39)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
C(39)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
C(41)-C(45)-H(45A)	109.5
C(41)-C(45)-H(45B)	109.5
H(45A)-C(45)-H(45B)	109.5
C(41)-C(45)-H(45C)	109.5
H(45A)-C(45)-H(45C)	109.5
H(45B)-C(45)-H(45C)	109.5
C(43)-C(46)-H(46A)	109.5
C(43)-C(46)-H(46B)	109.5
H(46A)-C(46)-H(46B)	109.5
C(43)-C(46)-H(46C)	109.5
H(46A)-C(46)-H(46C)	109.5
H(46B)-C(46)-H(46C)	109.5
C(48)-C(47)-C(52)	123.1(6)
C(48)-C(47)-N(5)	119.4(5)
C(52)-C(47)-N(5)	117.4(6)

C(47)-C(48)-C(49)	117.6(6)
C(47)-C(48)-C(53)	123.5(6)
C(49)-C(48)-C(53)	118.9(6)
C(50)-C(49)-C(48)	121.7(6)
C(50)-C(49)-H(49)	119.1
C(48)-C(49)-H(49)	119.1
C(49)-C(50)-C(51)	118.2(7)
C(49)-C(50)-C(54)	121.4(7)
C(51)-C(50)-C(54)	120.5(7)
C(50)-C(51)-C(52)	122.7(7)
C(50)-C(51)-H(51)	118.6
C(52)-C(51)-H(51)	118.6
C(51)-C(52)-C(47)	116.6(6)
C(51)-C(52)-C(55)	121.1(6)
C(47)-C(52)-C(55)	122.3(6)
C(48)-C(53)-H(53A)	109.5
C(48)-C(53)-H(53B)	109.5
H(53A)-C(53)-H(53B)	109.5
C(48)-C(53)-H(53C)	109.5
H(53A)-C(53)-H(53C)	109.5
H(53B)-C(53)-H(53C)	109.5
C(50)-C(54)-H(54A)	109.5
C(50)-C(54)-H(54B)	109.5
H(54A)-C(54)-H(54B)	109.5
C(50)-C(54)-H(54C)	109.5
H(54A)-C(54)-H(54C)	109.5
H(54B)-C(54)-H(54C)	109.5
C(52)-C(55)-H(55A)	109.5
C(52)-C(55)-H(55B)	109.5
H(55A)-C(55)-H(55B)	109.5
C(52)-C(55)-H(55C)	109.5
H(55A)-C(55)-H(55C)	109.5
H(55B)-C(55)-H(55C)	109.5
Cl(3)-C(1X)-Cl(2)	113.0(8)
Cl(3)-C(1X)-H(1X1)	109.0
Cl(2)-C(1X)-H(1X1)	109.0
Cl(3)-C(1X)-H(1X2)	109.0
Cl(2)-C(1X)-H(1X2)	109.0
H(1X1)-C(1X)-H(1X2)	107.8
Cl(4)-C(2X)-Cl(5)	111.9(4)
Cl(4)-C(2X)-H(2X1)	109.2
Cl(5)-C(2X)-H(2X1)	109.2
Cl(4)-C(2X)-H(2X2)	109.2
Cl(5)-C(2X)-H(2X2)	109.2
H(2X1)-C(2X)-H(2X2)	107.9
Cl(6)-C(3X)-Cl(7)	112.2(5)
Cl(6)-C(3X)-H(3X1)	109.2

Cl(7)-C(3X)-H(3X1)	109.2
Cl(6)-C(3X)-H(3X2)	109.2
Cl(7)-C(3X)-H(3X2)	109.2
H(3X1)-C(3X)-H(3X2)	107.9
Cl(9)-C(4X)-Cl(8)	116.7(11)
Cl(9)-C(4X)-H(4X1)	108.1
Cl(8)-C(4X)-H(4X1)	108.1
Cl(9)-C(4X)-H(4X2)	108.1
Cl(8)-C(4X)-H(4X2)	108.1
H(4X1)-C(4X)-H(4X2)	107.3

Table S5: Anisotropic displacement parameters (A^2 x 10^3) for complex 2. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$.

	U11	U22	U33	U23	U13	U12
W(1)	24(1)	11(1)	14(1)	0(1)	8(1)	0(1)
Cl(1)	34(1)	14(1)	23(1)	1(1)	13(1)	-1(1)
N(1)	15(2)	23(3)	18(2)	3(2)	10(2)	-1(2)
C(1)	18(3)	15(3)	25(3)	2(2)	6(2)	0(2)
N(2)	36(3)	15(2)	16(2)	-1(2)	9(2)	3(2)
C(2)	24(3)	24(3)	26(3)	6(3)	7(2)	0(2)
N(3)	25(3)	15(2)	19(2)	0(2)	7(2)	2(2)
C(3)	32(4)	25(3)	33(3)	8(3)	14(3)	2(3)
C(4)	30(3)	18(3)	53(4)	4(3)	19(3)	-1(3)
C(5)	26(3)	32(4)	42(4)	-8(3)	15(3)	-7(3)
C(6)	23(3)	22(3)	30(3)	-1(3)	11(3)	-3(2)
C(7)	35(4)	26(3)	22(3)	1(3)	14(3)	-4(3)
C(8)	57(5)	50(5)	28(4)	1(3)	4(3)	1(4)
C(9)	42(4)	42(4)	45(4)	-8(4)	21(4)	-3(4)
C(10)	31(3)	20(3)	31(3)	-4(3)	13(3)	-6(3)
C(11)	41(4)	21(3)	39(4)	-6(3)	20(3)	-1(3)
C(12)	42(4)	35(4)	30(3)	-8(3)	14(3)	-1(3)
C(13)	11(2)	18(3)	18(3)	-5(2)	5(2)	-4(2)
C(14)	20(3)	17(3)	17(3)	2(2)	5(2)	2(2)
C(15)	25(3)	20(3)	37(4)	10(3)	10(3)	4(2)
C(16)	33(3)	20(3)	24(3)	-1(2)	9(3)	6(3)
C(17)	21(3)	15(3)	25(3)	-4(2)	8(2)	4(2)
C(18)	32(3)	25(3)	22(3)	-5(2)	13(3)	4(3)
C(19)	28(3)	36(4)	32(3)	-10(3)	5(3)	10(3)
C(20)	28(4)	33(4)	40(4)	-19(3)	2(3)	0(3)
C(21)	23(3)	15(3)	51(4)	-8(3)	15(3)	2(2)
C(22)	30(3)	16(3)	29(3)	-1(2)	13(3)	3(2)
C(23)	38(4)	23(3)	22(3)	-1(3)	3(3)	5(3)
C(24)	59(5)	33(4)	16(3)	1(3)	3(3)	12(3)
C(25)	72(6)	38(4)	16(3)	6(3)	23(3)	18(4)
C(26)	51(4)	19(3)	22(3)	3(2)	20(3)	8(3)
C(27)	33(4)	34(4)	24(3)	-2(3)	-4(3)	4(3)
C(28)	43(4)	29(4)	35(4)	9(3)	29(3)	8(3)
C(29)	28(3)	16(3)	29(3)	1(2)	14(3)	-2(2)
C(30)	41(4)	15(3)	34(3)	-3(3)	24(3)	-4(3)
C(31)	41(4)	20(3)	23(3)	-2(2)	16(3)	-1(3)
C(32)	31(3)	14(3)	17(3)	1(2)	9(2)	-3(2)
C(33)	28(3)	29(4)	30(3)	-9(3)	9(3)	-2(3)
C(34)	36(4)	23(3)	15(3)	-6(2)	4(2)	0(3)
N(4)	30(3)	14(2)	20(2)	-4(2)	11(2)	1(2)
N(5)	23(3)	19(3)	20(2)	-2(2)	6(2)	2(2)
C(35)	32(3)	17(3)	15(3)	2(2)	13(2)	-1(2)
C(36)	36(4)	26(4)	48(4)	-17(3)	9(3)	6(3)
C(37)	40(4)	27(4)	34(4)	-13(3)	16(3)	-3(3)

C(38)	20(3)	19(3)	14(3)	-2(2)	4(2)	5(2)
C(39)	27(3)	19(3)	18(3)	4(2)	8(2)	7(2)
C(40)	31(3)	18(3)	18(3)	4(2)	9(2)	5(2)
C(41)	31(3)	15(3)	21(3)	1(2)	9(2)	4(2)
C(42)	30(3)	23(3)	14(3)	1(2)	5(2)	1(2)
C(43)	33(3)	17(3)	18(3)	1(2)	10(2)	1(2)
C(44)	35(4)	31(4)	20(3)	1(3)	15(3)	4(3)
C(45)	34(4)	28(3)	25(3)	0(3)	12(3)	1(3)
C(46)	36(4)	33(4)	18(3)	4(3)	8(3)	-8(3)
C(47)	27(3)	17(3)	26(3)	-6(2)	11(3)	-4(2)
C(48)	34(4)	22(3)	26(3)	0(3)	6(3)	-5(3)
C(49)	30(4)	30(4)	34(4)	3(3)	-1(3)	-7(3)
C(50)	29(4)	39(4)	48(4)	-5(3)	10(3)	-4(3)
C(51)	40(4)	46(5)	43(4)	-7(3)	26(3)	-10(3)
C(52)	39(4)	21(3)	28(3)	-5(3)	18(3)	-4(3)
C(53)	40(4)	44(4)	27(3)	7(3)	9(3)	-5(3)
C(54)	36(5)	79(7)	70(6)	-15(6)	12(4)	-15(5)
C(55)	46(4)	28(4)	24(3)	-3(3)	21(3)	-9(3)
C(1X)	108(10)	64(7)	83(9)	-2(6)	57(8)	-5(7)
Cl(2)	98(2)	100(2)	69(2)	-31(2)	31(2)	-28(2)
Cl(3)	142(3)	177(4)	142(3)	-12(3)	55(3)	-59(3)
C(2X)	48(5)	34(4)	73(6)	-6(4)	31(4)	-9(4)
Cl(4)	49(1)	42(1)	79(2)	0(1)	34(1)	2(1)
Cl(5)	62(1)	63(1)	48(1)	-22(1)	25(1)	-30(1)
C(3X)	54(5)	50(5)	49(5)	11(4)	5(4)	-3(4)
Cl(6)	44(1)	80(2)	51(1)	9(1)	5(1)	-1(1)
Cl(7)	59(2)	91(2)	82(2)	25(2)	40(1)	8(1)
C(4X)	50(10)	53(11)	51(10)	-6(8)	23(8)	14(8)
Cl(8)	26(2)	72(3)	62(3)	-27(2)	-2(2)	-3(2)
Cl(9)	125(5)	51(3)	68(3)	19(3)	7(3)	7(3)

Table S6: Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for complex 2.

	x	y	z	U(eq)
H(3)	1375	3057	2686	35
H(4)	1174	2157	1645	39
H(5)	1541	2286	421	39
H(7)	2226	4676	2612	32
H(8A)	2219	3639	3904	70
H(8B)	2570	4393	4076	70
H(8C)	2832	3790	3564	70
H(9A)	1099	4742	2386	62
H(9B)	1477	4949	3363	62
H(9C)	1153	4183	3151	62
H(10)	2411	3755	-96	31
H(11A)	3072	2767	511	48
H(11B)	2895	2754	-524	48
H(11C)	2528	2239	-34	48
H(12A)	1475	2708	-924	52
H(12B)	1813	3255	-1416	52
H(12C)	1318	3537	-921	52
H(13)	4022	5172	1511	19
H(15A)	3624	3825	2697	41
H(15B)	4047	3197	2477	41
H(15C)	3394	3435	1777	41
H(16A)	3928	3645	646	39
H(16B)	4563	3329	1314	39
H(16C)	4588	4081	866	39
H(18)	4702	3795	3560	30
H(19)	5654	4198	4545	39
H(20)	6318	4987	4101	42
H(21)	6031	5403	2671	35
H(22)	5057	5023	1693	29
H(24)	1755	4877	-2136	45
H(25)	2932	4969	-2080	48
H(27A)	1453	5490	-230	50
H(27B)	1493	4651	-75	50
H(27C)	1097	4964	-998	50
H(28A)	3990	5255	-904	48
H(28B)	4008	4784	-71	48
H(28C)	3892	5621	-54	48
H(30)	1911	6434	3293	32
H(31)	3028	6126	4249	31
H(33A)	1297	6289	1627	44
H(33B)	1494	5541	1310	44
H(33C)	1772	6259	1029	44
H(34A)	3857	4922	3452	38
H(34B)	4092	5647	3959	38

H(34C)	4081	5569	2964	38
H(35)	7060	2043	2440	24
H(36A)	5931	3503	2889	45
H(36B)	6150	3744	2054	45
H(37A)	7113	4042	2999	39
H(37B)	6947	3626	3784	39
H(40)	4428	1554	1759	26
H(42)	5065	2084	-277	27
H(44A)	5368	2522	3283	41
H(44B)	5795	1819	3376	41
H(44C)	5031	1760	3195	41
H(45A)	3899	1767	-484	43
H(45B)	3708	1440	325	43
H(45C)	4137	990	-143	43
H(46A)	6564	2368	620	44
H(46B)	6329	3143	798	44
H(46C)	6013	2761	-112	44
H(49)	9302	2934	4857	40
H(51)	9150	3210	2328	48
H(53A)	7949	3309	4991	56
H(53B)	8404	2639	5331	56
H(53C)	7708	2530	4655	56
H(54A)	10223	3554	4029	94
H(54B)	10188	2971	3296	94
H(54C)	10256	2730	4271	94
H(55A)	8151	3361	1277	46
H(55B)	7543	3555	1608	46
H(55C)	7676	2749	1402	46
H(1X1)	1731	4808	6443	95
H(1X2)	1281	5457	6001	95
H(2X1)	2677	3589	8019	59
H(2X2)	2722	2823	7614	59
H(3X1)	261	4489	10813	64
H(3X2)	730	3835	10808	64
H(4X1)	-711	4355	6363	59
H(4X2)	-121	4085	6042	59

Table S7: Torsion angles [°] for complex 2

C(13)-W(1)-N(1)-C(1)	-170(15)
N(2)-W(1)-N(1)-C(1)	-67(15)
N(3)-W(1)-N(1)-C(1)	88(15)
Cl(1)-W(1)-N(1)-C(1)	12(15)
W(1)-N(1)-C(1)-C(6)	90(15)
W(1)-N(1)-C(1)-C(2)	-92(15)
N(1)-W(1)-N(2)-C(23)	51.9(5)
C(13)-W(1)-N(2)-C(23)	153.8(5)
N(3)-W(1)-N(2)-C(23)	-63.2(7)
Cl(1)-W(1)-N(2)-C(23)	-105.0(5)
N(1)-W(1)-N(2)-C(26)	-127.4(5)
C(13)-W(1)-N(2)-C(26)	-25.5(6)
N(3)-W(1)-N(2)-C(26)	117.5(6)
Cl(1)-W(1)-N(2)-C(26)	75.7(5)
N(1)-C(1)-C(2)-C(3)	-178.8(5)
C(6)-C(1)-C(2)-C(3)	-0.6(9)
N(1)-C(1)-C(2)-C(7)	1.6(9)
C(6)-C(1)-C(2)-C(7)	179.8(6)
N(1)-W(1)-N(3)-C(32)	95.5(5)
C(13)-W(1)-N(3)-C(32)	-6.1(6)
N(2)-W(1)-N(3)-C(32)	-149.1(5)
Cl(1)-W(1)-N(3)-C(32)	-107.4(5)
N(1)-W(1)-N(3)-C(29)	-75.9(4)
C(13)-W(1)-N(3)-C(29)	-177.5(4)
N(2)-W(1)-N(3)-C(29)	39.5(7)
Cl(1)-W(1)-N(3)-C(29)	81.2(4)
C(1)-C(2)-C(3)-C(4)	1.0(10)
C(7)-C(2)-C(3)-C(4)	-179.4(6)
C(2)-C(3)-C(4)-C(5)	-0.8(10)
C(3)-C(4)-C(5)-C(6)	0.3(11)
C(4)-C(5)-C(6)-C(1)	0.1(10)
C(4)-C(5)-C(6)-C(10)	178.2(6)
N(1)-C(1)-C(6)-C(5)	178.3(6)
C(2)-C(1)-C(6)-C(5)	0.1(9)
N(1)-C(1)-C(6)-C(10)	0.2(9)
C(2)-C(1)-C(6)-C(10)	-178.0(6)
C(3)-C(2)-C(7)-C(8)	65.9(8)
C(1)-C(2)-C(7)-C(8)	-114.4(7)
C(3)-C(2)-C(7)-C(9)	-58.1(8)
C(1)-C(2)-C(7)-C(9)	121.5(7)
C(5)-C(6)-C(10)-C(11)	-66.2(8)
C(1)-C(6)-C(10)-C(11)	111.9(7)
C(5)-C(6)-C(10)-C(12)	55.9(8)
C(1)-C(6)-C(10)-C(12)	-126.1(6)
N(1)-W(1)-C(13)-C(14)	2.3(7)
N(2)-W(1)-C(13)-C(14)	-97.0(7)

N(3)-W(1)-C(13)-C(14)	100.0(7)
Cl(1)-W(1)-C(13)-C(14)	-178.3(7)
W(1)-C(13)-C(14)-C(15)	-21.6(9)
W(1)-C(13)-C(14)-C(17)	-145.8(6)
W(1)-C(13)-C(14)-C(16)	96.3(7)
C(13)-C(14)-C(17)-C(18)	121.8(6)
C(15)-C(14)-C(17)-C(18)	-1.3(8)
C(16)-C(14)-C(17)-C(18)	-118.9(6)
C(13)-C(14)-C(17)-C(22)	-58.3(7)
C(15)-C(14)-C(17)-C(22)	178.5(5)
C(16)-C(14)-C(17)-C(22)	60.9(7)
C(22)-C(17)-C(18)-C(19)	1.2(9)
C(14)-C(17)-C(18)-C(19)	-179.0(5)
C(17)-C(18)-C(19)-C(20)	-1.4(10)
C(18)-C(19)-C(20)-C(21)	0.5(10)
C(19)-C(20)-C(21)-C(22)	0.5(10)
C(18)-C(17)-C(22)-C(21)	-0.2(9)
C(14)-C(17)-C(22)-C(21)	-180.0(5)
C(20)-C(21)-C(22)-C(17)	-0.7(9)
C(26)-N(2)-C(23)-C(24)	1.9(7)
W(1)-N(2)-C(23)-C(24)	-177.6(4)
C(26)-N(2)-C(23)-C(27)	-174.8(6)
W(1)-N(2)-C(23)-C(27)	5.8(9)
N(2)-C(23)-C(24)-C(25)	-1.2(8)
C(27)-C(23)-C(24)-C(25)	175.3(7)
C(23)-C(24)-C(25)-C(26)	0.0(8)
C(24)-C(25)-C(26)-N(2)	1.2(8)
C(24)-C(25)-C(26)-C(28)	-176.7(6)
C(23)-N(2)-C(26)-C(25)	-1.9(7)
W(1)-N(2)-C(26)-C(25)	177.5(5)
C(23)-N(2)-C(26)-C(28)	176.1(6)
W(1)-N(2)-C(26)-C(28)	-4.5(9)
C(32)-N(3)-C(29)-C(30)	-0.7(7)
W(1)-N(3)-C(29)-C(30)	172.7(4)
C(32)-N(3)-C(29)-C(33)	-178.3(6)
W(1)-N(3)-C(29)-C(33)	-4.9(8)
N(3)-C(29)-C(30)-C(31)	0.4(7)
C(33)-C(29)-C(30)-C(31)	177.8(6)
C(29)-C(30)-C(31)-C(32)	0.0(7)
C(29)-N(3)-C(32)-C(31)	0.7(7)
W(1)-N(3)-C(32)-C(31)	-171.4(4)
C(29)-N(3)-C(32)-C(34)	-179.6(5)
W(1)-N(3)-C(32)-C(34)	8.3(9)
C(30)-C(31)-C(32)-N(3)	-0.5(7)
C(30)-C(31)-C(32)-C(34)	179.9(6)
C(38)-N(4)-C(35)-N(5)	171.2(5)
C(36)-N(4)-C(35)-N(5)	6.0(7)

C(47)-N(5)-C(35)-N(4)	-168.0(5)
C(37)-N(5)-C(35)-N(4)	3.4(7)
C(35)-N(4)-C(36)-C(37)	-12.0(7)
C(38)-N(4)-C(36)-C(37)	-179.0(5)
C(35)-N(5)-C(37)-C(36)	-10.6(7)
C(47)-N(5)-C(37)-C(36)	161.3(6)
N(4)-C(36)-C(37)-N(5)	13.0(7)
C(35)-N(4)-C(38)-C(39)	112.2(7)
C(36)-N(4)-C(38)-C(39)	-83.8(7)
C(35)-N(4)-C(38)-C(43)	-74.5(8)
C(36)-N(4)-C(38)-C(43)	89.5(7)
C(43)-C(38)-C(39)-C(40)	1.6(9)
N(4)-C(38)-C(39)-C(40)	174.7(5)
C(43)-C(38)-C(39)-C(44)	-178.2(6)
N(4)-C(38)-C(39)-C(44)	-5.1(8)
C(38)-C(39)-C(40)-C(41)	-1.5(9)
C(44)-C(39)-C(40)-C(41)	178.4(6)
C(39)-C(40)-C(41)-C(42)	1.0(9)
C(39)-C(40)-C(41)-C(45)	179.8(6)
C(40)-C(41)-C(42)-C(43)	-0.7(9)
C(45)-C(41)-C(42)-C(43)	-179.5(6)
C(41)-C(42)-C(43)-C(38)	0.8(9)
C(41)-C(42)-C(43)-C(46)	-179.3(6)
C(39)-C(38)-C(43)-C(42)	-1.3(9)
N(4)-C(38)-C(43)-C(42)	-174.4(5)
C(39)-C(38)-C(43)-C(46)	178.9(6)
N(4)-C(38)-C(43)-C(46)	5.7(9)
C(35)-N(5)-C(47)-C(48)	-113.6(7)
C(37)-N(5)-C(47)-C(48)	76.0(8)
C(35)-N(5)-C(47)-C(52)	69.9(8)
C(37)-N(5)-C(47)-C(52)	-100.5(7)
C(52)-C(47)-C(48)-C(49)	-1.2(10)
N(5)-C(47)-C(48)-C(49)	-177.5(6)
C(52)-C(47)-C(48)-C(53)	177.0(6)
N(5)-C(47)-C(48)-C(53)	0.7(10)
C(47)-C(48)-C(49)-C(50)	-0.5(10)
C(53)-C(48)-C(49)-C(50)	-178.8(7)
C(48)-C(49)-C(50)-C(51)	1.9(11)
C(48)-C(49)-C(50)-C(54)	-178.0(8)
C(49)-C(50)-C(51)-C(52)	-1.6(12)
C(54)-C(50)-C(51)-C(52)	178.2(8)
C(50)-C(51)-C(52)-C(47)	0.0(11)
C(50)-C(51)-C(52)-C(55)	178.7(7)
C(48)-C(47)-C(52)-C(51)	1.5(10)
N(5)-C(47)-C(52)-C(51)	177.8(6)
C(48)-C(47)-C(52)-C(55)	-177.2(6)
N(5)-C(47)-C(52)-C(55)	-0.8(9)

Crystal data and structure refinement for complex 3.

Empirical formula	C62.50 H75 Cl3 F5 N5 O W
Formula weight	1297.47
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P 21/c
Unit cell dimensions	a = 11.2444(3) Å, α = 90°
	b = 26.1267(5) Å, β = 94.9910(10)°
	c = 20.6154(4) Å, γ = 90°
Volume	6033.4(2) $Å^3$
Z, Calculated density	4, 1.428 Mg/m^3
Absorption coefficient	2.107 mm^{-1}
F (000)	2652
Crystal size	0.21 x 0.17 x 0.16 mm
Theta range for data collection	1.56 to 28.30°
Limiting indices	-14<=h<=15, -30<=k<=34, -25<=l<=27
Reflections collected / unique	61583 / 14733 [R (int) = 0.0344]
Completeness to theta = 28.30	98.3 %
Absorption correction	Numerical
Max. and min. transmission	0.8546 and 0.7560
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	14733 / 0 / 736
Goodness-of-fit on F^2	1.024
Final R indices [I>2sigma (I)]	R1 = 0.0271, wR2 = 0.0545
R indices (all data)	R1 = 0.0400, wR2 = 0.0571
Largest diff. peak and hole	0.876 and -0.746 e. $Å^{-3}$

Table S8: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for complex 3. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
W(1)	1970(1)	4053(1)	7136(1)	14(1)
O(1)	2877(1)	3454(1)	6737(1)	19(1)
N(1)	872(2)	4384(1)	7525(1)	18(1)
F(1)	2751(2)	2669(1)	7653(1)	39(1)
C(1)	3789(2)	3147(1)	6902(1)	18(1)
N(2)	2930(2)	3792(1)	8012(1)	17(1)
F(2)	4671(2)	2098(1)	8003(1)	64(1)
C(2)	4844(2)	3186(1)	6598(1)	22(1)
N(3)	893(2)	3899(1)	6257(1)	16(1)
C(3)	5814(2)	2868(1)	6749(2)	37(1)
F(3)	6701(2)	2198(1)	7390(1)	75(1)
F(4)	6800(1)	2919(1)	6434(1)	57(1)
C(4)	5752(3)	2505(1)	7228(2)	44(1)
F(5)	4929(1)	3554(1)	6144(1)	30(1)
C(5)	4735(3)	2455(1)	7531(1)	38(1)
C(6)	3767(2)	2759(1)	7363(1)	26(1)
C(7)	-44(2)	4613(1)	7844(1)	25(1)
C(8)	210(3)	4803(1)	8484(1)	36(1)
C(9)	-735(4)	5040(1)	8771(1)	55(1)
C(10)	-1857(3)	5082(1)	8462(2)	57(1)
C(11)	-2088(3)	4893(1)	7840(2)	43(1)
C(12)	-1190(2)	4661(1)	7514(1)	28(1)
C(13)	1416(3)	4767(1)	8859(1)	41(1)
C(14)	1355(4)	4475(1)	9502(1)	56(1)
C(15)	1958(4)	5300(1)	9000(2)	63(1)
C(16)	-1464(2)	4490(1)	6815(1)	28(1)
C(17)	-1652(3)	4950(1)	6358(1)	39(1)

C(18)	-2544(2)	4136(1)	6723(2)	40(1)
C(19)	2877(2)	4622(1)	6901(1)	19(1)
C(20)	2992(2)	5205(1)	6960(1)	25(1)
C(21)	3919(3)	5331(1)	7539(1)	40(1)
C(22)	1809(3)	5449(1)	7097(1)	36(1)
C(23)	3475(2)	5416(1)	6336(1)	29(1)
C(24)	2839(3)	5764(1)	5930(1)	38(1)
C(25)	3277(3)	5921(1)	5347(2)	52(1)
C(26)	4350(3)	5748(1)	5174(2)	58(1)
C(27)	5021(3)	5415(1)	5584(2)	46(1)
C(28)	4579(2)	5253(1)	6156(1)	33(1)
C(29)	4138(2)	3831(1)	8225(1)	19(1)
C(30)	4334(2)	3624(1)	8837(1)	28(1)
C(31)	3221(2)	3451(1)	9021(1)	25(1)
C(32)	2381(2)	3551(1)	8513(1)	19(1)
C(33)	5057(2)	4066(1)	7837(1)	25(1)
C(34)	1102(2)	3399(1)	8469(1)	25(1)
C(35)	107(2)	3486(1)	6226(1)	20(1)
C(36)	-546(2)	3483(1)	5634(1)	25(1)
C(37)	-169(2)	3909(1)	5281(1)	26(1)
C(38)	710(2)	4155(1)	5668(1)	19(1)
C(39)	2(2)	3141(1)	6794(1)	26(1)
C(40)	1372(2)	4626(1)	5505(1)	24(1)
N(4)	3091(2)	2051(1)	9741(1)	22(1)
N(5)	2180(2)	1685(1)	8875(1)	22(1)
C(41)	2646(2)	2105(1)	9137(1)	21(1)
C(42)	2922(3)	1516(1)	9963(1)	29(1)
C(43)	2286(2)	1263(1)	9356(1)	25(1)
C(44)	3696(2)	2445(1)	10136(1)	22(1)

C(45)	4882(2)	2558(1)	10045(1)	26(1)
C(46)	5417(2)	2956(1)	10414(1)	30(1)
C(47)	4803(3)	3231(1)	10853(1)	32(1)
C(48)	3636(3)	3099(1)	10931(1)	30(1)
C(49)	3054(2)	2706(1)	10578(1)	24(1)
C(50)	5568(3)	2280(1)	9560(1)	41(1)
C(51)	5404(3)	3666(1)	11241(2)	48(1)
C(52)	1764(3)	2585(1)	10658(1)	36(1)
C(53)	1426(2)	1659(1)	8273(1)	23(1)
C(54)	1851(2)	1416(1)	7737(1)	28(1)
C(55)	1095(3)	1408(1)	7165(1)	35(1)
C(56)	-26(3)	1631(1)	7123(1)	38(1)
C(57)	-423(3)	1853(1)	7674(1)	35(1)
C(58)	283(2)	1867(1)	8260(1)	28(1)
C(59)	3058(3)	1166(1)	7765(1)	39(1)
C(60)	-812(3)	1627(1)	6485(2)	57(1)
C(61)	-195(2)	2088(1)	8864(1)	34(1)
C(1X)	8010(3)	3723(1)	8902(1)	43(1)
Cl(1)	8495(1)	3509(1)	9694(1)	73(1)
Cl(2)	7799(1)	3206(1)	8362(1)	47(1)
C(2X)	-5256(7)	4588(3)	9804(3)	57(2)
Cl(3)	-5571(2)	5023(1)	10417(1)	75(1)
Cl(4)	-4182(2)	4831(1)	9330(1)	56(1)

Table S9: Bond lengths [Å] and angles [°] for complex 3.

W(1)-N(1)	1.7566(18)
W(1)-C(19)	1.889(2)
W(1)-O(1)	2.0775(15)
W(1)-N(3)	2.1274(18)
W(1)-N(2)	2.1348(18)
O(1)-C(1)	1.323(3)
N(1)-C(7)	1.403(3)
F(1)-C(6)	1.356(3)
C(1)-C(6)	1.391(3)
C(1)-C(2)	1.392(3)
N(2)-C(29)	1.394(3)
N(2)-C(32)	1.398(3)
F(2)-C(5)	1.355(3)
C(2)-F(5)	1.351(3)
C(2)-C(3)	1.383(3)
N(3)-C(38)	1.385(3)
N(3)-C(35)	1.393(3)
C(3)-F(4)	1.339(3)
C(3)-C(4)	1.376(4)
F(3)-C(4)	1.354(3)
C(4)-C(5)	1.356(5)
C(5)-C(6)	1.367(4)
C(7)-C(12)	1.408(4)
C(7)-C(8)	1.416(4)
C(8)-C(9)	1.405(4)
C(8)-C(13)	1.504(4)
C(9)-C(10)	1.367(5)
C(9)-H(9)	0.9500
C(10)-C(11)	1.379(5)
C(10)-H(10)	0.9500
C(11)-C(12)	1.398(3)
C(11)-H(11)	0.9500
C(12)-C(16)	1.515(4)
C(13)-C(14)	1.536(4)
C(13)-C(15)	1.538(4)
C(13)-H(13)	10.000
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-C(18)	1.526(4)
C(16)-C(17)	1.530(3)
C(16)-H(16)	10.000
C(17)-H(17A)	0.9800

C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-C(20)	1.534(3)
C(19)-H(19)	0.96(2)
C(20)-C(22)	1.524(4)
C(20)-C(23)	1.540(3)
C(20)-C(21)	1.551(3)
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-C(24)	1.392(4)
C(23)-C(28)	1.393(4)
C(24)-C(25)	1.398(4)
C(24)-H(24)	0.9500
C(25)-C(26)	1.365(5)
C(25)-H(25)	0.9500
C(26)-C(27)	1.389(4)
C(26)-H(26)	0.9500
C(27)-C(28)	1.386(4)
C(27)-H(27)	0.9500
C(28)-H(28)	0.9500
C(29)-C(30)	1.372(3)
C(29)-C(33)	1.493(3)
C(30)-C(31)	1.412(4)
C(30)-H(30)	0.9500
C(31)-C(32)	1.373(3)
C(31)-H(31)	0.9500
C(32)-C(34)	1.488(3)
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(35)-C(36)	1.368(3)
C(35)-C(39)	1.491(3)
C(36)-C(37)	1.416(3)
C(36)-H(36)	0.9500
C(37)-C(38)	1.375(3)
C(37)-H(37)	0.9500
C(38)-C(40)	1.491(3)

C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
C(40)-H(40A)	0.9800
C(40)-H(40B)	0.9800
C(40)-H(40C)	0.9800
N(4)-C(41)	1.308(3)
N(4)-C(44)	1.445(3)
N(4)-C(42)	1.487(3)
N(5)-C(41)	1.311(3)
N(5)-C(53)	1.443(3)
N(5)-C(43)	1.483(3)
C(41)-H(41)	0.91(2)
C(42)-C(43)	1.536(3)
C(42)-H(42A)	0.9900
C(42)-H(42B)	0.9900
C(43)-H(43A)	0.9900
C(43)-H(43B)	0.9900
C(44)-C(49)	1.389(3)
C(44)-C(45)	1.394(3)
C(45)-C(46)	1.393(3)
C(45)-C(50)	1.502(4)
C(46)-C(47)	1.387(4)
C(46)-H(46)	0.9500
C(47)-C(48)	1.379(4)
C(47)-C(51)	1.514(4)
C(48)-C(49)	1.391(3)
C(48)-H(48)	0.9500
C(49)-C(52)	1.507(4)
C(50)-H(50A)	0.9800
C(50)-H(50B)	0.9800
C(50)-H(50C)	0.9800
C(51)-H(51A)	0.9800
C(51)-H(51B)	0.9800
C(51)-H(51C)	0.9800
C(52)-H(52A)	0.9800
C(52)-H(52B)	0.9800
C(52)-H(52C)	0.9800
C(53)-C(58)	1.393(4)
C(53)-C(54)	1.394(3)
C(54)-C(55)	1.393(4)
C(54)-C(59)	1.503(4)
C(55)-C(56)	1.385(4)
C(55)-H(55)	0.9500
C(56)-C(57)	1.384(4)
C(56)-C(60)	1.519(4)
C(57)-C(58)	1.387(4)

C(57)-H(57)	0.9500
C(58)-C(61)	1.512(4)
C(59)-H(59A)	0.9800
C(59)-H(59B)	0.9800
C(59)-H(59C)	0.9800
C(60)-H(60A)	0.9800
C(60)-H(60B)	0.9800
C(60)-H(60C)	0.9800
C(61)-H(61A)	0.9800
C(61)-H(61B)	0.9800
C(61)-H(61C)	0.9800
C(1X)-Cl(2)	1.755(3)
C(1X)-Cl(1)	1.767(3)
C(1X)-H(1X1)	0.9900
C(1X)-H(1X2)	0.9900
C(2X)-Cl(3)#1	1.475(7)
C(2X)-Cl(4)	1.738(6)
C(2X)-Cl(3)	1.759(7)
C(2X)-H(2X1)	0.9712
C(2X)-H(2X2)	0.9789
Cl(3)-Cl(4)#1	0.7198(19)
Cl(3)-C(2X)#1	1.475(7)
Cl(3)-Cl(3)#1	2.239(4)
Cl(4)-Cl(3)#1	0.7197(19)

N(1)-W(1)-C(19)	98.47(10)
N(1)-W(1)-O(1)	160.06(8)
C(19)-W(1)-O(1)	101.37(9)
N(1)-W(1)-N(3)	96.41(8)
C(19)-W(1)-N(3)	102.18(8)
O(1)-W(1)-N(3)	77.49(6)
N(1)-W(1)-N(2)	95.36(8)
C(19)-W(1)-N(2)	102.91(8)
O(1)-W(1)-N(2)	82.21(6)
N(3)-W(1)-N(2)	150.30(7)
C(1)-O(1)-W(1)	138.77(14)
C(7)-N(1)-W(1)	175.84(17)
O(1)-C(1)-C(6)	123.9(2)
O(1)-C(1)-C(2)	120.8(2)
C(6)-C(1)-C(2)	115.2(2)
C(29)-N(2)-C(32)	106.29(18)
C(29)-N(2)-W(1)	130.58(14)
C(32)-N(2)-W(1)	123.09(15)
F(5)-C(2)-C(3)	118.7(2)
F(5)-C(2)-C(1)	118.5(2)
C(3)-C(2)-C(1)	122.8(2)
C(38)-N(3)-C(35)	106.71(18)

C(38)-N(3)-W(1)	133.24(15)
C(35)-N(3)-W(1)	119.87(14)
F(4)-C(3)-C(4)	120.7(3)
F(4)-C(3)-C(2)	120.2(3)
C(4)-C(3)-C(2)	119.1(3)
F(3)-C(4)-C(5)	120.5(3)
F(3)-C(4)-C(3)	119.9(3)
C(5)-C(4)-C(3)	119.6(2)
F(2)-C(5)-C(4)	119.8(3)
F(2)-C(5)-C(6)	119.4(3)
C(4)-C(5)-C(6)	120.7(3)
F(1)-C(6)-C(5)	118.0(2)
F(1)-C(6)-C(1)	119.6(2)
C(5)-C(6)-C(1)	122.4(3)
N(1)-C(7)-C(12)	119.4(2)
N(1)-C(7)-C(8)	119.3(2)
C(12)-C(7)-C(8)	121.4(2)
C(9)-C(8)-C(7)	116.7(3)
C(9)-C(8)-C(13)	119.5(3)
C(7)-C(8)-C(13)	123.8(2)
C(10)-C(9)-C(8)	122.7(3)
C(10)-C(9)-H(9)	118.6
C(8)-C(9)-H(9)	118.6
C(9)-C(10)-C(11)	119.7(3)
C(9)-C(10)-H(10)	120.1
C(11)-C(10)-H(10)	120.1
C(10)-C(11)-C(12)	121.1(3)
C(10)-C(11)-H(11)	119.4
C(12)-C(11)-H(11)	119.4
C(11)-C(12)-C(7)	118.4(3)
C(11)-C(12)-C(16)	119.2(3)
C(7)-C(12)-C(16)	122.3(2)
C(8)-C(13)-C(14)	111.6(3)
C(8)-C(13)-C(15)	111.5(3)
C(14)-C(13)-C(15)	109.4(2)
C(8)-C(13)-H(13)	108.1
C(14)-C(13)-H(13)	108.1
C(15)-C(13)-H(13)	108.1
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(12)-C(16)-C(18)	113.0(2)
C(12)-C(16)-C(17)	111.2(2)
C(18)-C(16)-C(17)	109.5(2)
C(12)-C(16)-H(16)	107.6
C(18)-C(16)-H(16)	107.6
C(17)-C(16)-H(16)	107.6
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(16)-C(18)-H(18A)	109.5
C(16)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(16)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(20)-C(19)-W(1)	143.67(19)
C(20)-C(19)-H(19)	111.5(14)
W(1)-C(19)-H(19)	104.8(14)
C(22)-C(20)-C(19)	111.1(2)
C(22)-C(20)-C(23)	112.5(2)
C(19)-C(20)-C(23)	108.8(2)
C(22)-C(20)-C(21)	107.9(2)
C(19)-C(20)-C(21)	108.5(2)
C(23)-C(20)-C(21)	107.8(2)
C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(20)-C(22)-H(22A)	109.5
C(20)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(20)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(24)-C(23)-C(28)	117.5(2)
C(24)-C(23)-C(20)	122.4(3)
C(28)-C(23)-C(20)	120.0(2)
C(23)-C(24)-C(25)	120.5(3)
C(23)-C(24)-H(24)	119.7

C(25)-C(24)-H(24)	119.7
C(26)-C(25)-C(24)	120.9(3)
C(26)-C(25)-H(25)	119.6
C(24)-C(25)-H(25)	119.6
C(25)-C(26)-C(27)	119.6(3)
C(25)-C(26)-H(26)	120.2
C(27)-C(26)-H(26)	120.2
C(28)-C(27)-C(26)	119.6(3)
C(28)-C(27)-H(27)	120.2
C(26)-C(27)-H(27)	120.2
C(27)-C(28)-C(23)	121.8(3)
C(27)-C(28)-H(28)	119.1
C(23)-C(28)-H(28)	119.1
C(30)-C(29)-N(2)	109.5(2)
C(30)-C(29)-C(33)	126.2(2)
N(2)-C(29)-C(33)	124.20(19)
C(29)-C(30)-C(31)	107.3(2)
C(29)-C(30)-H(30)	126.3
C(31)-C(30)-H(30)	126.3
C(32)-C(31)-C(30)	107.5(2)
C(32)-C(31)-H(31)	126.2
C(30)-C(31)-H(31)	126.2
C(31)-C(32)-N(2)	109.3(2)
C(31)-C(32)-C(34)	126.3(2)
N(2)-C(32)-C(34)	124.2(2)
C(29)-C(33)-H(33A)	109.5
C(29)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(29)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(32)-C(34)-H(34A)	109.5
C(32)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(32)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(36)-C(35)-N(3)	109.6(2)
C(36)-C(35)-C(39)	128.6(2)
N(3)-C(35)-C(39)	121.7(2)
C(35)-C(36)-C(37)	107.0(2)
C(35)-C(36)-H(36)	126.5
C(37)-C(36)-H(36)	126.5
C(38)-C(37)-C(36)	107.4(2)
C(38)-C(37)-H(37)	126.3
C(36)-C(37)-H(37)	126.3
C(37)-C(38)-N(3)	109.2(2)

C(37)-C(38)-C(40)	126.9(2)
N(3)-C(38)-C(40)	123.9(2)
C(35)-C(39)-H(39A)	109.5
C(35)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(35)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(38)-C(40)-H(40A)	109.5
C(38)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(38)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
C(41)-N(4)-C(44)	125.52(19)
C(41)-N(4)-C(42)	110.24(19)
C(44)-N(4)-C(42)	124.20(18)
C(41)-N(5)-C(53)	125.3(2)
C(41)-N(5)-C(43)	109.97(19)
C(53)-N(5)-C(43)	123.15(19)
N(4)-C(41)-N(5)	114.0(2)
N(4)-C(41)-H(41)	123.9(15)
N(5)-C(41)-H(41)	122.1(15)
N(4)-C(42)-C(43)	102.59(18)
N(4)-C(42)-H(42A)	111.2
C(43)-C(42)-H(42A)	111.2
N(4)-C(42)-H(42B)	111.2
C(43)-C(42)-H(42B)	111.2
H(42A)-C(42)-H(42B)	109.2
N(5)-C(43)-C(42)	103.15(18)
N(5)-C(43)-H(43A)	111.1
C(42)-C(43)-H(43A)	111.1
N(5)-C(43)-H(43B)	111.1
C(42)-C(43)-H(43B)	111.1
H(43A)-C(43)-H(43B)	109.1
C(49)-C(44)-C(45)	122.8(2)
C(49)-C(44)-N(4)	118.2(2)
C(45)-C(44)-N(4)	118.9(2)
C(46)-C(45)-C(44)	117.2(2)
C(46)-C(45)-C(50)	120.1(2)
C(44)-C(45)-C(50)	122.7(2)
C(47)-C(46)-C(45)	121.9(3)
C(47)-C(46)-H(46)	119.1
C(45)-C(46)-H(46)	119.1
C(48)-C(47)-C(46)	118.7(2)
C(48)-C(47)-C(51)	120.7(3)
C(46)-C(47)-C(51)	120.6(3)

C(47)-C(48)-C(49)	122.1(2)
C(47)-C(48)-H(48)	118.9
C(49)-C(48)-H(48)	118.9
C(44)-C(49)-C(48)	117.3(2)
C(44)-C(49)-C(52)	122.0(2)
C(48)-C(49)-C(52)	120.6(2)
C(45)-C(50)-H(50A)	109.5
C(45)-C(50)-H(50B)	109.5
H(50A)-C(50)-H(50B)	109.5
C(45)-C(50)-H(50C)	109.5
H(50A)-C(50)-H(50C)	109.5
H(50B)-C(50)-H(50C)	109.5
C(47)-C(51)-H(51A)	109.5
C(47)-C(51)-H(51B)	109.5
H(51A)-C(51)-H(51B)	109.5
C(47)-C(51)-H(51C)	109.5
H(51A)-C(51)-H(51C)	109.5
H(51B)-C(51)-H(51C)	109.5
C(49)-C(52)-H(52A)	109.5
C(49)-C(52)-H(52B)	109.5
H(52A)-C(52)-H(52B)	109.5
C(49)-C(52)-H(52C)	109.5
H(52A)-C(52)-H(52C)	109.5
H(52B)-C(52)-H(52C)	109.5
C(58)-C(53)-C(54)	122.8(2)
C(58)-C(53)-N(5)	118.0(2)
C(54)-C(53)-N(5)	119.2(2)
C(55)-C(54)-C(53)	116.9(3)
C(55)-C(54)-C(59)	120.6(2)
C(53)-C(54)-C(59)	122.6(2)
C(56)-C(55)-C(54)	122.1(3)
C(56)-C(55)-H(55)	118.9
C(54)-C(55)-H(55)	118.9
C(57)-C(56)-C(55)	118.9(2)
C(57)-C(56)-C(60)	120.5(3)
C(55)-C(56)-C(60)	120.6(3)
C(56)-C(57)-C(58)	121.7(3)
C(56)-C(57)-H(57)	119.2
C(58)-C(57)-H(57)	119.2
C(57)-C(58)-C(53)	117.6(3)
C(57)-C(58)-C(61)	120.6(3)
C(53)-C(58)-C(61)	121.8(2)
C(54)-C(59)-H(59A)	109.5
C(54)-C(59)-H(59B)	109.5
H(59A)-C(59)-H(59B)	109.5
C(54)-C(59)-H(59C)	109.5
H(59A)-C(59)-H(59C)	109.5

H(59B)-C(59)-H(59C)	109.5
C(56)-C(60)-H(60A)	109.5
C(56)-C(60)-H(60B)	109.5
H(60A)-C(60)-H(60B)	109.5
C(56)-C(60)-H(60C)	109.5
H(60A)-C(60)-H(60C)	109.5
H(60B)-C(60)-H(60C)	109.5
C(58)-C(61)-H(61A)	109.5
C(58)-C(61)-H(61B)	109.5
H(61A)-C(61)-H(61B)	109.5
C(58)-C(61)-H(61C)	109.5
H(61A)-C(61)-H(61C)	109.5
H(61B)-C(61)-H(61C)	109.5
Cl(2)-C(1X)-Cl(1)	110.84(17)
Cl(2)-C(1X)-H(1X1)	109.5
Cl(1)-C(1X)-H(1X1)	109.5
Cl(2)-C(1X)-H(1X2)	109.5
Cl(1)-C(1X)-H(1X2)	109.5
H(1X1)-C(1X)-H(1X2)	108.1
Cl(3)#1-C(2X)-Cl(4)	24.16(13)
Cl(3)#1-C(2X)-Cl(3)	87.1(3)
Cl(4)-C(2X)-Cl(3)	111.2(4)
Cl(3)#1-C(2X)-H(2X1)	119.7
Cl(4)-C(2X)-H(2X1)	110.5
Cl(3)-C(2X)-H(2X1)	109.9
Cl(3)#1-C(2X)-H(2X2)	122.7
Cl(4)-C(2X)-H(2X2)	110.0
Cl(3)-C(2X)-H(2X2)	109.3
H(2X1)-C(2X)-H(2X2)	105.8
Cl(4)#1-Cl(3)-C(2X)#1	98.8(4)
Cl(4)#1-Cl(3)-C(2X)	167.4(4)
C(2X)#1-Cl(3)-C(2X)	92.9(3)
Cl(4)#1-Cl(3)-Cl(3)#1	150.3(4)
C(2X)#1-Cl(3)-Cl(3)#1	51.7(3)
C(2X)-Cl(3)-Cl(3)#1	41.1(2)
Cl(3)#1-Cl(4)-C(2X)	57.0(3)

Symmetry transformations used to generate equivalent atoms: #1 -x-1,-y+1,-z+2.

Table S10: Anisotropic displacement parameters (A^2 x 10^3) for complex 3. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$.

	U11	U22	U33	U23	U13	U12
W(1)	15(1)	15(1)	12(1)	0(1)	2(1)	0(1)
O(1)	20(1)	21(1)	17(1)	-2(1)	1(1)	5(1)
N(1)	23(1)	19(1)	12(1)	1(1)	3(1)	2(1)
F(1)	63(1)	24(1)	31(1)	2(1)	19(1)	-9(1)
C(1)	24(1)	15(1)	14(1)	-4(1)	-2(1)	2(1)
N(2)	19(1)	18(1)	15(1)	0(1)	2(1)	-3(1)
F(2)	115(2)	24(1)	46(1)	12(1)	-26(1)	7(1)
C(2)	21(1)	21(1)	22(1)	-3(1)	1(1)	0(1)
N(3)	15(1)	19(1)	14(1)	-3(1)	2(1)	1(1)
C(3)	19(1)	36(2)	54(2)	-20(1)	-3(1)	3(1)
F(3)	55(1)	46(1)	115(2)	-18(1)	-43(1)	33(1)
F(4)	20(1)	58(1)	95(2)	-28(1)	11(1)	3(1)
C(4)	43(2)	27(2)	56(2)	-13(1)	-28(2)	19(1)
F(5)	30(1)	37(1)	26(1)	2(1)	9(1)	-5(1)
C(5)	60(2)	17(1)	32(2)	0(1)	-16(1)	7(1)
C(6)	40(2)	19(1)	20(1)	-4(1)	2(1)	0(1)
C(7)	36(2)	21(1)	21(1)	3(1)	15(1)	9(1)
C(8)	62(2)	26(1)	22(1)	1(1)	15(1)	13(1)
C(9)	99(3)	44(2)	25(2)	2(1)	31(2)	28(2)
C(10)	72(3)	56(2)	49(2)	18(2)	42(2)	38(2)
C(11)	41(2)	43(2)	49(2)	18(2)	28(2)	20(1)
C(12)	30(1)	27(1)	30(1)	10(1)	17(1)	10(1)
C(13)	73(2)	32(2)	17(1)	-9(1)	3(1)	9(2)
C(14)	101(3)	47(2)	19(1)	-4(1)	5(2)	24(2)
C(15)	116(4)	39(2)	33(2)	-13(2)	-7(2)	1(2)
C(16)	20(1)	36(1)	29(1)	11(1)	9(1)	10(1)
C(17)	38(2)	45(2)	35(2)	18(1)	11(1)	7(1)
C(18)	25(1)	50(2)	45(2)	17(1)	4(1)	1(1)
C(19)	21(1)	22(1)	15(1)	0(1)	-3(1)	-2(1)
C(20)	31(1)	19(1)	24(1)	2(1)	-3(1)	-6(1)
C(21)	57(2)	30(2)	29(1)	-1(1)	-13(1)	-16(1)
C(22)	50(2)	18(1)	39(2)	-5(1)	6(1)	1(1)
C(23)	29(1)	24(1)	30(1)	7(1)	-11(1)	-14(1)
C(24)	33(2)	33(2)	45(2)	17(1)	-13(1)	-12(1)
C(25)	45(2)	54(2)	52(2)	38(2)	-19(2)	-21(2)
C(26)	40(2)	80(2)	50(2)	39(2)	-11(2)	-33(2)
C(27)	29(2)	63(2)	46(2)	23(2)	-3(1)	-22(2)
C(28)	26(1)	39(2)	33(1)	15(1)	-9(1)	-15(1)
C(29)	21(1)	17(1)	19(1)	1(1)	-2(1)	0(1)
C(30)	27(1)	30(1)	24(1)	6(1)	-5(1)	2(1)
C(31)	34(1)	22(1)	18(1)	6(1)	2(1)	0(1)
C(32)	25(1)	16(1)	17(1)	1(1)	5(1)	-1(1)
C(33)	19(1)	30(1)	24(1)	1(1)	-1(1)	-3(1)
C(34)	29(1)	26(1)	19(1)	7(1)	4(1)	-3(1)

C(35)	20(1)	19(1)	23(1)	-2(1)	2(1)	0(1)
C(36)	21(1)	27(1)	26(1)	-6(1)	-4(1)	-3(1)
C(37)	25(1)	33(1)	18(1)	-1(1)	-3(1)	2(1)
C(38)	17(1)	25(1)	15(1)	-1(1)	3(1)	4(1)
C(39)	24(1)	24(1)	29(1)	0(1)	1(1)	-7(1)
C(40)	24(1)	29(1)	18(1)	4(1)	0(1)	1(1)
N(4)	30(1)	17(1)	19(1)	3(1)	0(1)	-6(1)
N(5)	28(1)	18(1)	19(1)	1(1)	0(1)	-5(1)
C(41)	25(1)	18(1)	21(1)	2(1)	2(1)	-2(1)
C(42)	42(2)	19(1)	25(1)	5(1)	-4(1)	-6(1)
C(43)	36(2)	17(1)	22(1)	1(1)	1(1)	-4(1)
C(44)	32(1)	16(1)	16(1)	3(1)	-4(1)	-5(1)
C(45)	32(1)	23(1)	24(1)	4(1)	0(1)	-5(1)
C(46)	29(1)	28(1)	34(1)	6(1)	-4(1)	-10(1)
C(47)	45(2)	24(1)	25(1)	3(1)	-7(1)	-10(1)
C(48)	45(2)	24(1)	21(1)	-2(1)	2(1)	-4(1)
C(49)	34(1)	21(1)	17(1)	4(1)	1(1)	-4(1)
C(50)	37(2)	41(2)	46(2)	-8(1)	11(1)	-8(1)
C(51)	62(2)	36(2)	44(2)	-8(1)	-9(2)	-20(2)
C(52)	37(2)	36(2)	37(2)	-8(1)	11(1)	-7(1)
C(53)	30(1)	20(1)	18(1)	3(1)	-2(1)	-7(1)
C(54)	38(2)	23(1)	22(1)	2(1)	3(1)	-10(1)
C(55)	56(2)	28(1)	21(1)	-1(1)	-1(1)	-14(1)
C(56)	49(2)	30(2)	31(2)	6(1)	-15(1)	-18(1)
C(57)	35(2)	29(1)	41(2)	11(1)	-8(1)	-7(1)
C(58)	34(2)	20(1)	29(1)	6(1)	-3(1)	-6(1)
C(59)	47(2)	43(2)	29(2)	-6(1)	10(1)	-3(1)
C(60)	72(3)	53(2)	41(2)	6(2)	-28(2)	-22(2)
C(61)	32(2)	31(2)	40(2)	4(1)	3(1)	5(1)
C(1X)	36(2)	56(2)	39(2)	3(2)	5(1)	10(2)
Cl(1)	65(1)	121(1)	33(1)	11(1)	5(1)	-22(1)
Cl(2)	44(1)	49(1)	47(1)	4(1)	-8(1)	7(1)
C(2X)	60(5)	59(4)	58(4)	-18(4)	33(4)	-19(4)
Cl(3)	65(1)	101(2)	63(1)	-41(1)	27(1)	4(1)
Cl(4)	56(1)	64(1)	49(1)	-19(1)	22(1)	-24(1)

Table S11: Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for complex 3.

	x	y	z	U(eq)
H(9)	-589	5177	9197	66
H(10)	-2474	5241	8676	68
H(11)	-2870	4920	7628	52
H(13)	1959	4574	8587	49
H(14A)	845	4663	9782	83
H(14B)	2160	4443	9722	83
H(14C)	1021	4134	9412	83
H(15A)	1991	5487	8590	95
H(15B)	2767	5263	9213	95
H(15C)	1462	5489	9286	95
H(16)	-755	4296	6685	34
H(17A)	-2373	5135	6456	59
H(17B)	-1744	4830	5905	59
H(17C)	-961	5178	6418	59
H(18A)	-2422	3841	7016	60
H(18B)	-2641	4016	6271	60
H(18C)	-3262	4322	6824	60
H(19)	3510(20)	4479(9)	6676(11)	19(6)
H(21A)	3664	5177	7938	60
H(21B)	3979	5703	7594	60
H(21C)	4699	5192	7452	60
H(22A)	1199	5363	6745	53
H(22B)	1903	5821	7123	53
H(22C)	1563	5319	7510	53
H(24)	2102	5896	6049	45
H(25)	2822	6151	5069	62
H(26)	4636	5854	4775	69
H(27)	5779	5300	5473	56
H(28)	5042	5024	6433	40
H(30)	5079	3601	9090	33
H(31)	3080	3293	9422	30
H(33A)	5166	4427	7960	37
H(33B)	4794	4043	7372	37
H(33C)	5816	3884	7924	37
H(34A)	967	3118	8155	37
H(34B)	603	3692	8325	37
H(34C)	892	3285	8898	37
H(36)	-1140	3241	5488	30
H(37)	-469	4007	4853	31
H(39A)	-589	2874	6676	38
H(39B)	-251	3340	7161	38
H(39C)	778	2982	6919	38
H(40A)	1223	4897	5815	35
H(40B)	1098	4737	5063	35

H(40C)	2229	4551	5528	35
H(41)	2640(20)	2407(9)	8914(11)	16(6)
H(42A)	2423	1505	10335	35
H(42B)	3698	1349	10090	35
H(43A)	2765	977	9201	30
H(43B)	1491	1132	9446	30
H(46)	6224	3041	10363	36
H(48)	3216	3284	11237	36
H(50A)	5393	2434	9128	62
H(50B)	5333	1919	9544	62
H(50C)	6425	2307	9689	62
H(51A)	4871	3963	11225	72
H(51B)	6148	3757	11054	72
H(51C)	5583	3558	11694	72
H(52A)	1295	2618	10237	54
H(52B)	1460	2824	10971	54
H(52C)	1700	2234	10820	54
H(55)	1358	1245	6791	43
H(57)	-1200	1999	7651	42
H(59A)	3559	1297	8141	59
H(59B)	3435	1243	7365	59
H(59C)	2967	795	7806	59
H(60A)	-1613	1507	6563	86
H(60B)	-466	1398	6176	86
H(60C)	-864	1975	6306	86
H(61A)	-1062	2132	8788	51
H(61B)	179	2421	8963	51
H(61C)	-13	1855	9231	51
H(1X1)	7251	3914	8914	52
H(1X2)	8612	3960	8746	52
H(2X1)	-5983	4507	9534	69
H(2X2)	-4981	4265	10004	69

Table S12: Torsion angles [°] for complex 3.

N(1)-W(1)-O(1)-C(1)	-98.5(3)
C(19)-W(1)-O(1)-C(1)	87.4(2)
N(3)-W(1)-O(1)-C(1)	-172.4(2)
N(2)-W(1)-O(1)-C(1)	-14.2(2)
C(19)-W(1)-N(1)-C(7)	178(100)
O(1)-W(1)-N(1)-C(7)	3(3)
N(3)-W(1)-N(1)-C(7)	74(2)
N(2)-W(1)-N(1)-C(7)	-78(2)
W(1)-O(1)-C(1)-C(6)	70.8(3)
W(1)-O(1)-C(1)-C(2)	-111.2(2)
N(1)-W(1)-N(2)-C(29)	-127.78(19)
C(19)-W(1)-N(2)-C(29)	-27.8(2)
O(1)-W(1)-N(2)-C(29)	72.15(19)
N(3)-W(1)-N(2)-C(29)	119.2(2)
N(1)-W(1)-N(2)-C(32)	49.59(17)
C(19)-W(1)-N(2)-C(32)	149.57(17)
O(1)-W(1)-N(2)-C(32)	-110.49(17)
N(3)-W(1)-N(2)-C(32)	-63.4(2)
O(1)-C(1)-C(2)-F(5)	1.8(3)
C(6)-C(1)-C(2)-F(5)	179.96(19)
O(1)-C(1)-C(2)-C(3)	-179.2(2)
C(6)-C(1)-C(2)-C(3)	-1.0(3)
N(1)-W(1)-N(3)-C(38)	92.5(2)
C(19)-W(1)-N(3)-C(38)	-7.7(2)
O(1)-W(1)-N(3)-C(38)	-106.8(2)
N(2)-W(1)-N(3)-C(38)	-154.80(18)
N(1)-W(1)-N(3)-C(35)	-81.85(17)
C(19)-W(1)-N(3)-C(35)	178.02(17)
O(1)-W(1)-N(3)-C(35)	78.89(16)
N(2)-W(1)-N(3)-C(35)	30.9(2)
F(5)-C(2)-C(3)-F(4)	-1.9(4)
C(1)-C(2)-C(3)-F(4)	179.0(2)
F(5)-C(2)-C(3)-C(4)	177.6(2)
C(1)-C(2)-C(3)-C(4)	-1.5(4)
F(4)-C(3)-C(4)-F(3)	0.7(4)
C(2)-C(3)-C(4)-F(3)	-178.8(2)
F(4)-C(3)-C(4)-C(5)	-178.6(2)
C(2)-C(3)-C(4)-C(5)	1.9(4)
F(3)-C(4)-C(5)-F(2)	0.7(4)
C(3)-C(4)-C(5)-F(2)	-180.0(2)
F(3)-C(4)-C(5)-C(6)	-179.0(2)
C(3)-C(4)-C(5)-C(6)	0.3(4)
F(2)-C(5)-C(6)-F(1)	-3.9(4)
C(4)-C(5)-C(6)-F(1)	175.9(2)
F(2)-C(5)-C(6)-C(1)	177.3(2)
C(4)-C(5)-C(6)-C(1)	-2.9(4)

O(1)-C(1)-C(6)-F(1)	2.5(3)
C(2)-C(1)-C(6)-F(1)	-175.6(2)
O(1)-C(1)-C(6)-C(5)	-178.7(2)
C(2)-C(1)-C(6)-C(5)	3.2(3)
W(1)-N(1)-C(7)-C(12)	-75(2)
W(1)-N(1)-C(7)-C(8)	107(2)
N(1)-C(7)-C(8)-C(9)	178.4(2)
C(12)-C(7)-C(8)-C(9)	-0.1(4)
N(1)-C(7)-C(8)-C(13)	-1.0(4)
C(12)-C(7)-C(8)-C(13)	-179.4(2)
C(7)-C(8)-C(9)-C(10)	1.2(5)
C(13)-C(8)-C(9)-C(10)	-179.4(3)
C(8)-C(9)-C(10)-C(11)	-0.9(5)
C(9)-C(10)-C(11)-C(12)	-0.5(5)
C(10)-C(11)-C(12)-C(7)	1.6(4)
C(10)-C(11)-C(12)-C(16)	-176.0(3)
N(1)-C(7)-C(12)-C(11)	-179.7(2)
C(8)-C(7)-C(12)-C(11)	-1.3(4)
N(1)-C(7)-C(12)-C(16)	-2.2(4)
C(8)-C(7)-C(12)-C(16)	176.2(2)
C(9)-C(8)-C(13)-C(14)	58.9(3)
C(7)-C(8)-C(13)-C(14)	-121.7(3)
C(9)-C(8)-C(13)-C(15)	-63.7(4)
C(7)-C(8)-C(13)-C(15)	115.6(3)
C(11)-C(12)-C(16)-C(18)	-54.4(3)
C(7)-C(12)-C(16)-C(18)	128.2(3)
C(11)-C(12)-C(16)-C(17)	69.3(3)
C(7)-C(12)-C(16)-C(17)	-108.2(3)
N(1)-W(1)-C(19)-C(20)	3.8(3)
O(1)-W(1)-C(19)-C(20)	-178.3(3)
N(3)-W(1)-C(19)-C(20)	102.3(3)
N(2)-W(1)-C(19)-C(20)	-93.8(3)
W(1)-C(19)-C(20)-C(22)	-22.9(4)
W(1)-C(19)-C(20)-C(23)	-147.3(2)
W(1)-C(19)-C(20)-C(21)	95.6(3)
C(22)-C(20)-C(23)-C(24)	-4.1(3)
C(19)-C(20)-C(23)-C(24)	119.5(3)
C(21)-C(20)-C(23)-C(24)	-123.0(3)
C(22)-C(20)-C(23)-C(28)	176.8(2)
C(19)-C(20)-C(23)-C(28)	-59.6(3)
C(21)-C(20)-C(23)-C(28)	57.9(3)
C(28)-C(23)-C(24)-C(25)	3.1(4)
C(20)-C(23)-C(24)-C(25)	-176.0(2)
C(23)-C(24)-C(25)-C(26)	-1.9(5)
C(24)-C(25)-C(26)-C(27)	-0.6(5)
C(25)-C(26)-C(27)-C(28)	1.7(5)
C(26)-C(27)-C(28)-C(23)	-0.3(5)

C(24)-C(23)-C(28)-C(27)	-2.1(4)
C(20)-C(23)-C(28)-C(27)	177.0(2)
C(32)-N(2)-C(29)-C(30)	-0.2(2)
W(1)-N(2)-C(29)-C(30)	177.46(16)
C(32)-N(2)-C(29)-C(33)	-180.0(2)
W(1)-N(2)-C(29)-C(33)	-2.3(3)
N(2)-C(29)-C(30)-C(31)	-0.3(3)
C(33)-C(29)-C(30)-C(31)	179.5(2)
C(29)-C(30)-C(31)-C(32)	0.7(3)
C(30)-C(31)-C(32)-N(2)	-0.9(3)
C(30)-C(31)-C(32)-C(34)	175.0(2)
C(29)-N(2)-C(32)-C(31)	0.7(2)
W(1)-N(2)-C(32)-C(31)	-177.23(15)
C(29)-N(2)-C(32)-C(34)	-175.3(2)
W(1)-N(2)-C(32)-C(34)	6.8(3)
C(38)-N(3)-C(35)-C(36)	0.2(2)
W(1)-N(3)-C(35)-C(36)	175.83(15)
C(38)-N(3)-C(35)-C(39)	-176.2(2)
W(1)-N(3)-C(35)-C(39)	-0.6(3)
N(3)-C(35)-C(36)-C(37)	-0.4(3)
C(39)-C(35)-C(36)-C(37)	175.7(2)
C(35)-C(36)-C(37)-C(38)	0.5(3)
C(36)-C(37)-C(38)-N(3)	-0.4(3)
C(36)-C(37)-C(38)-C(40)	-179.7(2)
C(35)-N(3)-C(38)-C(37)	0.2(2)
W(1)-N(3)-C(38)-C(37)	-174.68(16)
C(35)-N(3)-C(38)-C(40)	179.5(2)
W(1)-N(3)-C(38)-C(40)	4.6(3)
C(44)-N(4)-C(41)-N(5)	177.5(2)
C(42)-N(4)-C(41)-N(5)	-0.6(3)
C(53)-N(5)-C(41)-N(4)	166.8(2)
C(43)-N(5)-C(41)-N(4)	0.6(3)
C(41)-N(4)-C(42)-C(43)	0.4(3)
C(44)-N(4)-C(42)-C(43)	-177.8(2)
C(41)-N(5)-C(43)-C(42)	-0.3(3)
C(53)-N(5)-C(43)-C(42)	-166.9(2)
N(4)-C(42)-C(43)-N(5)	0.0(3)
C(41)-N(4)-C(44)-C(49)	99.5(3)
C(42)-N(4)-C(44)-C(49)	-82.5(3)
C(41)-N(4)-C(44)-C(45)	-78.7(3)
C(42)-N(4)-C(44)-C(45)	99.3(3)
C(49)-C(44)-C(45)-C(46)	-1.0(4)
N(4)-C(44)-C(45)-C(46)	177.1(2)
C(49)-C(44)-C(45)-C(50)	-179.1(2)
N(4)-C(44)-C(45)-C(50)	-0.9(4)
C(44)-C(45)-C(46)-C(47)	0.0(4)
C(50)-C(45)-C(46)-C(47)	178.1(2)

C(45)-C(46)-C(47)-C(48)	1.0(4)
C(45)-C(46)-C(47)-C(51)	-179.3(2)
C(46)-C(47)-C(48)-C(49)	-0.9(4)
C(51)-C(47)-C(48)-C(49)	179.3(2)
C(45)-C(44)-C(49)-C(48)	1.0(4)
N(4)-C(44)-C(49)-C(48)	-177.1(2)
C(45)-C(44)-C(49)-C(52)	178.7(2)
N(4)-C(44)-C(49)-C(52)	0.6(3)
C(47)-C(48)-C(49)-C(44)	0.0(4)
C(47)-C(48)-C(49)-C(52)	-177.8(2)
C(41)-N(5)-C(53)-C(58)	-69.2(3)
C(43)-N(5)-C(53)-C(58)	95.2(3)
C(41)-N(5)-C(53)-C(54)	112.5(3)
C(43)-N(5)-C(53)-C(54)	-83.0(3)
C(58)-C(53)-C(54)-C(55)	2.9(4)
N(5)-C(53)-C(54)-C(55)	-179.0(2)
C(58)-C(53)-C(54)-C(59)	-176.4(2)
N(5)-C(53)-C(54)-C(59)	1.7(3)
C(53)-C(54)-C(55)-C(56)	0.1(4)
C(59)-C(54)-C(55)-C(56)	179.4(2)
C(54)-C(55)-C(56)-C(57)	-2.1(4)
C(54)-C(55)-C(56)-C(60)	178.3(2)
C(55)-C(56)-C(57)-C(58)	1.4(4)
C(60)-C(56)-C(57)-C(58)	-179.1(3)
C(56)-C(57)-C(58)-C(53)	1.4(4)
C(56)-C(57)-C(58)-C(61)	-176.9(2)
C(54)-C(53)-C(58)-C(57)	-3.6(4)
N(5)-C(53)-C(58)-C(57)	178.2(2)
C(54)-C(53)-C(58)-C(61)	174.6(2)
N(5)-C(53)-C(58)-C(61)	-3.5(3)
Cl(3)#1-C(2X)-Cl(3)-Cl(4)#1	159(2)
Cl(4)-C(2X)-Cl(3)-Cl(4)#1	161(2)
Cl(3)#1-C(2X)-Cl(3)-C(2X)#1	0.001(2)
Cl(4)-C(2X)-Cl(3)-C(2X)#1	2.0(2)
Cl(4)-C(2X)-Cl(3)-Cl(3)#1	2.0(2)
Cl(3)-C(2X)-Cl(4)-Cl(3)#1	-4.9(5)

Symmetry transformations used to generate equivalent atoms: #1 -x-1,-y+1,-z+2.

Crystal data and structure refinement for complex 4.

Empirical formula	C55 H76 Cl2 N4 W
Formula weight	1047.95
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 10.5591(3) Å, α = 86.879(2)°
	b = 13.6270(5) Å, β = 81.476(2)°
	c = 21.2326(7) Å, γ = 88.576(2)°
Volume	3016.47(17) $Å^3$
Z, Calculated density	2, 1.154 Mg/m^3
Absorption coefficient	2.036 mm^{-1}
F(000)	1084
Crystal size	0.29 x 0.27 x 0.06 mm
Theta range for data collection	1.74 to 28.40°
Limiting indices	-14<=h<=14, -18<=k<=18, -28<=l<=28
Reflections collected / unique	52893 / 14996 [R(int) = 0.0440]
Completeness to theta = 28.40	99.0 %
Absorption correction	Numerical
Max. and min. transmission	0.9120 and 0.6301
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	14996 / 26 / 581
Goodness-of-fit on F^2	1.041
Final R indices [I>2sigma(I)]	R1 = 0.0297, wR2 = 0.0532
R indices (all data)	R1 = 0.0404, wR2 = 0.0550
Largest diff. peak and hole	0.885 and -0.916 e. $Å^{-3}$

Table S13:Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) complex 4. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
W(1)	1562(1)	2280(1)	2356(1)	12(1)
Cl(1)	2655(1)	678(1)	2272(1)	22(1)
N(1)	976(2)	3267(2)	2804(1)	15(1)
C(1)	651(2)	4038(2)	3210(1)	17(1)
Cl(2)	-289(1)	1243(1)	2707(1)	22(1)
N(2)	3479(2)	2704(2)	2303(1)	25(1)
C(2)	1144(2)	4987(2)	3021(1)	21(1)
C(3)	766(3)	5742(2)	3429(1)	31(1)
C(4)	-38(3)	5577(2)	4001(2)	38(1)
C(5)	-468(3)	4639(2)	4185(1)	32(1)
C(6)	-143(2)	3858(2)	3798(1)	22(1)
C(7)	2075(2)	5185(2)	2421(1)	24(1)
C(8)	1669(3)	6084(2)	2027(1)	32(1)
C(9)	3434(3)	5315(2)	2567(2)	32(1)
C(10)	-653(2)	2842(2)	3997(1)	23(1)
C(11)	-2041(3)	2784(2)	3880(2)	37(1)
C(12)	-515(3)	2537(2)	4689(1)	31(1)
C(13)	4036(3)	2746(2)	2856(2)	38(1)
C(14)	5320(3)	2941(2)	2671(2)	49(1)
C(15)	5571(3)	3017(2)	2020(2)	51(1)
C(16)	4453(3)	2853(2)	1786(2)	38(1)
C(17)	3298(3)	2540(3)	3500(2)	54(1)
C(18)	4256(3)	2784(3)	1113(2)	60(1)
C(19)	1118(2)	2692(2)	1554(1)	14(1)
C(20)	354(2)	3470(2)	1227(1)	20(1)
C(21)	1299(3)	4206(2)	844(1)	33(1)
C(22)	-574(3)	4024(2)	1719(1)	28(1)
C(23)	-476(2)	2994(2)	797(1)	20(1)
C(24)	-657(3)	3410(2)	207(2)	44(1)
C(25)	-1488(3)	3011(2)	-151(2)	45(1)
C(26)	-2147(3)	2180(2)	71(1)	29(1)
C(27)	-1953(2)	1742(2)	644(1)	29(1)
C(28)	-1131(2)	2149(2)	1008(1)	24(1)
N(3)	6092(2)	-507(1)	3076(1)	13(1)
N(4)	6708(2)	-482(1)	2041(1)	13(1)
C(29)	6468(2)	-1017(2)	2575(1)	13(1)
C(30)	6067(2)	556(2)	2891(1)	16(1)
C(31)	6412(2)	574(2)	2159(1)	15(1)
C(32)	5763(2)	-898(2)	3722(1)	16(1)
C(33)	4478(2)	-1109(2)	3940(1)	20(1)
C(34)	4179(3)	-1493(2)	4562(1)	32(1)
C(35)	5110(3)	-1628(3)	4952(1)	42(1)
C(36)	6373(3)	-1398(2)	4726(1)	36(1)
C(37)	6730(2)	-1029(2)	4104(1)	21(1)

C(38)	3447(2)	-955(2)	3520(1)	21(1)
C(39)	2255(2)	-427(2)	3855(1)	33(1)
C(40)	3098(3)	-1924(2)	3268(2)	40(1)
C(41)	8113(2)	-780(2)	3860(1)	22(1)
C(42)	8922(3)	-1728(2)	3747(2)	33(1)
C(43)	8682(3)	-141(2)	4315(1)	29(1)
C(44)	7068(2)	-866(2)	1418(1)	16(1)
C(45)	6094(2)	-1142(2)	1086(1)	20(1)
C(46)	6471(2)	-1564(2)	502(1)	31(1)
C(47)	7753(2)	-1672(2)	258(1)	32(1)
C(48)	8685(2)	-1364(2)	590(1)	28(1)
C(49)	8370(2)	-951(2)	1178(1)	20(1)
C(50)	4682(2)	-972(2)	1319(1)	21(1)
C(51)	3952(2)	-1931(2)	1432(1)	30(1)
C(52)	4126(2)	-270(2)	843(1)	30(1)
C(53)	9398(2)	-622(2)	1542(1)	23(1)
C(54)	10525(2)	-158(2)	1101(1)	35(1)
C(55)	9876(3)	-1469(3)	1944(2)	43(1)

Table S15: Bond lengths [Å] and angles [°] for complex 4.

W(1)-N(1)	1.739(2)
W(1)-C(19)	1.886(2)
W(1)-N(2)	2.104(2)
W(1)-Cl(2)	2.4418(6)
W(1)-Cl(1)	2.4458(6)
N(1)-C(1)	1.398(3)
C(1)-C(6)	1.410(3)
C(1)-C(2)	1.421(3)
N(2)-C(13)	1.392(4)
N(2)-C(16)	1.399(4)
C(2)-C(3)	1.394(4)
C(2)-C(7)	1.506(4)
C(3)-C(4)	1.385(4)
C(3)-H(3)	0.9500
C(4)-C(5)	1.383(4)
C(4)-H(4)	0.9500
C(5)-C(6)	1.385(4)
C(5)-H(5)	0.9500
C(6)-C(10)	1.515(4)
C(7)-C(9)	1.529(4)
C(7)-C(8)	1.534(4)
C(7)-H(7)	1.0
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-C(11)	1.527(4)
C(10)-C(12)	1.531(4)
C(10)-H(10)	1.0
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(14)	1.382(4)
C(13)-C(17)	1.486(5)
C(14)-C(15)	1.367(5)
C(14)-H(14)	0.9500
C(15)-C(16)	1.374(4)
C(15)-H(15)	0.9500
C(16)-C(18)	1.482(5)
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800

C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-C(20)	1.516(3)
C(19)-H(19)	0.952(10)
C(20)-C(23)	1.534(3)
C(20)-C(22)	1.540(4)
C(20)-C(21)	1.544(4)
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-C(28)	1.377(4)
C(23)-C(24)	1.385(4)
C(24)-C(25)	1.382(4)
C(24)-H(24)	0.9500
C(25)-C(26)	1.369(4)
C(25)-H(25)	0.9500
C(26)-C(27)	1.367(4)
C(26)-H(26)	0.9500
C(27)-C(28)	1.389(3)
C(27)-H(27)	0.9500
C(28)-H(28)	0.9500
N(3)-C(29)	1.311(3)
N(3)-C(32)	1.439(3)
N(3)-C(30)	1.481(3)
N(4)-C(29)	1.309(3)
N(4)-C(44)	1.444(3)
N(4)-C(31)	1.491(3)
C(29)-H(29)	0.949(10)
C(30)-C(31)	1.542(3)
C(30)-H(30A)	0.9900
C(30)-H(30B)	0.9900
C(31)-H(31A)	0.9900
C(31)-H(31B)	0.9900
C(32)-C(37)	1.398(3)
C(32)-C(33)	1.399(3)
C(33)-C(34)	1.389(3)
C(33)-C(38)	1.510(3)
C(34)-C(35)	1.378(4)
C(34)-H(34)	0.9500
C(35)-C(36)	1.386(4)
C(35)-H(35)	0.9500
C(36)-C(37)	1.389(4)

C(36)-H(36)	0.9500
C(37)-C(41)	1.517(3)
C(38)-C(40)	1.524(4)
C(38)-C(39)	1.534(4)
C(38)-H(38)	1.0
C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
C(40)-H(40A)	0.9800
C(40)-H(40B)	0.9800
C(40)-H(40C)	0.9800
C(41)-C(43)	1.531(4)
C(41)-C(42)	1.540(4)
C(41)-H(41)	1.0
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
C(43)-H(43A)	0.9800
C(43)-H(43B)	0.9800
C(43)-H(43C)	0.9800
C(44)-C(49)	1.398(3)
C(44)-C(45)	1.400(3)
C(45)-C(46)	1.396(3)
C(45)-C(50)	1.515(3)
C(46)-C(47)	1.384(3)
C(46)-H(46)	0.9500
C(47)-C(48)	1.379(4)
C(47)-H(47)	0.9500
C(48)-C(49)	1.388(3)
C(48)-H(48)	0.9500
C(49)-C(53)	1.512(3)
C(50)-C(51)	1.524(4)
C(50)-C(52)	1.525(4)
C(50)-H(50)	1.0
C(51)-H(51A)	0.9800
C(51)-H(51B)	0.9800
C(51)-H(51C)	0.9800
C(52)-H(52A)	0.9800
C(52)-H(52B)	0.9800
C(52)-H(52C)	0.9800
C(53)-C(55)	1.519(4)
C(53)-C(54)	1.528(4)
C(53)-H(53)	1.0
C(54)-H(54A)	0.9800
C(54)-H(54B)	0.9800
C(54)-H(54C)	0.9800
C(55)-H(55A)	0.9800

C(55)-H(55B)	0.9800
C(55)-H(55C)	0.9800

N(1)-W(1)-C(19)	100.61(10)
N(1)-W(1)-N(2)	93.24(9)
C(19)-W(1)-N(2)	104.16(9)
N(1)-W(1)-Cl(2)	95.26(6)
C(19)-W(1)-Cl(2)	97.01(7)
N(2)-W(1)-Cl(2)	155.30(6)
N(1)-W(1)-Cl(1)	150.37(7)
C(19)-W(1)-Cl(1)	109.02(7)
N(2)-W(1)-Cl(1)	79.51(6)
Cl(2)-W(1)-Cl(1)	81.68(2)
C(1)-N(1)-W(1)	171.99(17)
N(1)-C(1)-C(6)	119.7(2)
N(1)-C(1)-C(2)	119.0(2)
C(6)-C(1)-C(2)	121.4(2)
C(13)-N(2)-C(16)	107.2(2)
C(13)-N(2)-W(1)	120.4(2)
C(16)-N(2)-W(1)	131.9(2)
C(3)-C(2)-C(1)	117.2(2)
C(3)-C(2)-C(7)	120.1(2)
C(1)-C(2)-C(7)	122.6(2)
C(4)-C(3)-C(2)	121.7(3)
C(4)-C(3)-H(3)	119.1
C(2)-C(3)-H(3)	119.1
C(5)-C(4)-C(3)	119.9(3)
C(5)-C(4)-H(4)	120.0
C(3)-C(4)-H(4)	120.0
C(4)-C(5)-C(6)	121.2(3)
C(4)-C(5)-H(5)	119.4
C(6)-C(5)-H(5)	119.4
C(5)-C(6)-C(1)	118.4(2)
C(5)-C(6)-C(10)	120.6(2)
C(1)-C(6)-C(10)	121.0(2)
C(2)-C(7)-C(9)	111.5(2)
C(2)-C(7)-C(8)	111.9(2)
C(9)-C(7)-C(8)	110.0(2)
C(2)-C(7)-H(7)	107.8
C(9)-C(7)-H(7)	107.8
C(8)-C(7)-H(7)	107.8
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5

C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(6)-C(10)-C(11)	109.9(2)
C(6)-C(10)-C(12)	112.6(2)
C(11)-C(10)-C(12)	111.5(2)
C(6)-C(10)-H(10)	107.5
C(11)-C(10)-H(10)	107.5
C(12)-C(10)-H(10)	107.5
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(14)-C(13)-N(2)	107.4(3)
C(14)-C(13)-C(17)	130.6(3)
N(2)-C(13)-C(17)	121.9(3)
C(15)-C(14)-C(13)	109.1(3)
C(15)-C(14)-H(14)	125.4
C(13)-C(14)-H(14)	125.4
C(14)-C(15)-C(16)	108.1(3)
C(14)-C(15)-H(15)	126.0
C(16)-C(15)-H(15)	126.0
C(15)-C(16)-N(2)	108.2(3)
C(15)-C(16)-C(18)	128.4(3)
N(2)-C(16)-C(18)	123.3(3)
C(13)-C(17)-H(17A)	109.5
C(13)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(13)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(16)-C(18)-H(18A)	109.5
C(16)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(16)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5

H(18B)-C(18)-H(18C)	109.5
C(20)-C(19)-W(1)	142.41(18)
C(20)-C(19)-H(19)	115.8(15)
W(1)-C(19)-H(19)	101.4(15)
C(19)-C(20)-C(23)	110.5(2)
C(19)-C(20)-C(22)	110.9(2)
C(23)-C(20)-C(22)	106.3(2)
C(19)-C(20)-C(21)	108.4(2)
C(23)-C(20)-C(21)	111.6(2)
C(22)-C(20)-C(21)	109.1(2)
C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(20)-C(22)-H(22A)	109.5
C(20)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(20)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(28)-C(23)-C(24)	117.4(2)
C(28)-C(23)-C(20)	120.0(2)
C(24)-C(23)-C(20)	122.4(2)
C(25)-C(24)-C(23)	121.5(3)
C(25)-C(24)-H(24)	119.3
C(23)-C(24)-H(24)	119.3
C(26)-C(25)-C(24)	120.2(3)
C(26)-C(25)-H(25)	119.9
C(24)-C(25)-H(25)	119.9
C(27)-C(26)-C(25)	119.1(3)
C(27)-C(26)-H(26)	120.4
C(25)-C(26)-H(26)	120.4
C(26)-C(27)-C(28)	120.7(3)
C(26)-C(27)-H(27)	119.7
C(28)-C(27)-H(27)	119.7
C(23)-C(28)-C(27)	121.0(3)
C(23)-C(28)-H(28)	119.5
C(27)-C(28)-H(28)	119.5
C(29)-N(3)-C(32)	126.1(2)
C(29)-N(3)-C(30)	110.27(19)
C(32)-N(3)-C(30)	123.65(19)
C(29)-N(4)-C(44)	125.0(2)
C(29)-N(4)-C(31)	110.20(19)
C(44)-N(4)-C(31)	124.47(19)
N(4)-C(29)-N(3)	113.9(2)

N(4)-C(29)-H(29)	122.4(15)
N(3)-C(29)-H(29)	123.6(15)
N(3)-C(30)-C(31)	102.96(18)
N(3)-C(30)-H(30A)	111.2
C(31)-C(30)-H(30A)	111.2
N(3)-C(30)-H(30B)	111.2
C(31)-C(30)-H(30B)	111.2
H(30A)-C(30)-H(30B)	109.1
N(4)-C(31)-C(30)	102.32(18)
N(4)-C(31)-H(31A)	111.3
C(30)-C(31)-H(31A)	111.3
N(4)-C(31)-H(31B)	111.3
C(30)-C(31)-H(31B)	111.3
H(31A)-C(31)-H(31B)	109.2
C(37)-C(32)-C(33)	123.1(2)
C(37)-C(32)-N(3)	118.9(2)
C(33)-C(32)-N(3)	118.0(2)
C(34)-C(33)-C(32)	117.2(2)
C(34)-C(33)-C(38)	120.5(2)
C(32)-C(33)-C(38)	122.2(2)
C(35)-C(34)-C(33)	121.0(2)
C(35)-C(34)-H(34)	119.5
C(33)-C(34)-H(34)	119.5
C(34)-C(35)-C(36)	120.5(3)
C(34)-C(35)-H(35)	119.8
C(36)-C(35)-H(35)	119.8
C(35)-C(36)-C(37)	120.9(3)
C(35)-C(36)-H(36)	119.5
C(37)-C(36)-H(36)	119.5
C(36)-C(37)-C(32)	117.2(2)
C(36)-C(37)-C(41)	120.7(2)
C(32)-C(37)-C(41)	122.1(2)
C(33)-C(38)-C(40)	111.1(2)
C(33)-C(38)-C(39)	112.4(2)
C(40)-C(38)-C(39)	111.1(2)
C(33)-C(38)-H(38)	107.3
C(40)-C(38)-H(38)	107.3
C(39)-C(38)-H(38)	107.3
C(38)-C(39)-H(39A)	109.5
C(38)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(38)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(38)-C(40)-H(40A)	109.5
C(38)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5

C(38)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
C(37)-C(41)-C(43)	111.8(2)
C(37)-C(41)-C(42)	110.2(2)
C(43)-C(41)-C(42)	110.4(2)
C(37)-C(41)-H(41)	108.1
C(43)-C(41)-H(41)	108.1
C(42)-C(41)-H(41)	108.1
C(41)-C(42)-H(42A)	109.5
C(41)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(41)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(41)-C(43)-H(43A)	109.5
C(41)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43B)	109.5
C(41)-C(43)-H(43C)	109.5
H(43A)-C(43)-H(43C)	109.5
H(43B)-C(43)-H(43C)	109.5
C(49)-C(44)-C(45)	123.2(2)
C(49)-C(44)-N(4)	118.5(2)
C(45)-C(44)-N(4)	118.3(2)
C(46)-C(45)-C(44)	117.0(2)
C(46)-C(45)-C(50)	119.6(2)
C(44)-C(45)-C(50)	123.4(2)
C(47)-C(46)-C(45)	120.9(2)
C(47)-C(46)-H(46)	119.5
C(45)-C(46)-H(46)	119.5
C(48)-C(47)-C(46)	120.3(2)
C(48)-C(47)-H(47)	119.8
C(46)-C(47)-H(47)	119.8
C(47)-C(48)-C(49)	121.4(2)
C(47)-C(48)-H(48)	119.3
C(49)-C(48)-H(48)	119.3
C(48)-C(49)-C(44)	117.1(2)
C(48)-C(49)-C(53)	121.1(2)
C(44)-C(49)-C(53)	121.9(2)
C(45)-C(50)-C(51)	112.1(2)
C(45)-C(50)-C(52)	108.9(2)
C(51)-C(50)-C(52)	111.7(2)
C(45)-C(50)-H(50)	108.0
C(51)-C(50)-H(50)	108.0
C(52)-C(50)-H(50)	108.0
C(50)-C(51)-H(51A)	109.5
C(50)-C(51)-H(51B)	109.5

H(51A)-C(51)-H(51B)	109.5
C(50)-C(51)-H(51C)	109.5
H(51A)-C(51)-H(51C)	109.5
H(51B)-C(51)-H(51C)	109.5
C(50)-C(52)-H(52A)	109.5
C(50)-C(52)-H(52B)	109.5
H(52A)-C(52)-H(52B)	109.5
C(50)-C(52)-H(52C)	109.5
H(52A)-C(52)-H(52C)	109.5
H(52B)-C(52)-H(52C)	109.5
C(49)-C(53)-C(55)	111.3(2)
C(49)-C(53)-C(54)	112.2(2)
C(55)-C(53)-C(54)	109.7(2)
C(49)-C(53)-H(53)	107.8
C(55)-C(53)-H(53)	107.8
C(54)-C(53)-H(53)	107.8
C(53)-C(54)-H(54A)	109.5
C(53)-C(54)-H(54B)	109.5
H(54A)-C(54)-H(54B)	109.5
C(53)-C(54)-H(54C)	109.5
H(54A)-C(54)-H(54C)	109.5
H(54B)-C(54)-H(54C)	109.5
C(53)-C(55)-H(55A)	109.5
C(53)-C(55)-H(55B)	109.5
H(55A)-C(55)-H(55B)	109.5
C(53)-C(55)-H(55C)	109.5
H(55A)-C(55)-H(55C)	109.5
H(55B)-C(55)-H(55C)	109.5

Table S15: Anisotropic displacement parameters (A^2 x 10^3) for complex 4 the anisotropic displacement factor exponent takes the form:-2 π^2 [h^2 a^{*2} U_{11} + ... + 2 h k a* b* U_{12}]

	U11	U22	U33	U23	U13	U12
W(1)	15(1)	10(1)	12(1)	1(1)	-5(1)	0(1)
Cl(1)	27(1)	15(1)	25(1)	-2(1)	-9(1)	6(1)
N(1)	18(1)	14(1)	14(1)	1(1)	-7(1)	-4(1)
C(1)	22(1)	14(1)	17(1)	-4(1)	-9(1)	-1(1)
Cl(2)	26(1)	18(1)	20(1)	-5(1)	3(1)	-9(1)
N(2)	21(1)	17(1)	39(1)	3(1)	-14(1)	0(1)
C(2)	28(1)	14(1)	24(1)	-3(1)	-12(1)	-1(1)
C(3)	42(2)	14(1)	38(2)	-4(1)	-13(1)	-1(1)
C(4)	52(2)	25(2)	37(2)	-18(1)	-6(2)	5(2)
C(5)	44(2)	27(2)	25(2)	-10(1)	1(1)	-2(1)
C(6)	26(1)	20(1)	20(1)	-8(1)	-6(1)	-1(1)
C(7)	29(1)	15(1)	28(2)	3(1)	-9(1)	-6(1)
C(8)	39(2)	23(2)	36(2)	7(1)	-16(1)	-7(1)
C(9)	32(2)	24(2)	43(2)	3(1)	-11(1)	-4(1)
C(10)	28(1)	26(2)	14(1)	-4(1)	1(1)	-3(1)
C(11)	37(2)	38(2)	37(2)	0(2)	-10(1)	-9(2)
C(12)	44(2)	30(2)	21(2)	-3(1)	-5(1)	-8(1)
C(13)	37(2)	20(2)	67(2)	-7(2)	-36(2)	6(1)
C(14)	36(2)	25(2)	98(2)	-12(2)	-43(2)	0(1)
C(15)	23(1)	32(2)	98(2)	7(2)	-12(2)	-2(1)
C(16)	20(1)	28(2)	62(2)	7(1)	0(1)	-1(1)
C(17)	65(2)	58(2)	49(2)	-8(2)	-40(2)	15(2)
C(18)	28(2)	82(3)	57(2)	24(2)	22(2)	5(2)
C(19)	14(1)	12(1)	15(1)	-2(1)	-2(1)	2(1)
C(20)	28(1)	17(1)	19(1)	2(1)	-13(1)	0(1)
C(21)	52(2)	23(2)	28(2)	9(1)	-21(1)	-11(1)
C(22)	32(2)	24(2)	33(2)	-10(1)	-18(1)	12(1)
C(23)	24(1)	18(1)	21(1)	-3(1)	-10(1)	5(1)
C(24)	77(2)	24(2)	40(2)	8(1)	-38(2)	-10(2)
C(25)	77(2)	32(2)	36(2)	8(2)	-42(2)	-5(2)
C(26)	26(1)	39(2)	28(2)	-13(1)	-16(1)	8(1)
C(27)	25(1)	41(2)	23(2)	-2(1)	-5(1)	-12(1)
C(28)	21(1)	39(2)	15(1)	4(1)	-5(1)	-7(1)
N(3)	13(1)	13(1)	14(1)	1(1)	0(1)	0(1)
N(4)	11(1)	13(1)	15(1)	-2(1)	0(1)	0(1)
C(29)	8(1)	13(1)	20(1)	0(1)	-4(1)	0(1)
C(30)	21(1)	12(1)	15(1)	0(1)	1(1)	1(1)
C(31)	17(1)	14(1)	14(1)	2(1)	0(1)	1(1)
C(32)	18(1)	16(1)	13(1)	4(1)	0(1)	0(1)
C(33)	15(1)	27(2)	16(1)	4(1)	-3(1)	-2(1)
C(34)	18(1)	56(2)	21(2)	14(1)	-2(1)	-6(1)
C(35)	29(2)	74(3)	21(2)	24(2)	-5(1)	-10(2)
C(36)	26(2)	59(2)	23(2)	15(2)	-12(1)	-8(2)
C(37)	17(1)	28(2)	19(1)	4(1)	-4(1)	-2(1)

C(38)	14(1)	31(2)	17(1)	6(1)	-4(1)	-3(1)
C(39)	19(1)	50(2)	28(2)	6(1)	-1(1)	0(1)
C(40)	41(2)	41(2)	42(2)	-5(2)	-19(2)	-5(2)
C(41)	16(1)	28(2)	22(1)	6(1)	-6(1)	-3(1)
C(42)	27(2)	34(2)	39(2)	-9(1)	-7(1)	2(1)
C(43)	23(1)	29(2)	37(2)	-5(1)	-5(1)	-3(1)
C(44)	16(1)	19(1)	13(1)	-5(1)	-1(1)	-1(1)
C(45)	13(1)	26(2)	20(1)	-7(1)	0(1)	-2(1)
C(46)	19(1)	51(2)	24(2)	-19(1)	-7(1)	-2(1)
C(47)	21(1)	54(2)	23(2)	-23(1)	2(1)	-1(1)
C(48)	12(1)	46(2)	27(2)	-17(1)	1(1)	-3(1)
C(49)	15(1)	25(2)	20(1)	-8(1)	-2(1)	-1(1)
C(50)	11(1)	35(2)	18(1)	-9(1)	-2(1)	-1(1)
C(51)	19(1)	41(2)	29(2)	0(1)	-2(1)	-8(1)
C(52)	17(1)	45(2)	26(2)	-3(1)	0(1)	0(1)
C(53)	13(1)	33(2)	26(2)	-14(1)	-4(1)	1(1)
C(54)	20(1)	44(2)	41(2)	-19(2)	-1(1)	-9(1)
C(55)	30(2)	57(2)	47(2)	-3(2)	-18(2)	5(2)

Table S16: Hydrogen coordinates (x10^4) and isotropic displacement parameters (A^2 x 10^3) for complex 4.

	x	y	z	U(eq)
H(3)	1068	6387	3312	37
H(4)	-294	6107	4266	45
H(5)	-997	4529	4584	39
H(7)	2087	4600	2155	28
H(8A)	806	5988	1926	47
H(8B)	2271	6168	1631	47
H(8C)	1669	6672	2273	47
H(9A)	3444	5872	2839	48
H(9B)	4015	5441	2168	48
H(9C)	3713	4716	2788	48
H(10)	-136	2365	3718	27
H(11A)	-2574	3247	4146	55
H(11B)	-2350	2115	3988	55
H(11C)	-2091	2954	3429	55
H(12A)	379	2604	4752	47
H(12B)	-770	1852	4780	47
H(12C)	-1065	2961	4976	47
H(14)	5930	3010	2951	59
H(15)	6377	3159	1772	61
H(17A)	3881	2517	3819	81
H(17B)	2873	1907	3511	81
H(17C)	2652	3062	3594	81
H(18A)	5080	2846	834	90
H(18B)	3672	3313	1000	90
H(18C)	3885	2147	1060	90
H(19)	1450(20)	2163(13)	1301(10)	16
H(21A)	1888	4430	1120	49
H(21B)	821	4771	688	49
H(21C)	1788	3884	481	49
H(22A)	-1130	3553	1987	42
H(22B)	-1100	4489	1497	42
H(22C)	-84	4382	1987	42
H(24)	-199	3984	44	53
H(25)	-1603	3315	-553	54
H(26)	-2730	1910	-171	35
H(27)	-2386	1153	795	35
H(28)	-1019	1841	1408	29
H(29)	6530(20)	-1714(8)	2590(11)	16
H(30A)	6705	913	3085	19
H(30B)	5207	850	3019	19
H(31A)	5683	817	1947	18
H(31B)	7165	988	2009	18
H(34)	3321	-1665	4722	39
H(35)	4884	-1881	5379	51
H(36)	7003	-1494	5001	43

H(38)	3808	-523	3143	25
H(39A)	1786	-879	4177	49
H(39B)	1702	-210	3541	49
H(39C)	2516	144	4062	49
H(40A)	3867	-2227	3036	60
H(40B)	2459	-1800	2981	60
H(40C)	2744	-2367	3627	60
H(41)	8140	-401	3441	26
H(42A)	8921	-2107	4153	49
H(42B)	9803	-1558	3568	49
H(42C)	8556	-2123	3448	49
H(43A)	8075	390	4448	44
H(43B)	9485	141	4098	44
H(43C)	8850	-545	4691	44
H(46)	5838	-1781	269	37
H(47)	7993	-1960	-141	39
H(48)	9561	-1436	414	34
H(50)	4604	-647	1735	25
H(51A)	4033	-2272	1033	45
H(51B)	3045	-1789	1581	45
H(51C)	4307	-2350	1756	45
H(52A)	4613	340	786	45
H(52B)	3228	-121	1004	45
H(52C)	4181	-577	433	45
H(53)	9009	-113	1837	28
H(54A)	10999	-666	849	52
H(54B)	11094	144	1358	52
H(54C)	10204	346	815	52
H(55A)	9150	-1769	2222	65
H(55B)	10480	-1222	2204	65
H(55C)	10309	-1962	1664	65

Table S17: Torsion angles [°] for complex 4.

C(19)-W(1)-N(1)-C(1)	-145.2(13)
N(2)-W(1)-N(1)-C(1)	-40.1(13)
Cl(2)-W(1)-N(1)-C(1)	116.7(13)
Cl(1)-W(1)-N(1)-C(1)	34.2(13)
W(1)-N(1)-C(1)-C(6)	-89.7(13)
W(1)-N(1)-C(1)-C(2)	89.6(13)
N(1)-W(1)-N(2)-C(13)	61.9(2)
C(19)-W(1)-N(2)-C(13)	163.7(2)
Cl(2)-W(1)-N(2)-C(13)	-48.1(3)
Cl(1)-W(1)-N(2)-C(13)	-89.1(2)
N(1)-W(1)-N(2)-C(16)	-127.8(2)
C(19)-W(1)-N(2)-C(16)	-26.0(3)
Cl(2)-W(1)-N(2)-C(16)	122.1(2)
Cl(1)-W(1)-N(2)-C(16)	81.1(2)
N(1)-C(1)-C(2)-C(3)	178.0(2)
C(6)-C(1)-C(2)-C(3)	-2.7(4)
N(1)-C(1)-C(2)-C(7)	-4.2(4)
C(6)-C(1)-C(2)-C(7)	175.2(2)
C(1)-C(2)-C(3)-C(4)	1.1(4)
C(7)-C(2)-C(3)-C(4)	-176.8(3)
C(2)-C(3)-C(4)-C(5)	1.2(5)
C(3)-C(4)-C(5)-C(6)	-2.1(5)
C(4)-C(5)-C(6)-C(1)	0.6(4)
C(4)-C(5)-C(6)-C(10)	-178.2(3)
N(1)-C(1)-C(6)-C(5)	-178.8(2)
C(2)-C(1)-C(6)-C(5)	1.8(4)
N(1)-C(1)-C(6)-C(10)	-0.1(4)
C(2)-C(1)-C(6)-C(10)	-179.4(2)
C(3)-C(2)-C(7)-C(9)	73.2(3)
C(1)-C(2)-C(7)-C(9)	-104.6(3)
C(3)-C(2)-C(7)-C(8)	-50.5(3)
C(1)-C(2)-C(7)-C(8)	131.8(3)
C(5)-C(6)-C(10)-C(11)	77.8(3)
C(1)-C(6)-C(10)-C(11)	-100.9(3)
C(5)-C(6)-C(10)-C(12)	-47.2(3)
C(1)-C(6)-C(10)-C(12)	134.1(3)
C(16)-N(2)-C(13)-C(14)	1.4(3)
W(1)-N(2)-C(13)-C(14)	173.77(19)
C(16)-N(2)-C(13)-C(17)	-175.2(3)
W(1)-N(2)-C(13)-C(17)	-2.8(4)
N(2)-C(13)-C(14)-C(15)	-0.2(4)
C(17)-C(13)-C(14)-C(15)	176.0(3)
C(13)-C(14)-C(15)-C(16)	-1.1(4)
C(14)-C(15)-C(16)-N(2)	2.0(4)
C(14)-C(15)-C(16)-C(18)	-175.0(3)
C(13)-N(2)-C(16)-C(15)	-2.1(3)

W(1)-N(2)-C(16)-C(15)	-173.3(2)
C(13)-N(2)-C(16)-C(18)	175.1(3)
W(1)-N(2)-C(16)-C(18)	3.9(5)
N(1)-W(1)-C(19)-C(20)	-9.5(3)
N(2)-W(1)-C(19)-C(20)	-105.6(3)
Cl(2)-W(1)-C(19)-C(20)	87.3(3)
Cl(1)-W(1)-C(19)-C(20)	170.8(3)
W(1)-C(19)-C(20)-C(23)	-132.2(3)
W(1)-C(19)-C(20)-C(22)	-14.6(4)
W(1)-C(19)-C(20)-C(21)	105.2(3)
C(19)-C(20)-C(23)-C(28)	42.5(3)
C(22)-C(20)-C(23)-C(28)	-77.8(3)
C(21)-C(20)-C(23)-C(28)	163.2(2)
C(19)-C(20)-C(23)-C(24)	-141.0(3)
C(22)-C(20)-C(23)-C(24)	98.6(3)
C(21)-C(20)-C(23)-C(24)	-20.3(4)
C(28)-C(23)-C(24)-C(25)	1.7(5)
C(20)-C(23)-C(24)-C(25)	-174.8(3)
C(23)-C(24)-C(25)-C(26)	-0.7(5)
C(24)-C(25)-C(26)-C(27)	-1.1(5)
C(25)-C(26)-C(27)-C(28)	2.0(4)
C(24)-C(23)-C(28)-C(27)	-0.8(4)
C(20)-C(23)-C(28)-C(27)	175.8(2)
C(26)-C(27)-C(28)-C(23)	-1.0(4)
C(44)-N(4)-C(29)-N(3)	-176.42(19)
C(31)-N(4)-C(29)-N(3)	-2.9(3)
C(32)-N(3)-C(29)-N(4)	180.0(2)
C(30)-N(3)-C(29)-N(4)	-0.9(3)
C(29)-N(3)-C(30)-C(31)	4.1(2)
C(32)-N(3)-C(30)-C(31)	-176.8(2)
C(29)-N(4)-C(31)-C(30)	5.2(2)
C(44)-N(4)-C(31)-C(30)	178.72(19)
N(3)-C(30)-C(31)-N(4)	-5.3(2)
C(29)-N(3)-C(32)-C(37)	88.6(3)
C(30)-N(3)-C(32)-C(37)	-90.4(3)
C(29)-N(3)-C(32)-C(33)	-92.8(3)
C(30)-N(3)-C(32)-C(33)	88.2(3)
C(37)-C(32)-C(33)-C(34)	-1.9(4)
N(3)-C(32)-C(33)-C(34)	179.5(2)
C(37)-C(32)-C(33)-C(38)	179.6(3)
N(3)-C(32)-C(33)-C(38)	1.1(4)
C(32)-C(33)-C(34)-C(35)	2.1(5)
C(38)-C(33)-C(34)-C(35)	-179.4(3)
C(33)-C(34)-C(35)-C(36)	-1.1(5)
C(34)-C(35)-C(36)-C(37)	-0.1(5)
C(35)-C(36)-C(37)-C(32)	0.3(5)
C(35)-C(36)-C(37)-C(41)	-179.9(3)

C(33)-C(32)-C(37)-C(36)	0.8(4)
N(3)-C(32)-C(37)-C(36)	179.3(3)
C(33)-C(32)-C(37)-C(41)	-179.0(2)
N(3)-C(32)-C(37)-C(41)	-0.5(4)
C(34)-C(33)-C(38)-C(40)	-77.2(3)
C(32)-C(33)-C(38)-C(40)	101.2(3)
C(34)-C(33)-C(38)-C(39)	48.0(4)
C(32)-C(33)-C(38)-C(39)	-133.6(3)
C(36)-C(37)-C(41)-C(43)	-49.6(4)
C(32)-C(37)-C(41)-C(43)	130.2(3)
C(36)-C(37)-C(41)-C(42)	73.7(3)
C(32)-C(37)-C(41)-C(42)	-106.5(3)
C(29)-N(4)-C(44)-C(49)	-94.5(3)
C(31)-N(4)-C(44)-C(49)	92.9(3)
C(29)-N(4)-C(44)-C(45)	85.0(3)
C(31)-N(4)-C(44)-C(45)	-87.5(3)
C(49)-C(44)-C(45)-C(46)	3.2(4)
N(4)-C(44)-C(45)-C(46)	-176.3(2)
C(49)-C(44)-C(45)-C(50)	-174.7(3)
N(4)-C(44)-C(45)-C(50)	5.8(4)
C(44)-C(45)-C(46)-C(47)	-2.1(4)
C(50)-C(45)-C(46)-C(47)	175.9(3)
C(45)-C(46)-C(47)-C(48)	0.2(5)
C(46)-C(47)-C(48)-C(49)	0.7(5)
C(47)-C(48)-C(49)-C(44)	0.3(4)
C(47)-C(48)-C(49)-C(53)	179.5(3)
C(45)-C(44)-C(49)-C(48)	-2.4(4)
N(4)-C(44)-C(49)-C(48)	177.1(2)
C(45)-C(44)-C(49)-C(53)	178.5(3)
N(4)-C(44)-C(49)-C(53)	-2.0(4)
C(46)-C(45)-C(50)-C(51)	63.0(3)
C(44)-C(45)-C(50)-C(51)	-119.2(3)
C(46)-C(45)-C(50)-C(52)	-61.2(3)
C(44)-C(45)-C(50)-C(52)	116.6(3)
C(48)-C(49)-C(53)-C(55)	-85.5(3)
C(44)-C(49)-C(53)-C(55)	93.6(3)
C(48)-C(49)-C(53)-C(54)	38.0(4)
C(44)-C(49)-C(53)-C(54)	-142.9(3)

Crystal data and structure refinement for complex 6.

Empirical formula	C40.50 H58 Cl F6 N5 O6 S2 W
Formula weight	1108.34
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 11.7112(7) Å, α = 103.305(3)°
	b = 20.3641(13) Å, β = 97.459(2)°
	c = 21.9201(14) Å, γ = 100.855(3)°
Volume	4913.6(5) $Å^3$
Z, Calculated density	4, 1.498 Mg/m^3
Absorption coefficient	2.560 mm^{-1}
F(000)	2244
Crystal size	0.45 x 0.32 x 0.28 mm
Theta range for data collection	1.61 to 30.66°
Limiting indices	-16<=h<=16, -29<=k<=29, -31<=l<=31
Reflections collected / unique	107760 / 29954 [R(int) = 0.0329]
Completeness to theta = 30.66	98.5 %
Absorption correction	Numerical
Max. and min. transmission	0.6740 and 0.5205
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	29954 / 18 / 1168
Goodness-of-fit on F^2	1.052
Final R indices [I>2sigma(I)]	R1 = 0.0276, wR2 = 0.0598
R indices (all data)	R1 = 0.0419, wR2 = 0.0633
Largest diff. peak and hole	1.623 and -0.990 e. $Å^{-3}$

Table S18: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) complex 6. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
W(1A)	6283(1)	2089(1)	8200(1)	12(1)
S(1A)	8985(1)	3254(1)	8339(1)	16(1)
F(1A)	10591(1)	2995(1)	9150(1)	32(1)
O(1A)	8237(1)	2593(1)	8358(1)	16(1)
C(1A)	6674(2)	1572(1)	7239(1)	18(1)
N(1A)	7890(2)	2211(1)	6608(1)	21(1)
S(2A)	6771(1)	592(1)	8635(1)	20(1)
F(2A)	11289(1)	3653(1)	8584(1)	34(1)
O(2A)	8986(2)	3352(1)	7711(1)	24(1)
N(2A)	8730(2)	1541(1)	7048(1)	20(1)
C(2A)	7732(2)	1778(1)	6986(1)	18(1)
F(3A)	10647(1)	2561(1)	8167(1)	36(1)
O(3A)	8909(2)	3837(1)	8829(1)	23(1)
N(3A)	7606(2)	3636(1)	9859(1)	20(1)
C(3A)	8998(2)	2255(1)	6431(1)	24(1)
O(4A)	7250(1)	1216(1)	8442(1)	17(1)
F(4A)	7814(2)	-357(1)	8910(1)	44(1)
N(4A)	8661(2)	2894(1)	9937(1)	18(1)
C(4A)	9515(2)	1828(1)	6701(1)	23(1)
N(5A)	4853(2)	1586(1)	8105(1)	15(1)
O(5A)	6617(2)	725(1)	9288(1)	26(1)
F(5A)	9024(2)	603(1)	8956(1)	44(1)
F(6A)	8184(2)	-94(1)	8045(1)	51(1)
O(6A)	5846(2)	101(1)	8171(1)	45(1)
C(5A)	7068(2)	2624(2)	6448(1)	28(1)
C(6A)	8920(2)	1030(2)	7392(1)	29(1)
C(7A)	9420(3)	2716(2)	6032(1)	32(1)
C(8A)	10688(2)	1649(2)	6668(1)	34(1)
C(9A)	6630(2)	2412(1)	9280(1)	18(1)
C(10A)	7615(2)	2962(1)	9669(1)	16(1)
C(11A)	8671(2)	4001(1)	10256(1)	27(1)
C(12A)	9326(2)	3536(2)	10309(1)	25(1)
C(13A)	6620(3)	3925(2)	9669(1)	36(1)
C(14A)	8986(2)	2226(1)	9881(1)	26(1)
C(15A)	8907(3)	4761(2)	10547(2)	47(1)
C(16A)	10527(2)	3623(2)	10682(1)	41(1)
C(17A)	3716(2)	1160(1)	8024(1)	17(1)
C(18A)	3196(2)	699(1)	7418(1)	19(1)
C(19A)	2092(2)	264(1)	7354(1)	23(1)
C(20A)	1495(2)	284(1)	7857(1)	24(1)
C(21A)	1992(2)	752(1)	8440(1)	23(1)
C(22A)	3091(2)	1198(1)	8538(1)	19(1)
C(23A)	3805(2)	677(1)	6846(1)	21(1)
C(24A)	4221(3)	8(2)	6655(1)	35(1)

C(25A)	3046(3)	799(2)	6278(1)	33(1)
C(26A)	3600(2)	1713(1)	9180(1)	23(1)
C(27A)	4127(3)	1368(2)	9662(1)	32(1)
C(28A)	2688(3)	2096(2)	9447(2)	40(1)
C(29A)	5898(2)	2909(1)	8020(1)	19(1)
C(30A)	4848(2)	3221(1)	7848(1)	24(1)
C(31A)	3689(3)	2791(2)	7936(2)	65(1)
C(32A)	4725(3)	3233(2)	7143(2)	56(1)
C(33A)	5103(2)	3974(1)	8247(1)	20(1)
C(34A)	6091(3)	4449(2)	8200(2)	37(1)
C(35A)	6330(3)	5134(2)	8578(2)	64(1)
C(36A)	5569(5)	5324(2)	8999(2)	79(2)
C(37A)	4632(4)	4868(2)	9041(2)	69(1)
C(38A)	4394(3)	4204(2)	8672(2)	44(1)
C(39A)	10453(2)	3105(1)	8572(1)	21(1)
C(40A)	8020(3)	171(2)	8633(1)	32(1)
W(1B)	-480(1)	2821(1)	3298(1)	12(1)
S(1B)	-1637(1)	3025(1)	1821(1)	15(1)
O(1B)	-1740(1)	2854(1)	2434(1)	16(1)
F(1B)	-3764(1)	2232(1)	1348(1)	33(1)
N(1B)	-2719(2)	4183(1)	3199(1)	17(1)
C(1B)	-945(2)	3849(1)	3707(1)	17(1)
S(2B)	-2677(1)	2265(1)	4137(1)	24(1)
O(2B)	-1202(2)	2533(1)	1386(1)	22(1)
F(2B)	-3756(1)	3272(1)	1848(1)	34(1)
C(2B)	-1548(2)	4232(1)	3332(1)	15(1)
N(2B)	-1030(2)	4730(1)	3085(1)	17(1)
N(3B)	-2601(2)	1165(1)	1860(1)	17(1)
O(3B)	-1152(2)	3742(1)	1884(1)	22(1)
F(3B)	-3284(2)	3068(1)	917(1)	41(1)
C(3B)	-2950(2)	4665(1)	2865(1)	19(1)
O(4B)	-2414(1)	2452(1)	3560(1)	18(1)
F(4B)	-4766(1)	2533(1)	3911(1)	32(1)
N(4B)	-838(2)	1211(1)	1662(1)	17(1)
C(4B)	-1891(2)	5004(1)	2788(1)	19(1)
N(5B)	279(2)	2749(1)	4013(1)	15(1)
F(5B)	-4701(1)	1506(1)	3431(1)	43(1)
O(5B)	-2448(2)	2846(1)	4689(1)	40(1)
O(6B)	-2302(2)	1661(1)	4229(1)	44(1)
F(6B)	-4690(2)	1774(1)	4436(1)	60(1)
C(5B)	-3615(2)	3709(1)	3391(1)	25(1)
C(6B)	226(2)	4921(1)	3084(1)	24(1)
C(7B)	-4166(2)	4742(2)	2664(2)	30(1)
C(8B)	-1589(3)	5550(2)	2449(1)	31(1)
C(9B)	-965(2)	1676(1)	2805(1)	16(1)
C(10B)	-1448(2)	1376(1)	2128(1)	15(1)
C(11B)	-2721(2)	855(1)	1210(1)	19(1)

C(12B)	-1614(2)	886(1)	1087(1)	19(1)
C(13B)	-3565(2)	1212(1)	2214(1)	24(1)
C(14B)	440(2)	1394(1)	1744(1)	25(1)
C(15B)	-3891(2)	568(1)	782(1)	27(1)
C(16B)	-1191(3)	624(1)	484(1)	28(1)
C(17B)	958(2)	2704(1)	4572(1)	16(1)
C(18B)	1535(2)	3324(1)	5048(1)	20(1)
C(19B)	2319(2)	3277(1)	5561(1)	25(1)
C(20B)	2534(2)	2643(2)	5613(1)	29(1)
C(21B)	1933(2)	2042(1)	5166(1)	25(1)
C(22B)	1130(2)	2056(1)	4639(1)	19(1)
C(23B)	485(2)	1382(1)	4160(1)	24(1)
C(24B)	1306(3)	1110(2)	3721(1)	31(1)
C(25B)	-34(3)	831(2)	4494(2)	35(1)
C(26B)	1271(2)	4013(1)	5009(1)	21(1)
C(27B)	2305(2)	4631(2)	5299(2)	33(1)
C(28B)	197(2)	4116(1)	5321(1)	26(1)
C(29B)	851(2)	3120(1)	2925(1)	18(1)
C(30B)	2210(2)	3306(1)	3051(1)	21(1)
C(31B)	2644(2)	4083(2)	3129(2)	39(1)
C(32B)	2737(2)	3162(2)	3671(1)	32(1)
C(33B)	2642(2)	2897(1)	2481(1)	22(1)
C(34B)	2467(3)	3052(2)	1894(1)	38(1)
C(35B)	2801(3)	2681(2)	1365(2)	57(1)
C(36B)	3332(3)	2141(2)	1409(2)	66(1)
C(37B)	3522(3)	1973(2)	1985(2)	55(1)
C(38B)	3176(2)	2351(2)	2522(1)	32(1)
C(39B)	-3192(2)	2891(1)	1468(1)	21(1)
C(40B)	-4299(2)	2002(2)	3966(1)	26(1)
C(1X)	6964(3)	773(2)	5196(2)	40(1)
Cl(1X)	5654(1)	915(1)	5461(1)	43(1)
Cl(2X)	7623(1)	245(1)	5590(1)	57(1)

Table S19: Bond lengths [A] and angles [°] for complex 6.

W(1A)-N(5A)	1.750(2)
W(1A)-C(29A)	1.920(2)
W(1A)-C(9A)	2.266(2)
W(1A)-O(1A)	2.2704(16)
W(1A)-C(1A)	2.274(2)
W(1A)-O(4A)	2.4005(16)
S(1A)-O(3A)	1.4312(17)
S(1A)-O(2A)	1.4347(18)
S(1A)-O(1A)	1.4743(18)
S(1A)-C(39A)	1.830(2)
F(1A)-C(39A)	1.331(3)
C(1A)-C(2A)	1.452(3)
C(1A)-H(1A1)	0.96(3)
C(1A)-H(1A2)	0.93(3)
N(1A)-C(2A)	1.347(3)
N(1A)-C(3A)	1.395(3)
N(1A)-C(5A)	1.452(3)
S(2A)-O(6A)	1.430(2)
S(2A)-O(5A)	1.4363(19)
S(2A)-O(4A)	1.4648(18)
S(2A)-C(40A)	1.830(3)
F(2A)-C(39A)	1.332(3)
N(2A)-C(2A)	1.348(3)
N(2A)-C(4A)	1.395(3)
N(2A)-C(6A)	1.452(3)
F(3A)-C(39A)	1.327(3)
N(3A)-C(10A)	1.341(3)
N(3A)-C(11A)	1.392(3)
N(3A)-C(13A)	1.448(3)
C(3A)-C(4A)	1.347(4)
C(3A)-C(7A)	1.486(4)
F(4A)-C(40A)	1.350(3)
N(4A)-C(10A)	1.334(3)
N(4A)-C(12A)	1.392(3)
N(4A)-C(14A)	1.464(3)
C(4A)-C(8A)	1.492(3)
N(5A)-C(17A)	1.411(3)
F(5A)-C(40A)	1.329(4)
F(6A)-C(40A)	1.333(3)
C(5A)-H(5A1)	0.9800
C(5A)-H(5A2)	0.9800
C(5A)-H(5A3)	0.9800
C(6A)-H(6A1)	0.9800
C(6A)-H(6A2)	0.9800
C(6A)-H(6A3)	0.9800
C(7A)-H(7A1)	0.9800

C(7A)-H(7A2)	0.9800
C(7A)-H(7A3)	0.9800
C(8A)-H(8A1)	0.9800
C(8A)-H(8A2)	0.9800
C(8A)-H(8A3)	0.9800
C(9A)-C(10A)	1.460(3)
C(9A)-H(9A1)	0.97(3)
C(9A)-H(9A2)	0.96(3)
C(11A)-C(12A)	1.341(4)
C(11A)-C(15A)	1.490(4)
C(12A)-C(16A)	1.490(4)
C(13A)-H(13A)	0.9800
C(13A)-H(13B)	0.9800
C(13A)-H(13C)	0.9800
C(14A)-H(14A)	0.9800
C(14A)-H(14B)	0.9800
C(14A)-H(14C)	0.9800
C(15A)-H(15A)	0.9800
C(15A)-H(15B)	0.9800
C(15A)-H(15C)	0.9800
C(16A)-H(16A)	0.9800
C(16A)-H(16B)	0.9800
C(16A)-H(16C)	0.9800
C(17A)-C(22A)	1.417(3)
C(17A)-C(18A)	1.420(3)
C(18A)-C(19A)	1.394(3)
C(18A)-C(23A)	1.518(3)
C(19A)-C(20A)	1.377(4)
C(19A)-H(19A)	0.9500
C(20A)-C(21A)	1.384(4)
C(20A)-H(20A)	0.9500
C(21A)-C(22A)	1.388(4)
C(21A)-H(21A)	0.9500
C(22A)-C(26A)	1.517(3)
C(23A)-C(24A)	1.520(4)
C(23A)-C(25A)	1.530(4)
C(23A)-H(23A)	10.000
C(24A)-H(24A)	0.9800
C(24A)-H(24B)	0.9800
C(24A)-H(24C)	0.9800
C(25A)-H(25A)	0.9800
C(25A)-H(25B)	0.9800
C(25A)-H(25C)	0.9800
C(26A)-C(27A)	1.526(4)
C(26A)-C(28A)	1.535(3)
C(26A)-H(26A)	10.000
C(27A)-H(27A)	0.9800

C(27A)-H(27B)	0.9800
C(27A)-H(27C)	0.9800
C(28A)-H(28A)	0.9800
C(28A)-H(28B)	0.9800
C(28A)-H(28C)	0.9800
C(29A)-C(30A)	1.530(3)
C(29A)-H(29A)	0.9500
C(30A)-C(31A)	1.531(4)
C(30A)-C(33A)	1.533(3)
C(30A)-C(32A)	1.539(4)
C(31A)-H(31A)	0.9800
C(31A)-H(31B)	0.9800
C(31A)-H(31C)	0.9800
C(32A)-H(32A)	0.9800
C(32A)-H(32B)	0.9800
C(32A)-H(32C)	0.9800
C(33A)-C(38A)	1.387(4)
C(33A)-C(34A)	1.392(4)
C(34A)-C(35A)	1.404(5)
C(34A)-H(34A)	0.9500
C(35A)-C(36A)	1.405(7)
C(35A)-H(35A)	0.9500
C(36A)-C(37A)	1.324(7)
C(36A)-H(36A)	0.9500
C(37A)-C(38A)	1.362(5)
C(37A)-H(37A)	0.9500
C(38A)-H(38A)	0.9500
W(1B)-N(5B)	1.7491(19)
W(1B)-C(29B)	1.918(2)
W(1B)-C(9B)	2.261(2)
W(1B)-O(1B)	2.2671(15)
W(1B)-C(1B)	2.274(2)
W(1B)-O(4B)	2.4321(16)
S(1B)-O(3B)	1.4307(18)
S(1B)-O(2B)	1.4317(17)
S(1B)-O(1B)	1.4780(17)
S(1B)-C(39B)	1.827(2)
F(1B)-C(39B)	1.331(3)
N(1B)-C(2B)	1.344(3)
N(1B)-C(3B)	1.397(3)
N(1B)-C(5B)	1.460(3)
C(1B)-C(2B)	1.461(3)
C(1B)-H(1B1)	0.92(3)
C(1B)-H(1B2)	0.95(3)
S(2B)-O(6B)	1.429(2)
S(2B)-O(5B)	1.439(2)
S(2B)-O(4B)	1.4576(18)

S(2B)-C(40B)	1.837(3)
F(2B)-C(39B)	1.331(3)
C(2B)-N(2B)	1.341(3)
N(2B)-C(4B)	1.399(3)
N(2B)-C(6B)	1.449(3)
N(3B)-C(10B)	1.345(3)
N(3B)-C(11B)	1.396(3)
N(3B)-C(13B)	1.457(3)
F(3B)-C(39B)	1.333(3)
C(3B)-C(4B)	1.352(4)
C(3B)-C(7B)	1.483(3)
F(4B)-C(40B)	1.322(3)
N(4B)-C(10B)	1.337(3)
N(4B)-C(12B)	1.396(3)
N(4B)-C(14B)	1.449(3)
C(4B)-C(8B)	1.488(4)
N(5B)-C(17B)	1.404(3)
F(5B)-C(40B)	1.323(3)
F(6B)-C(40B)	1.323(3)
C(5B)-H(5B1)	0.9800
C(5B)-H(5B2)	0.9800
C(5B)-H(5B3)	0.9800
C(6B)-H(6B1)	0.9800
C(6B)-H(6B2)	0.9800
C(6B)-H(6B3)	0.9800
C(7B)-H(7B1)	0.9800
C(7B)-H(7B2)	0.9800
C(7B)-H(7B3)	0.9800
C(8B)-H(8B1)	0.9800
C(8B)-H(8B2)	0.9800
C(8B)-H(8B3)	0.9800
C(9B)-C(10B)	1.459(3)
C(9B)-H(9B1)	0.95(3)
C(9B)-H(9B2)	0.92(3)
C(11B)-C(12B)	1.351(3)
C(11B)-C(15B)	1.487(3)
C(12B)-C(16B)	1.491(3)
C(13B)-H(13D)	0.9800
C(13B)-H(13E)	0.9800
C(13B)-H(13F)	0.9800
C(14B)-H(14D)	0.9800
C(14B)-H(14E)	0.9800
C(14B)-H(14F)	0.9800
C(15B)-H(15D)	0.9800
C(15B)-H(15E)	0.9800
C(15B)-H(15F)	0.9800
C(16B)-H(16D)	0.9800

C(16B)-H(16E)	0.9800
C(16B)-H(16F)	0.9800
C(17B)-C(22B)	1.410(3)
C(17B)-C(18B)	1.424(3)
C(18B)-C(19B)	1.389(3)
C(18B)-C(26B)	1.511(3)
C(19B)-C(20B)	1.389(4)
C(19B)-H(19B)	0.9500
C(20B)-C(21B)	1.378(4)
C(20B)-H(20B)	0.9500
C(21B)-C(22B)	1.400(3)
C(21B)-H(21B)	0.9500
C(22B)-C(23B)	1.515(3)
C(23B)-C(24B)	1.533(4)
C(23B)-C(25B)	1.547(4)
C(23B)-H(23B)	10.000
C(24B)-H(24D)	0.9800
C(24B)-H(24E)	0.9800
C(24B)-H(24F)	0.9800
C(25B)-H(25D)	0.9800
C(25B)-H(25E)	0.9800
C(25B)-H(25F)	0.9800
C(26B)-C(27B)	1.521(4)
C(26B)-C(28B)	1.534(3)
C(26B)-H(26B)	10.000
C(27B)-H(27D)	0.9800
C(27B)-H(27E)	0.9800
C(27B)-H(27F)	0.9800
C(28B)-H(28D)	0.9800
C(28B)-H(28E)	0.9800
C(28B)-H(28F)	0.9800
C(29B)-C(30B)	1.536(3)
C(29B)-H(29B)	0.9500
C(30B)-C(31B)	1.531(4)
C(30B)-C(32B)	1.532(4)
C(30B)-C(33B)	1.535(3)
C(31B)-H(31D)	0.9800
C(31B)-H(31E)	0.9800
C(31B)-H(31F)	0.9800
C(32B)-H(32D)	0.9800
C(32B)-H(32E)	0.9800
C(32B)-H(32F)	0.9800
C(33B)-C(38B)	1.389(4)
C(33B)-C(34B)	1.392(4)
C(34B)-C(35B)	1.377(5)
C(34B)-H(34B)	0.9500
C(35B)-C(36B)	1.376(6)

C(35B)-H(35B)	0.9500
C(36B)-C(37B)	1.383(6)
C(36B)-H(36B)	0.9500
C(37B)-C(38B)	1.401(4)
C(37B)-H(37B)	0.9500
C(38B)-H(38B)	0.9500
C(1X)-Cl(2X)	1.751(3)
C(1X)-Cl(1X)	1.759(3)
C(1X)-H(1X1)	0.9900
C(1X)-H(1X2)	0.9900

N(5A)-W(1A)-C(29A)	99.29(10)
N(5A)-W(1A)-C(9A)	96.47(9)
C(29A)-W(1A)-C(9A)	100.35(10)
N(5A)-W(1A)-O(1A)	170.81(7)
C(29A)-W(1A)-O(1A)	89.90(8)
C(9A)-W(1A)-O(1A)	81.84(8)
N(5A)-W(1A)-C(1A)	96.99(9)
C(29A)-W(1A)-C(1A)	99.95(10)
C(9A)-W(1A)-C(1A)	153.42(9)
O(1A)-W(1A)-C(1A)	81.22(7)
N(5A)-W(1A)-O(4A)	94.66(7)
C(29A)-W(1A)-O(4A)	166.02(8)
C(9A)-W(1A)-O(4A)	78.83(7)
O(1A)-W(1A)-O(4A)	76.14(6)
C(1A)-W(1A)-O(4A)	77.33(8)
O(3A)-S(1A)-O(2A)	116.81(11)
O(3A)-S(1A)-O(1A)	113.97(11)
O(2A)-S(1A)-O(1A)	114.59(10)
O(3A)-S(1A)-C(39A)	104.41(11)
O(2A)-S(1A)-C(39A)	104.12(11)
O(1A)-S(1A)-C(39A)	100.24(11)
S(1A)-O(1A)-W(1A)	138.26(9)
C(2A)-C(1A)-W(1A)	126.05(17)
C(2A)-C(1A)-H(1A1)	108.3(15)
W(1A)-C(1A)-H(1A1)	104.0(16)
C(2A)-C(1A)-H(1A2)	104.9(18)
W(1A)-C(1A)-H(1A2)	105.7(17)
H(1A1)-C(1A)-H(1A2)	106(2)
C(2A)-N(1A)-C(3A)	110.7(2)
C(2A)-N(1A)-C(5A)	125.0(2)
C(3A)-N(1A)-C(5A)	124.1(2)
O(6A)-S(2A)-O(5A)	117.22(13)
O(6A)-S(2A)-O(4A)	114.50(12)
O(5A)-S(2A)-O(4A)	114.02(11)
O(6A)-S(2A)-C(40A)	103.93(15)
O(5A)-S(2A)-C(40A)	103.02(12)

O(4A)-S(2A)-C(40A)	101.34(12)
C(2A)-N(2A)-C(4A)	110.0(2)
C(2A)-N(2A)-C(6A)	124.5(2)
C(4A)-N(2A)-C(6A)	125.4(2)
N(1A)-C(2A)-N(2A)	105.8(2)
N(1A)-C(2A)-C(1A)	127.0(2)
N(2A)-C(2A)-C(1A)	127.1(2)
C(10A)-N(3A)-C(11A)	109.9(2)
C(10A)-N(3A)-C(13A)	123.9(2)
C(11A)-N(3A)-C(13A)	126.3(2)
C(4A)-C(3A)-N(1A)	106.1(2)
C(4A)-C(3A)-C(7A)	131.8(2)
N(1A)-C(3A)-C(7A)	122.0(2)
S(2A)-O(4A)-W(1A)	129.43(9)
C(10A)-N(4A)-C(12A)	109.9(2)
C(10A)-N(4A)-C(14A)	123.4(2)
C(12A)-N(4A)-C(14A)	126.5(2)
C(3A)-C(4A)-N(2A)	107.3(2)
C(3A)-C(4A)-C(8A)	130.6(3)
N(2A)-C(4A)-C(8A)	122.2(2)
C(17A)-N(5A)-W(1A)	178.03(16)
N(1A)-C(5A)-H(5A1)	109.5
N(1A)-C(5A)-H(5A2)	109.5
H(5A1)-C(5A)-H(5A2)	109.5
N(1A)-C(5A)-H(5A3)	109.5
H(5A1)-C(5A)-H(5A3)	109.5
H(5A2)-C(5A)-H(5A3)	109.5
N(2A)-C(6A)-H(6A1)	109.5
N(2A)-C(6A)-H(6A2)	109.5
H(6A1)-C(6A)-H(6A2)	109.5
N(2A)-C(6A)-H(6A3)	109.5
H(6A1)-C(6A)-H(6A3)	109.5
H(6A2)-C(6A)-H(6A3)	109.5
C(3A)-C(7A)-H(7A1)	109.5
C(3A)-C(7A)-H(7A2)	109.5
H(7A1)-C(7A)-H(7A2)	109.5
C(3A)-C(7A)-H(7A3)	109.5
H(7A1)-C(7A)-H(7A3)	109.5
H(7A2)-C(7A)-H(7A3)	109.5
C(4A)-C(8A)-H(8A1)	109.5
C(4A)-C(8A)-H(8A2)	109.5
H(8A1)-C(8A)-H(8A2)	109.5
C(4A)-C(8A)-H(8A3)	109.5
H(8A1)-C(8A)-H(8A3)	109.5
H(8A2)-C(8A)-H(8A3)	109.5
C(10A)-C(9A)-W(1A)	124.08(17)
C(10A)-C(9A)-H(9A1)	105.3(17)

W(1A)-C(9A)-H(9A1)	104.8(16)
C(10A)-C(9A)-H(9A2)	106(2)
W(1A)-C(9A)-H(9A2)	107(2)
H(9A1)-C(9A)-H(9A2)	108(3)
N(4A)-C(10A)-N(3A)	106.6(2)
N(4A)-C(10A)-C(9A)	127.4(2)
N(3A)-C(10A)-C(9A)	125.9(2)
C(12A)-C(11A)-N(3A)	106.6(2)
C(12A)-C(11A)-C(15A)	131.5(3)
N(3A)-C(11A)-C(15A)	121.8(3)
C(11A)-C(12A)-N(4A)	107.0(2)
C(11A)-C(12A)-C(16A)	130.6(3)
N(4A)-C(12A)-C(16A)	122.4(3)
N(3A)-C(13A)-H(13A)	109.5
N(3A)-C(13A)-H(13B)	109.5
H(13A)-C(13A)-H(13B)	109.5
N(3A)-C(13A)-H(13C)	109.5
H(13A)-C(13A)-H(13C)	109.5
H(13B)-C(13A)-H(13C)	109.5
N(4A)-C(14A)-H(14A)	109.5
N(4A)-C(14A)-H(14B)	109.5
H(14A)-C(14A)-H(14B)	109.5
N(4A)-C(14A)-H(14C)	109.5
H(14A)-C(14A)-H(14C)	109.5
H(14B)-C(14A)-H(14C)	109.5
C(11A)-C(15A)-H(15A)	109.5
C(11A)-C(15A)-H(15B)	109.5
H(15A)-C(15A)-H(15B)	109.5
C(11A)-C(15A)-H(15C)	109.5
H(15A)-C(15A)-H(15C)	109.5
H(15B)-C(15A)-H(15C)	109.5
C(12A)-C(16A)-H(16A)	109.5
C(12A)-C(16A)-H(16B)	109.5
H(16A)-C(16A)-H(16B)	109.5
C(12A)-C(16A)-H(16C)	109.5
H(16A)-C(16A)-H(16C)	109.5
H(16B)-C(16A)-H(16C)	109.5
N(5A)-C(17A)-C(22A)	120.5(2)
N(5A)-C(17A)-C(18A)	119.2(2)
C(22A)-C(17A)-C(18A)	120.3(2)
C(19A)-C(18A)-C(17A)	118.3(2)
C(19A)-C(18A)-C(23A)	119.9(2)
C(17A)-C(18A)-C(23A)	121.8(2)
C(20A)-C(19A)-C(18A)	121.6(2)
C(20A)-C(19A)-H(19A)	119.2
C(18A)-C(19A)-H(19A)	119.2
C(19A)-C(20A)-C(21A)	119.5(2)

C(19A)-C(20A)-H(20A)	120.2
C(21A)-C(20A)-H(20A)	120.2
C(20A)-C(21A)-C(22A)	122.0(2)
C(20A)-C(21A)-H(21A)	119.0
C(22A)-C(21A)-H(21A)	119.0
C(21A)-C(22A)-C(17A)	118.2(2)
C(21A)-C(22A)-C(26A)	120.6(2)
C(17A)-C(22A)-C(26A)	121.3(2)
C(18A)-C(23A)-C(24A)	111.5(2)
C(18A)-C(23A)-C(25A)	112.9(2)
C(24A)-C(23A)-C(25A)	111.1(2)
C(18A)-C(23A)-H(23A)	107.0
C(24A)-C(23A)-H(23A)	107.0
C(25A)-C(23A)-H(23A)	107.0
C(23A)-C(24A)-H(24A)	109.5
C(23A)-C(24A)-H(24B)	109.5
H(24A)-C(24A)-H(24B)	109.5
C(23A)-C(24A)-H(24C)	109.5
H(24A)-C(24A)-H(24C)	109.5
H(24B)-C(24A)-H(24C)	109.5
C(23A)-C(25A)-H(25A)	109.5
C(23A)-C(25A)-H(25B)	109.5
H(25A)-C(25A)-H(25B)	109.5
C(23A)-C(25A)-H(25C)	109.5
H(25A)-C(25A)-H(25C)	109.5
H(25B)-C(25A)-H(25C)	109.5
C(22A)-C(26A)-C(27A)	111.5(2)
C(22A)-C(26A)-C(28A)	112.3(2)
C(27A)-C(26A)-C(28A)	110.4(2)
C(22A)-C(26A)-H(26A)	107.4
C(27A)-C(26A)-H(26A)	107.4
C(28A)-C(26A)-H(26A)	107.4
C(26A)-C(27A)-H(27A)	109.5
C(26A)-C(27A)-H(27B)	109.5
H(27A)-C(27A)-H(27B)	109.5
C(26A)-C(27A)-H(27C)	109.5
H(27A)-C(27A)-H(27C)	109.5
H(27B)-C(27A)-H(27C)	109.5
C(26A)-C(28A)-H(28A)	109.5
C(26A)-C(28A)-H(28B)	109.5
H(28A)-C(28A)-H(28B)	109.5
C(26A)-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)-W(1A)	142.27(19)
C(30A)-C(29A)-H(29A)	108.9
W(1A)-C(29A)-H(29A)	108.9

C(29A)-C(30A)-C(31A)	111.5(2)
C(29A)-C(30A)-C(33A)	108.85(19)
C(31A)-C(30A)-C(33A)	112.1(2)
C(29A)-C(30A)-C(32A)	109.2(2)
C(31A)-C(30A)-C(32A)	107.8(3)
C(33A)-C(30A)-C(32A)	107.2(2)
C(30A)-C(31A)-H(31A)	109.5
C(30A)-C(31A)-H(31B)	109.5
H(31A)-C(31A)-H(31B)	109.5
C(30A)-C(31A)-H(31C)	109.5
H(31A)-C(31A)-H(31C)	109.5
H(31B)-C(31A)-H(31C)	109.5
C(30A)-C(32A)-H(32A)	109.5
C(30A)-C(32A)-H(32B)	109.5
H(32A)-C(32A)-H(32B)	109.5
C(30A)-C(32A)-H(32C)	109.5
H(32A)-C(32A)-H(32C)	109.5
H(32B)-C(32A)-H(32C)	109.5
C(38A)-C(33A)-C(34A)	117.8(3)
C(38A)-C(33A)-C(30A)	122.2(3)
C(34A)-C(33A)-C(30A)	120.0(2)
C(33A)-C(34A)-C(35A)	119.5(4)
C(33A)-C(34A)-H(34A)	120.3
C(35A)-C(34A)-H(34A)	120.3
C(34A)-C(35A)-C(36A)	119.1(4)
C(34A)-C(35A)-H(35A)	120.5
C(36A)-C(35A)-H(35A)	120.5
C(37A)-C(36A)-C(35A)	121.0(4)
C(37A)-C(36A)-H(36A)	119.5
C(35A)-C(36A)-H(36A)	119.5
C(36A)-C(37A)-C(38A)	120.0(4)
C(36A)-C(37A)-H(37A)	120.0
C(38A)-C(37A)-H(37A)	120.0
C(37A)-C(38A)-C(33A)	122.6(4)
C(37A)-C(38A)-H(38A)	118.7
C(33A)-C(38A)-H(38A)	118.7
F(3A)-C(39A)-F(1A)	107.8(2)
F(3A)-C(39A)-F(2A)	107.6(2)
F(1A)-C(39A)-F(2A)	107.7(2)
F(3A)-C(39A)-S(1A)	111.62(17)
F(1A)-C(39A)-S(1A)	111.60(16)
F(2A)-C(39A)-S(1A)	110.41(17)
F(5A)-C(40A)-F(6A)	107.9(3)
F(5A)-C(40A)-F(4A)	107.6(2)
F(6A)-C(40A)-F(4A)	107.2(2)
F(5A)-C(40A)-S(2A)	112.17(19)
F(6A)-C(40A)-S(2A)	112.1(2)

F(4A)-C(40A)-S(2A)	109.6(2)
N(5B)-W(1B)-C(29B)	98.81(10)
N(5B)-W(1B)-C(9B)	96.31(8)
C(29B)-W(1B)-C(9B)	100.63(9)
N(5B)-W(1B)-O(1B)	170.49(8)
C(29B)-W(1B)-O(1B)	90.70(8)
C(9B)-W(1B)-O(1B)	81.63(7)
N(5B)-W(1B)-C(1B)	96.83(8)
C(29B)-W(1B)-C(1B)	100.99(10)
C(9B)-W(1B)-C(1B)	152.58(9)
O(1B)-W(1B)-C(1B)	81.44(7)
N(5B)-W(1B)-O(4B)	93.50(7)
C(29B)-W(1B)-O(4B)	167.69(8)
C(9B)-W(1B)-O(4B)	77.52(8)
O(1B)-W(1B)-O(4B)	76.99(6)
C(1B)-W(1B)-O(4B)	77.75(8)
O(3B)-S(1B)-O(2B)	116.81(11)
O(3B)-S(1B)-O(1B)	113.94(10)
O(2B)-S(1B)-O(1B)	113.72(10)
O(3B)-S(1B)-C(39B)	104.46(11)
O(2B)-S(1B)-C(39B)	104.34(11)
O(1B)-S(1B)-C(39B)	101.21(11)
S(1B)-O(1B)-W(1B)	136.57(10)
C(2B)-N(1B)-C(3B)	110.1(2)
C(2B)-N(1B)-C(5B)	125.0(2)
C(3B)-N(1B)-C(5B)	124.96(19)
C(2B)-C(1B)-W(1B)	124.79(16)
C(2B)-C(1B)-H(1B1)	109.8(17)
W(1B)-C(1B)-H(1B1)	103.0(18)
C(2B)-C(1B)-H(1B2)	108.8(16)
W(1B)-C(1B)-H(1B2)	103.3(15)
H(1B1)-C(1B)-H(1B2)	106(2)
O(6B)-S(2B)-O(5B)	116.51(15)
O(6B)-S(2B)-O(4B)	114.45(12)
O(5B)-S(2B)-O(4B)	113.91(12)
O(6B)-S(2B)-C(40B)	104.54(13)
O(5B)-S(2B)-C(40B)	102.78(12)
O(4B)-S(2B)-C(40B)	102.20(11)
N(2B)-C(2B)-N(1B)	106.74(19)
N(2B)-C(2B)-C(1B)	126.3(2)
N(1B)-C(2B)-C(1B)	126.9(2)
C(2B)-N(2B)-C(4B)	109.82(19)
C(2B)-N(2B)-C(6B)	125.0(2)
C(4B)-N(2B)-C(6B)	125.1(2)
C(10B)-N(3B)-C(11B)	110.0(2)
C(10B)-N(3B)-C(13B)	124.1(2)
C(11B)-N(3B)-C(13B)	125.8(2)

C(4B)-C(3B)-N(1B)	106.5(2)
C(4B)-C(3B)-C(7B)	131.2(2)
N(1B)-C(3B)-C(7B)	122.3(2)
S(2B)-O(4B)-W(1B)	127.72(9)
C(10B)-N(4B)-C(12B)	109.9(2)
C(10B)-N(4B)-C(14B)	124.2(2)
C(12B)-N(4B)-C(14B)	125.7(2)
C(3B)-C(4B)-N(2B)	106.8(2)
C(3B)-C(4B)-C(8B)	130.8(2)
N(2B)-C(4B)-C(8B)	122.3(2)
C(17B)-N(5B)-W(1B)	176.29(18)
N(1B)-C(5B)-H(5B1)	109.5
N(1B)-C(5B)-H(5B2)	109.5
H(5B1)-C(5B)-H(5B2)	109.5
N(1B)-C(5B)-H(5B3)	109.5
H(5B1)-C(5B)-H(5B3)	109.5
H(5B2)-C(5B)-H(5B3)	109.5
N(2B)-C(6B)-H(6B1)	109.5
N(2B)-C(6B)-H(6B2)	109.5
H(6B1)-C(6B)-H(6B2)	109.5
N(2B)-C(6B)-H(6B3)	109.5
H(6B1)-C(6B)-H(6B3)	109.5
H(6B2)-C(6B)-H(6B3)	109.5
C(3B)-C(7B)-H(7B1)	109.5
C(3B)-C(7B)-H(7B2)	109.5
H(7B1)-C(7B)-H(7B2)	109.5
C(3B)-C(7B)-H(7B3)	109.5
H(7B1)-C(7B)-H(7B3)	109.5
H(7B2)-C(7B)-H(7B3)	109.5
C(4B)-C(8B)-H(8B1)	109.5
C(4B)-C(8B)-H(8B2)	109.5
H(8B1)-C(8B)-H(8B2)	109.5
C(4B)-C(8B)-H(8B3)	109.5
H(8B1)-C(8B)-H(8B3)	109.5
H(8B2)-C(8B)-H(8B3)	109.5
C(10B)-C(9B)-W(1B)	125.18(17)
C(10B)-C(9B)-H(9B1)	107.2(17)
W(1B)-C(9B)-H(9B1)	103.7(17)
C(10B)-C(9B)-H(9B2)	109.9(19)
W(1B)-C(9B)-H(9B2)	102.1(19)
H(9B1)-C(9B)-H(9B2)	108(2)
N(4B)-C(10B)-N(3B)	106.74(19)
N(4B)-C(10B)-C(9B)	126.7(2)
N(3B)-C(10B)-C(9B)	126.4(2)
C(12B)-C(11B)-N(3B)	106.5(2)
C(12B)-C(11B)-C(15B)	130.9(2)
N(3B)-C(11B)-C(15B)	122.7(2)

C(11B)-C(12B)-N(4B)	107.0(2)
C(11B)-C(12B)-C(16B)	130.8(2)
N(4B)-C(12B)-C(16B)	122.2(2)
N(3B)-C(13B)-H(13D)	109.5
N(3B)-C(13B)-H(13E)	109.5
H(13D)-C(13B)-H(13E)	109.5
N(3B)-C(13B)-H(13F)	109.5
H(13D)-C(13B)-H(13F)	109.5
H(13E)-C(13B)-H(13F)	109.5
N(4B)-C(14B)-H(14D)	109.5
N(4B)-C(14B)-H(14E)	109.5
H(14D)-C(14B)-H(14E)	109.5
N(4B)-C(14B)-H(14F)	109.5
H(14D)-C(14B)-H(14F)	109.5
H(14E)-C(14B)-H(14F)	109.5
C(11B)-C(15B)-H(15D)	109.5
C(11B)-C(15B)-H(15E)	109.5
H(15D)-C(15B)-H(15E)	109.5
C(11B)-C(15B)-H(15F)	109.5
H(15D)-C(15B)-H(15F)	109.5
H(15E)-C(15B)-H(15F)	109.5
C(12B)-C(16B)-H(16D)	109.5
C(12B)-C(16B)-H(16E)	109.5
H(16D)-C(16B)-H(16E)	109.5
C(12B)-C(16B)-H(16F)	109.5
H(16D)-C(16B)-H(16F)	109.5
H(16E)-C(16B)-H(16F)	109.5
N(5B)-C(17B)-C(22B)	120.0(2)
N(5B)-C(17B)-C(18B)	119.2(2)
C(22B)-C(17B)-C(18B)	120.7(2)
C(19B)-C(18B)-C(17B)	118.4(2)
C(19B)-C(18B)-C(26B)	120.7(2)
C(17B)-C(18B)-C(26B)	120.9(2)
C(18B)-C(19B)-C(20B)	121.1(2)
C(18B)-C(19B)-H(19B)	119.4
C(20B)-C(19B)-H(19B)	119.4
C(21B)-C(20B)-C(19B)	120.1(2)
C(21B)-C(20B)-H(20B)	119.9
C(19B)-C(20B)-H(20B)	119.9
C(20B)-C(21B)-C(22B)	121.3(2)
C(20B)-C(21B)-H(21B)	119.3
C(22B)-C(21B)-H(21B)	119.3
C(21B)-C(22B)-C(17B)	118.2(2)
C(21B)-C(22B)-C(23B)	119.5(2)
C(17B)-C(22B)-C(23B)	122.3(2)
C(22B)-C(23B)-C(24B)	110.4(2)
C(22B)-C(23B)-C(25B)	111.6(2)

C(24B)-C(23B)-C(25B)	111.0(2)
C(22B)-C(23B)-H(23B)	107.9
C(24B)-C(23B)-H(23B)	107.9
C(25B)-C(23B)-H(23B)	107.9
C(23B)-C(24B)-H(24D)	109.5
C(23B)-C(24B)-H(24E)	109.5
H(24D)-C(24B)-H(24E)	109.5
C(23B)-C(24B)-H(24F)	109.5
H(24D)-C(24B)-H(24F)	109.5
H(24E)-C(24B)-H(24F)	109.5
C(23B)-C(25B)-H(25D)	109.5
C(23B)-C(25B)-H(25E)	109.5
H(25D)-C(25B)-H(25E)	109.5
C(23B)-C(25B)-H(25F)	109.5
H(25D)-C(25B)-H(25F)	109.5
H(25E)-C(25B)-H(25F)	109.5
C(18B)-C(26B)-C(27B)	114.3(2)
C(18B)-C(26B)-C(28B)	109.4(2)
C(27B)-C(26B)-C(28B)	110.2(2)
C(18B)-C(26B)-H(26B)	107.6
C(27B)-C(26B)-H(26B)	107.6
C(28B)-C(26B)-H(26B)	107.6
C(26B)-C(27B)-H(27D)	109.5
C(26B)-C(27B)-H(27E)	109.5
H(27D)-C(27B)-H(27E)	109.5
C(26B)-C(27B)-H(27F)	109.5
H(27D)-C(27B)-H(27F)	109.5
H(27E)-C(27B)-H(27F)	109.5
C(26B)-C(28B)-H(28D)	109.5
C(26B)-C(28B)-H(28E)	109.5
H(28D)-C(28B)-H(28E)	109.5
C(26B)-C(28B)-H(28F)	109.5
H(28D)-C(28B)-H(28F)	109.5
H(28E)-C(28B)-H(28F)	109.5
C(30B)-C(29B)-W(1B)	142.42(19)
C(30B)-C(29B)-H(29B)	108.8
W(1B)-C(29B)-H(29B)	108.8
C(31B)-C(30B)-C(32B)	106.4(2)
C(31B)-C(30B)-C(33B)	109.5(2)
C(32B)-C(30B)-C(33B)	110.7(2)
C(31B)-C(30B)-C(29B)	109.2(2)
C(32B)-C(30B)-C(29B)	112.2(2)
C(33B)-C(30B)-C(29B)	108.77(19)
C(30B)-C(31B)-H(31D)	109.5
C(30B)-C(31B)-H(31E)	109.5
H(31D)-C(31B)-H(31E)	109.5
C(30B)-C(31B)-H(31F)	109.5

H(31D)-C(31B)-H(31F)	109.5
H(31E)-C(31B)-H(31F)	109.5
C(30B)-C(32B)-H(32D)	109.5
C(30B)-C(32B)-H(32E)	109.5
H(32D)-C(32B)-H(32E)	109.5
C(30B)-C(32B)-H(32F)	109.5
H(32D)-C(32B)-H(32F)	109.5
H(32E)-C(32B)-H(32F)	109.5
C(38B)-C(33B)-C(34B)	117.9(3)
C(38B)-C(33B)-C(30B)	121.9(2)
C(34B)-C(33B)-C(30B)	120.1(2)
C(35B)-C(34B)-C(33B)	121.9(3)
C(35B)-C(34B)-H(34B)	119.1
C(33B)-C(34B)-H(34B)	119.1
C(36B)-C(35B)-C(34B)	119.9(4)
C(36B)-C(35B)-H(35B)	120.0
C(34B)-C(35B)-H(35B)	120.0
C(35B)-C(36B)-C(37B)	119.7(3)
C(35B)-C(36B)-H(36B)	120.1
C(37B)-C(36B)-H(36B)	120.1
C(36B)-C(37B)-C(38B)	120.2(3)
C(36B)-C(37B)-H(37B)	119.9
C(38B)-C(37B)-H(37B)	119.9
C(33B)-C(38B)-C(37B)	120.3(3)
C(33B)-C(38B)-H(38B)	119.8
C(37B)-C(38B)-H(38B)	119.8
F(1B)-C(39B)-F(2B)	107.4(2)
F(1B)-C(39B)-F(3B)	107.6(2)
F(2B)-C(39B)-F(3B)	107.7(2)
F(1B)-C(39B)-S(1B)	111.96(17)
F(2B)-C(39B)-S(1B)	111.71(17)
F(3B)-C(39B)-S(1B)	110.24(18)
F(4B)-C(40B)-F(5B)	107.6(2)
F(4B)-C(40B)-F(6B)	107.8(2)
F(5B)-C(40B)-F(6B)	108.1(2)
F(4B)-C(40B)-S(2B)	110.74(19)
F(5B)-C(40B)-S(2B)	112.30(18)
F(6B)-C(40B)-S(2B)	110.15(18)
Cl(2X)-C(1X)-Cl(1X)	111.81(18)
Cl(2X)-C(1X)-H(1X1)	109.3
Cl(1X)-C(1X)-H(1X1)	109.3
Cl(2X)-C(1X)-H(1X2)	109.3
Cl(1X)-C(1X)-H(1X2)	109.3
H(1X1)-C(1X)-H(1X2)	107.9

Table S20: Anisotropic displacement parameters (A^2 x 10^3) for complex 6. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$.

	U11	U22	U33	U23	U13	U12
W(1A)	11(1)	12(1)	12(1)	-1(1)	-1(1)	3(1)
S(1A)	14(1)	16(1)	17(1)	3(1)	0(1)	2(1)
F(1A)	22(1)	53(1)	28(1)	22(1)	3(1)	13(1)
O(1A)	12(1)	15(1)	20(1)	3(1)	1(1)	2(1)
C(1A)	18(1)	20(1)	15(1)	0(1)	1(1)	3(1)
N(1A)	21(1)	24(1)	16(1)	3(1)	2(1)	6(1)
S(2A)	21(1)	16(1)	20(1)	4(1)	0(1)	1(1)
F(2A)	15(1)	35(1)	49(1)	17(1)	1(1)	-3(1)
O(2A)	24(1)	27(1)	20(1)	9(1)	0(1)	2(1)
N(2A)	22(1)	22(1)	19(1)	6(1)	6(1)	9(1)
C(2A)	20(1)	19(1)	13(1)	0(1)	2(1)	5(1)
F(3A)	24(1)	38(1)	40(1)	-5(1)	4(1)	15(1)
O(3A)	22(1)	18(1)	25(1)	0(1)	1(1)	4(1)
N(3A)	29(1)	14(1)	15(1)	-1(1)	1(1)	4(1)
C(3A)	23(1)	29(2)	20(1)	4(1)	5(1)	5(1)
O(4A)	16(1)	16(1)	20(1)	5(1)	3(1)	5(1)
F(4A)	81(1)	30(1)	40(1)	22(1)	28(1)	33(1)
N(4A)	16(1)	20(1)	14(1)	2(1)	-2(1)	0(1)
C(4A)	22(1)	31(2)	18(1)	5(1)	8(1)	8(1)
N(5A)	14(1)	14(1)	13(1)	-2(1)	0(1)	4(1)
O(5A)	30(1)	28(1)	26(1)	11(1)	11(1)	10(1)
F(5A)	30(1)	54(1)	58(1)	25(1)	10(1)	24(1)
F(6A)	101(2)	39(1)	38(1)	20(1)	39(1)	45(1)
O(6A)	47(1)	29(1)	41(1)	8(1)	-16(1)	-16(1)
C(5A)	26(1)	31(2)	30(1)	14(1)	3(1)	12(1)
C(6A)	31(1)	34(2)	33(2)	17(1)	14(1)	17(1)
C(7A)	33(2)	38(2)	30(2)	17(1)	10(1)	8(1)
C(8A)	29(2)	48(2)	33(2)	16(1)	15(1)	18(1)
C(9A)	16(1)	20(1)	13(1)	-1(1)	-1(1)	2(1)
C(10A)	18(1)	16(1)	11(1)	1(1)	3(1)	2(1)
C(11A)	35(2)	20(1)	15(1)	-2(1)	0(1)	-8(1)
C(12A)	21(1)	32(2)	13(1)	2(1)	-1(1)	-8(1)
C(13A)	55(2)	28(2)	26(1)	-2(1)	-1(1)	25(2)
C(14A)	22(1)	31(2)	25(1)	6(1)	0(1)	11(1)
C(15A)	74(3)	20(2)	34(2)	-7(1)	6(2)	-5(2)
C(16A)	23(1)	61(2)	24(1)	6(1)	-5(1)	-11(1)
C(17A)	13(1)	13(1)	21(1)	2(1)	-1(1)	3(1)
C(18A)	18(1)	15(1)	21(1)	0(1)	-1(1)	3(1)
C(19A)	20(1)	19(1)	26(1)	4(1)	-4(1)	1(1)
C(20A)	16(1)	21(1)	34(1)	13(1)	1(1)	0(1)
C(21A)	18(1)	27(1)	28(1)	12(1)	7(1)	7(1)
C(22A)	18(1)	21(1)	20(1)	5(1)	1(1)	7(1)
C(23A)	17(1)	21(1)	17(1)	-2(1)	1(1)	-2(1)
C(24A)	47(2)	40(2)	29(2)	11(1)	14(1)	24(2)

C(25A)	32(2)	43(2)	32(2)	16(1)	12(1)	16(1)
C(26A)	21(1)	28(1)	19(1)	1(1)	4(1)	7(1)
C(27A)	30(1)	41(2)	24(1)	6(1)	2(1)	12(1)
C(28A)	33(2)	52(2)	32(2)	-4(1)	7(1)	23(2)
C(29A)	15(1)	18(1)	20(1)	1(1)	-3(1)	5(1)
C(30A)	16(1)	16(1)	35(1)	2(1)	-6(1)	6(1)
C(31A)	14(1)	28(2)	155(4)	35(2)	-2(2)	5(1)
C(32A)	72(2)	63(2)	29(2)	-10(2)	-22(2)	52(2)
C(33A)	19(1)	18(1)	23(1)	5(1)	-4(1)	7(1)
C(34A)	25(1)	23(2)	58(2)	17(1)	-16(1)	-1(1)
C(35A)	48(2)	38(2)	89(3)	23(2)	-38(2)	-4(2)
C(36A)	90(3)	49(2)	80(3)	-15(2)	-30(2)	44(2)
C(37A)	68(2)	69(2)	58(2)	-19(2)	-7(2)	46(2)
C(38A)	40(2)	61(2)	34(2)	5(2)	0(1)	31(2)
C(39A)	15(1)	25(1)	22(1)	7(1)	3(1)	2(1)
C(40A)	53(2)	27(2)	28(1)	11(1)	15(1)	24(1)
W(1B)	11(1)	11(1)	12(1)	1(1)	0(1)	4(1)
S(1B)	17(1)	15(1)	13(1)	3(1)	2(1)	3(1)
O(1B)	16(1)	19(1)	14(1)	5(1)	1(1)	4(1)
F(1B)	23(1)	24(1)	45(1)	5(1)	-8(1)	-1(1)
N(1B)	14(1)	15(1)	23(1)	8(1)	5(1)	6(1)
C(1B)	18(1)	14(1)	19(1)	3(1)	2(1)	8(1)
S(2B)	16(1)	35(1)	23(1)	16(1)	1(1)	5(1)
O(2B)	26(1)	21(1)	17(1)	3(1)	7(1)	7(1)
F(2B)	26(1)	41(1)	32(1)	-1(1)	0(1)	17(1)
C(2B)	16(1)	11(1)	17(1)	0(1)	2(1)	5(1)
N(2B)	16(1)	16(1)	18(1)	3(1)	4(1)	4(1)
N(3B)	18(1)	14(1)	17(1)	1(1)	-2(1)	1(1)
O(3B)	28(1)	16(1)	21(1)	6(1)	3(1)	1(1)
F(3B)	35(1)	66(1)	27(1)	27(1)	-3(1)	10(1)
C(3B)	20(1)	16(1)	23(1)	7(1)	2(1)	7(1)
O(4B)	14(1)	21(1)	17(1)	5(1)	2(1)	5(1)
F(4B)	20(1)	30(1)	48(1)	12(1)	6(1)	9(1)
N(4B)	19(1)	14(1)	16(1)	1(1)	-1(1)	4(1)
C(4B)	22(1)	17(1)	20(1)	6(1)	3(1)	7(1)
N(5B)	13(1)	12(1)	16(1)	-2(1)	-1(1)	4(1)
F(5B)	24(1)	29(1)	63(1)	-5(1)	2(1)	-1(1)
O(5B)	22(1)	69(2)	19(1)	1(1)	2(1)	-1(1)
O(6B)	23(1)	56(2)	74(2)	51(1)	11(1)	14(1)
F(6B)	28(1)	106(2)	66(1)	66(1)	14(1)	8(1)
C(5B)	18(1)	25(1)	37(2)	16(1)	8(1)	6(1)
C(6B)	18(1)	21(1)	30(1)	5(1)	6(1)	1(1)
C(7B)	22(1)	26(2)	44(2)	15(1)	1(1)	10(1)
C(8B)	34(2)	28(2)	36(2)	18(1)	7(1)	5(1)
C(9B)	17(1)	11(1)	17(1)	1(1)	-3(1)	3(1)
C(10B)	18(1)	11(1)	16(1)	2(1)	-1(1)	4(1)
C(11B)	25(1)	13(1)	16(1)	2(1)	-2(1)	3(1)

C(12B)	29(1)	13(1)	13(1)	2(1)	-2(1)	4(1)
C(13B)	19(1)	27(1)	23(1)	5(1)	2(1)	1(1)
C(14B)	21(1)	25(1)	28(1)	1(1)	3(1)	8(1)
C(15B)	27(1)	25(1)	21(1)	1(1)	-9(1)	-1(1)
C(16B)	39(2)	26(1)	17(1)	3(1)	3(1)	10(1)
C(17B)	15(1)	20(1)	13(1)	1(1)	-2(1)	7(1)
C(18B)	17(1)	22(1)	17(1)	-1(1)	0(1)	6(1)
C(19B)	24(1)	26(1)	18(1)	-4(1)	-6(1)	5(1)
C(20B)	30(1)	35(2)	20(1)	3(1)	-9(1)	13(1)
C(21B)	29(1)	28(1)	20(1)	5(1)	-2(1)	14(1)
C(22B)	19(1)	22(1)	14(1)	1(1)	-1(1)	8(1)
C(23B)	25(1)	18(1)	24(1)	2(1)	-7(1)	6(1)
C(24B)	37(2)	26(2)	27(1)	-4(1)	-5(1)	17(1)
C(25B)	37(2)	29(2)	37(2)	14(1)	-7(1)	4(1)
C(26B)	21(1)	19(1)	19(1)	-2(1)	-1(1)	3(1)
C(27B)	25(1)	25(2)	40(2)	-3(1)	-4(1)	2(1)
C(28B)	29(1)	24(1)	26(1)	5(1)	7(1)	12(1)
C(29B)	15(1)	17(1)	19(1)	0(1)	1(1)	6(1)
C(30B)	13(1)	24(1)	25(1)	1(1)	5(1)	5(1)
C(31B)	19(1)	28(2)	66(2)	4(2)	16(1)	3(1)
C(32B)	13(1)	55(2)	22(1)	1(1)	0(1)	8(1)
C(33B)	12(1)	29(1)	22(1)	3(1)	4(1)	2(1)
C(34B)	36(2)	46(2)	27(2)	10(1)	6(1)	-2(1)
C(35B)	47(2)	87(3)	25(2)	3(2)	17(2)	-8(2)
C(36B)	26(2)	99(3)	44(2)	-30(2)	18(2)	-4(2)
C(37B)	25(2)	59(2)	64(2)	-25(2)	0(2)	22(2)
C(38B)	21(1)	35(2)	34(2)	-3(1)	-2(1)	12(1)
C(39B)	22(1)	25(1)	16(1)	5(1)	-1(1)	6(1)
C(40B)	18(1)	31(2)	32(1)	17(1)	6(1)	5(1)
C(1X)	54(2)	42(2)	30(2)	12(1)	11(1)	18(2)
Cl(1X)	47(1)	42(1)	38(1)	9(1)	9(1)	8(1)
Cl(2X)	75(1)	49(1)	46(1)	10(1)	-3(1)	27(1)

Table S21: Hydrogen coordinates (x10^4) and isotropic displacement parameters (A^2 x 10^3) for complex 6.

	x	y	z	U(eq)
H(1A1)	6590(20)	1095(14)	7241(12)	17(7)
H(1A2)	6050(20)	1590(14)	6935(14)	25(7)
H(5A1)	6312	2462	6572	42
H(5A2)	6943	2576	5987	42
H(5A3)	7394	3111	6675	42
H(6A1)	8822	1196	7834	44
H(6A2)	9722	957	7385	44
H(6A3)	8344	592	7188	44
H(7A1)	10210	2668	5957	48
H(7A2)	9453	3198	6253	48
H(7A3)	8874	2588	5623	48
H(8A1)	10572	1157	6452	51
H(8A2)	11135	1742	7101	51
H(8A3)	11129	1931	6431	51
H(9A1)	5920(20)	2555(14)	9392(13)	23(7)
H(9A2)	6690(30)	2006(17)	9424(16)	42(9)
H(13A)	6183	3643	9249	54
H(13B)	6916	4400	9645	54
H(13C)	6095	3927	9982	54
H(14A)	8518	1959	10119	39
H(14B)	9828	2302	10054	39
H(14C)	8828	1968	9430	39
H(15A)	9665	4912	10844	71
H(15B)	8273	4866	10777	71
H(15C)	8939	5005	10210	71
H(16A)	10818	4107	10931	61
H(16B)	11066	3501	10390	61
H(16C)	10487	3320	10970	61
H(19A)	1743	-55	6954	27
H(20A)	748	-22	7805	29
H(21A)	1568	768	8782	28
H(23A)	4527	1063	6979	25
H(24A)	4712	-56	7025	53
H(24B)	4687	30	6316	53
H(24C)	3534	-384	6499	53
H(25A)	2311	440	6144	49
H(25B)	3481	780	5923	49
H(25C)	2859	1255	6402	49
H(26A)	4257	2068	9115	28
H(27A)	3497	1033	9753	48
H(27B)	4514	1721	10057	48
H(27C)	4710	1128	9486	48
H(28A)	2287	2266	9114	60
H(28B)	3089	2488	9810	60
H(28C)	2105	1778	9587	60

H(29A)	6610	3236	8048	22
H(31A)	3566	2313	7679	98
H(31B)	3030	2989	7799	98
H(31C)	3728	2796	8386	98
H(32A)	5474	3479	7068	84
H(32B)	4099	3470	7041	84
H(32C)	4521	2757	6872	84
H(34A)	6600	4311	7916	45
H(35A)	6997	5465	8549	77
H(36A)	5729	5786	9258	95
H(37A)	4126	5004	9328	82
H(38A)	3716	3886	8707	53
H(1B1)	-1370(20)	3755(15)	4016(14)	25(8)
H(1B2)	-200(20)	4139(14)	3933(13)	18(7)
H(5B1)	-3793	3252	3086	38
H(5B2)	-4336	3888	3398	38
H(5B3)	-3319	3670	3817	38
H(6B1)	655	5110	3524	35
H(6B2)	377	5271	2846	35
H(6B3)	496	4510	2882	35
H(7B1)	-4145	5071	2401	45
H(7B2)	-4498	4913	3042	45
H(7B3)	-4660	4291	2417	45
H(8B1)	-2317	5652	2258	46
H(8B2)	-1153	5386	2114	46
H(8B3)	-1097	5971	2752	46
H(9B1)	-250(20)	1529(14)	2893(13)	23(7)
H(9B2)	-1480(30)	1504(16)	3046(15)	34(9)
H(13D)	-3487	964	2546	35
H(13E)	-4322	1004	1923	35
H(13F)	-3534	1700	2412	35
H(14D)	713	1899	1862	38
H(14E)	686	1197	1344	38
H(14F)	784	1209	2082	38
H(15D)	-3776	386	346	41
H(15E)	-4327	936	792	41
H(15F)	-4341	195	926	41
H(16D)	-1865	455	129	41
H(16E)	-806	244	524	41
H(16F)	-624	999	402	41
H(19B)	2715	3686	5881	30
H(20B)	3096	2623	5959	35
H(21B)	2067	1610	5215	30
H(23B)	-187	1478	3890	29
H(24D)	1573	1451	3491	47
H(24E)	877	674	3416	47
H(24F)	1991	1030	3977	47

H(25D)	612	716	4750	53
H(25E)	-486	413	4171	53
H(25F)	-555	1016	4770	53
H(26B)	1050	3992	4547	25
H(27D)	2504	4686	5759	50
H(27E)	2088	5050	5222	50
H(27F)	2991	4554	5102	50
H(28D)	-478	3729	5112	38
H(28E)	-2	4551	5276	38
H(28F)	384	4135	5774	38
H(29B)	572	3173	2516	21
H(31D)	2356	4344	3488	58
H(31E)	2345	4199	2738	58
H(31F)	3510	4203	3210	58
H(32D)	2418	2678	3663	48
H(32E)	2531	3469	4034	48
H(32F)	3599	3246	3713	48
H(34B)	2106	3425	1858	45
H(35B)	2666	2797	971	69
H(36B)	3566	1884	1046	79
H(37B)	3888	1601	2017	66
H(38B)	3308	2232	2916	38
H(1X1)	6783	552	4731	48
H(1X2)	7526	1224	5269	48

Table S22: Torsion angles [°] for complex 6.

O(3A)-S(1A)-O(1A)-W(1A)	67.54(17)
O(2A)-S(1A)-O(1A)-W(1A)	-70.73(17)
C(39A)-S(1A)-O(1A)-W(1A)	178.46(14)
N(5A)-W(1A)-O(1A)-S(1A)	179(6)
C(29A)-W(1A)-O(1A)-S(1A)	-0.54(16)
C(9A)-W(1A)-O(1A)-S(1A)	-101.01(16)
C(1A)-W(1A)-O(1A)-S(1A)	99.54(16)
O(4A)-W(1A)-O(1A)-S(1A)	178.56(16)
N(5A)-W(1A)-C(1A)-C(2A)	175.9(2)
C(29A)-W(1A)-C(1A)-C(2A)	75.1(2)
C(9A)-W(1A)-C(1A)-C(2A)	-64.2(3)
O(1A)-W(1A)-C(1A)-C(2A)	-13.2(2)
O(4A)-W(1A)-C(1A)-C(2A)	-90.9(2)
C(3A)-N(1A)-C(2A)-N(2A)	-0.3(3)
C(5A)-N(1A)-C(2A)-N(2A)	-175.6(2)
C(3A)-N(1A)-C(2A)-C(1A)	-176.5(2)
C(5A)-N(1A)-C(2A)-C(1A)	8.2(4)
C(4A)-N(2A)-C(2A)-N(1A)	-0.4(3)
C(6A)-N(2A)-C(2A)-N(1A)	-176.7(2)
C(4A)-N(2A)-C(2A)-C(1A)	175.8(2)
C(6A)-N(2A)-C(2A)-C(1A)	-0.5(4)
W(1A)-C(1A)-C(2A)-N(1A)	-93.0(3)
W(1A)-C(1A)-C(2A)-N(2A)	91.6(3)
C(2A)-N(1A)-C(3A)-C(4A)	0.9(3)
C(5A)-N(1A)-C(3A)-C(4A)	176.3(2)
C(2A)-N(1A)-C(3A)-C(7A)	-177.8(2)
C(5A)-N(1A)-C(3A)-C(7A)	-2.5(4)
O(6A)-S(2A)-O(4A)-W(1A)	62.67(17)
O(5A)-S(2A)-O(4A)-W(1A)	-76.22(14)
C(40A)-S(2A)-O(4A)-W(1A)	173.85(13)
N(5A)-W(1A)-O(4A)-S(2A)	-16.61(14)
C(29A)-W(1A)-O(4A)-S(2A)	167.0(3)
C(9A)-W(1A)-O(4A)-S(2A)	79.08(13)
O(1A)-W(1A)-O(4A)-S(2A)	163.32(13)
C(1A)-W(1A)-O(4A)-S(2A)	-112.74(14)
N(1A)-C(3A)-C(4A)-N(2A)	-1.1(3)
C(7A)-C(3A)-C(4A)-N(2A)	177.5(3)
N(1A)-C(3A)-C(4A)-C(8A)	178.6(3)
C(7A)-C(3A)-C(4A)-C(8A)	-2.9(5)
C(2A)-N(2A)-C(4A)-C(3A)	1.0(3)
C(6A)-N(2A)-C(4A)-C(3A)	177.3(2)
C(2A)-N(2A)-C(4A)-C(8A)	-178.7(2)
C(6A)-N(2A)-C(4A)-C(8A)	-2.4(4)
C(29A)-W(1A)-N(5A)-C(17A)	157(5)
C(9A)-W(1A)-N(5A)-C(17A)	-101(5)
O(1A)-W(1A)-N(5A)-C(17A)	-22(5)

C(1A)-W(1A)-N(5A)-C(17A)	56(5)
O(4A)-W(1A)-N(5A)-C(17A)	-22(5)
N(5A)-W(1A)-C(9A)-C(10A)	-167.2(2)
C(29A)-W(1A)-C(9A)-C(10A)	-66.4(2)
O(1A)-W(1A)-C(9A)-C(10A)	21.96(19)
C(1A)-W(1A)-C(9A)-C(10A)	72.8(3)
O(4A)-W(1A)-C(9A)-C(10A)	99.3(2)
C(12A)-N(4A)-C(10A)-N(3A)	0.5(3)
C(14A)-N(4A)-C(10A)-N(3A)	175.7(2)
C(12A)-N(4A)-C(10A)-C(9A)	-175.6(2)
C(14A)-N(4A)-C(10A)-C(9A)	-0.3(4)
C(11A)-N(3A)-C(10A)-N(4A)	0.0(3)
C(13A)-N(3A)-C(10A)-N(4A)	179.9(2)
C(11A)-N(3A)-C(10A)-C(9A)	176.1(2)
C(13A)-N(3A)-C(10A)-C(9A)	-4.0(4)
W(1A)-C(9A)-C(10A)-N(4A)	-96.0(3)
W(1A)-C(9A)-C(10A)-N(3A)	88.7(3)
C(10A)-N(3A)-C(11A)-C(12A)	-0.4(3)
C(13A)-N(3A)-C(11A)-C(12A)	179.7(3)
C(10A)-N(3A)-C(11A)-C(15A)	-179.2(3)
C(13A)-N(3A)-C(11A)-C(15A)	0.9(4)
N(3A)-C(11A)-C(12A)-N(4A)	0.7(3)
C(15A)-C(11A)-C(12A)-N(4A)	179.3(3)
N(3A)-C(11A)-C(12A)-C(16A)	-178.4(3)
C(15A)-C(11A)-C(12A)-C(16A)	0.2(5)
C(10A)-N(4A)-C(12A)-C(11A)	-0.8(3)
C(14A)-N(4A)-C(12A)-C(11A)	-175.8(2)
C(10A)-N(4A)-C(12A)-C(16A)	178.5(2)
C(14A)-N(4A)-C(12A)-C(16A)	3.4(4)
W(1A)-N(5A)-C(17A)-C(22A)	116(5)
W(1A)-N(5A)-C(17A)-C(18A)	-65(5)
N(5A)-C(17A)-C(18A)-C(19A)	177.6(2)
C(22A)-C(17A)-C(18A)-C(19A)	-3.4(3)
N(5A)-C(17A)-C(18A)-C(23A)	-3.0(3)
C(22A)-C(17A)-C(18A)-C(23A)	176.1(2)
C(17A)-C(18A)-C(19A)-C(20A)	1.5(4)
C(23A)-C(18A)-C(19A)-C(20A)	-178.0(2)
C(18A)-C(19A)-C(20A)-C(21A)	0.7(4)
C(19A)-C(20A)-C(21A)-C(22A)	-1.1(4)
C(20A)-C(21A)-C(22A)-C(17A)	-0.7(4)
C(20A)-C(21A)-C(22A)-C(26A)	178.9(2)
N(5A)-C(17A)-C(22A)-C(21A)	-178.0(2)
C(18A)-C(17A)-C(22A)-C(21A)	3.0(3)
N(5A)-C(17A)-C(22A)-C(26A)	2.4(3)
C(18A)-C(17A)-C(22A)-C(26A)	-176.6(2)
C(19A)-C(18A)-C(23A)-C(24A)	-70.1(3)
C(17A)-C(18A)-C(23A)-C(24A)	110.4(3)

C(19A)-C(18A)-C(23A)-C(25A)	55.8(3)
C(17A)-C(18A)-C(23A)-C(25A)	-123.6(3)
C(21A)-C(22A)-C(26A)-C(27A)	78.9(3)
C(17A)-C(22A)-C(26A)-C(27A)	-101.4(3)
C(21A)-C(22A)-C(26A)-C(28A)	-45.6(3)
C(17A)-C(22A)-C(26A)-C(28A)	134.0(3)
N(5A)-W(1A)-C(29A)-C(30A)	0.9(3)
C(9A)-W(1A)-C(29A)-C(30A)	-97.5(3)
O(1A)-W(1A)-C(29A)-C(30A)	-179.2(3)
C(1A)-W(1A)-C(29A)-C(30A)	99.8(3)
O(4A)-W(1A)-C(29A)-C(30A)	177.2(2)
W(1A)-C(29A)-C(30A)-C(31A)	12.4(4)
W(1A)-C(29A)-C(30A)-C(33A)	136.5(3)
W(1A)-C(29A)-C(30A)-C(32A)	-106.7(3)
C(29A)-C(30A)-C(33A)-C(38A)	-118.9(3)
C(31A)-C(30A)-C(33A)-C(38A)	5.0(4)
C(32A)-C(30A)-C(33A)-C(38A)	123.1(3)
C(29A)-C(30A)-C(33A)-C(34A)	59.5(3)
C(31A)-C(30A)-C(33A)-C(34A)	-176.7(3)
C(32A)-C(30A)-C(33A)-C(34A)	-58.6(3)
C(38A)-C(33A)-C(34A)-C(35A)	-0.2(4)
C(30A)-C(33A)-C(34A)-C(35A)	-178.6(3)
C(33A)-C(34A)-C(35A)-C(36A)	0.6(5)
C(34A)-C(35A)-C(36A)-C(37A)	-0.5(6)
C(35A)-C(36A)-C(37A)-C(38A)	0.0(7)
C(36A)-C(37A)-C(38A)-C(33A)	0.3(6)
C(34A)-C(33A)-C(38A)-C(37A)	-0.2(5)
C(30A)-C(33A)-C(38A)-C(37A)	178.1(3)
O(3A)-S(1A)-C(39A)-F(3A)	178.37(18)
O(2A)-S(1A)-C(39A)-F(3A)	-58.6(2)
O(1A)-S(1A)-C(39A)-F(3A)	60.2(2)
O(3A)-S(1A)-C(39A)-F(1A)	57.7(2)
O(2A)-S(1A)-C(39A)-F(1A)	-179.27(18)
O(1A)-S(1A)-C(39A)-F(1A)	-60.5(2)
O(3A)-S(1A)-C(39A)-F(2A)	-62.0(2)
O(2A)-S(1A)-C(39A)-F(2A)	61.04(19)
O(1A)-S(1A)-C(39A)-F(2A)	179.83(17)
O(6A)-S(2A)-C(40A)-F(5A)	168.9(2)
O(5A)-S(2A)-C(40A)-F(5A)	-68.4(2)
O(4A)-S(2A)-C(40A)-F(5A)	49.8(2)
O(6A)-S(2A)-C(40A)-F(6A)	47.3(3)
O(5A)-S(2A)-C(40A)-F(6A)	170.0(2)
O(4A)-S(2A)-C(40A)-F(6A)	-71.8(2)
O(6A)-S(2A)-C(40A)-F(4A)	-71.7(2)
O(5A)-S(2A)-C(40A)-F(4A)	51.1(2)
O(4A)-S(2A)-C(40A)-F(4A)	169.25(19)
O(3B)-S(1B)-O(1B)-W(1B)	-68.03(16)

O(2B)-S(1B)-O(1B)-W(1B)	69.20(17)
C(39B)-S(1B)-O(1B)-W(1B)	-179.53(14)
N(5B)-W(1B)-O(1B)-S(1B)	-178.5(4)
C(29B)-W(1B)-O(1B)-S(1B)	0.31(15)
C(9B)-W(1B)-O(1B)-S(1B)	-100.33(15)
C(1B)-W(1B)-O(1B)-S(1B)	101.32(15)
O(4B)-W(1B)-O(1B)-S(1B)	-179.37(15)
N(5B)-W(1B)-C(1B)-C(2B)	176.0(2)
C(29B)-W(1B)-C(1B)-C(2B)	75.7(2)
C(9B)-W(1B)-C(1B)-C(2B)	-65.8(3)
O(1B)-W(1B)-C(1B)-C(2B)	-13.4(2)
O(4B)-W(1B)-C(1B)-C(2B)	-91.8(2)
C(3B)-N(1B)-C(2B)-N(2B)	-0.5(3)
C(5B)-N(1B)-C(2B)-N(2B)	-179.0(2)
C(3B)-N(1B)-C(2B)-C(1B)	175.9(2)
C(5B)-N(1B)-C(2B)-C(1B)	-2.5(4)
W(1B)-C(1B)-C(2B)-N(2B)	-92.4(3)
W(1B)-C(1B)-C(2B)-N(1B)	91.8(3)
N(1B)-C(2B)-N(2B)-C(4B)	0.0(2)
C(1B)-C(2B)-N(2B)-C(4B)	-176.5(2)
N(1B)-C(2B)-N(2B)-C(6B)	-175.8(2)
C(1B)-C(2B)-N(2B)-C(6B)	7.7(4)
C(2B)-N(1B)-C(3B)-C(4B)	0.9(3)
C(5B)-N(1B)-C(3B)-C(4B)	179.3(2)
C(2B)-N(1B)-C(3B)-C(7B)	-178.8(2)
C(5B)-N(1B)-C(3B)-C(7B)	-0.4(4)
O(6B)-S(2B)-O(4B)-W(1B)	-64.58(16)
O(5B)-S(2B)-O(4B)-W(1B)	72.97(15)
C(40B)-S(2B)-O(4B)-W(1B)	-176.94(12)
N(5B)-W(1B)-O(4B)-S(2B)	0.64(13)
C(29B)-W(1B)-O(4B)-S(2B)	179.0(4)
C(9B)-W(1B)-O(4B)-S(2B)	96.34(13)
O(1B)-W(1B)-O(4B)-S(2B)	-179.51(13)
C(1B)-W(1B)-O(4B)-S(2B)	-95.60(13)
N(1B)-C(3B)-C(4B)-N(2B)	-0.9(3)
C(7B)-C(3B)-C(4B)-N(2B)	178.8(3)
N(1B)-C(3B)-C(4B)-C(8B)	177.2(3)
C(7B)-C(3B)-C(4B)-C(8B)	-3.1(5)
C(2B)-N(2B)-C(4B)-C(3B)	0.6(3)
C(6B)-N(2B)-C(4B)-C(3B)	176.4(2)
C(2B)-N(2B)-C(4B)-C(8B)	-177.7(2)
C(6B)-N(2B)-C(4B)-C(8B)	-1.9(4)
C(29B)-W(1B)-N(5B)-C(17B)	0(3)
C(9B)-W(1B)-N(5B)-C(17B)	102(3)
O(1B)-W(1B)-N(5B)-C(17B)	179(100)
C(1B)-W(1B)-N(5B)-C(17B)	-103(3)
O(4B)-W(1B)-N(5B)-C(17B)	179(100)

N(5B)-W(1B)-C(9B)-C(10B)	-168.4(2)
C(29B)-W(1B)-C(9B)-C(10B)	-68.2(2)
O(1B)-W(1B)-C(9B)-C(10B)	20.94(19)
C(1B)-W(1B)-C(9B)-C(10B)	73.3(3)
O(4B)-W(1B)-C(9B)-C(10B)	99.4(2)
C(12B)-N(4B)-C(10B)-N(3B)	-0.3(3)
C(14B)-N(4B)-C(10B)-N(3B)	175.5(2)
C(12B)-N(4B)-C(10B)-C(9B)	175.4(2)
C(14B)-N(4B)-C(10B)-C(9B)	-8.8(4)
C(11B)-N(3B)-C(10B)-N(4B)	0.4(3)
C(13B)-N(3B)-C(10B)-N(4B)	176.3(2)
C(11B)-N(3B)-C(10B)-C(9B)	-175.2(2)
C(13B)-N(3B)-C(10B)-C(9B)	0.7(4)
W(1B)-C(9B)-C(10B)-N(4B)	93.2(3)
W(1B)-C(9B)-C(10B)-N(3B)	-92.0(3)
C(10B)-N(3B)-C(11B)-C(12B)	-0.4(3)
C(13B)-N(3B)-C(11B)-C(12B)	-176.2(2)
C(10B)-N(3B)-C(11B)-C(15B)	179.9(2)
C(13B)-N(3B)-C(11B)-C(15B)	4.2(4)
N(3B)-C(11B)-C(12B)-N(4B)	0.2(3)
C(15B)-C(11B)-C(12B)-N(4B)	179.8(3)
N(3B)-C(11B)-C(12B)-C(16B)	178.2(3)
C(15B)-C(11B)-C(12B)-C(16B)	-2.2(5)
C(10B)-N(4B)-C(12B)-C(11B)	0.0(3)
C(14B)-N(4B)-C(12B)-C(11B)	-175.7(2)
C(10B)-N(4B)-C(12B)-C(16B)	-178.1(2)
C(14B)-N(4B)-C(12B)-C(16B)	6.1(4)
W(1B)-N(5B)-C(17B)-C(22B)	-100(3)
W(1B)-N(5B)-C(17B)-C(18B)	76(3)
N(5B)-C(17B)-C(18B)-C(19B)	-172.1(2)
C(22B)-C(17B)-C(18B)-C(19B)	3.4(4)
N(5B)-C(17B)-C(18B)-C(26B)	10.0(3)
C(22B)-C(17B)-C(18B)-C(26B)	-174.5(2)
C(17B)-C(18B)-C(19B)-C(20B)	-0.3(4)
C(26B)-C(18B)-C(19B)-C(20B)	177.6(3)
C(18B)-C(19B)-C(20B)-C(21B)	-2.5(4)
C(19B)-C(20B)-C(21B)-C(22B)	2.3(4)
C(20B)-C(21B)-C(22B)-C(17B)	0.7(4)
C(20B)-C(21B)-C(22B)-C(23B)	-179.7(3)
N(5B)-C(17B)-C(22B)-C(21B)	171.9(2)
C(18B)-C(17B)-C(22B)-C(21B)	-3.5(4)
N(5B)-C(17B)-C(22B)-C(23B)	-7.8(4)
C(18B)-C(17B)-C(22B)-C(23B)	176.8(2)
C(21B)-C(22B)-C(23B)-C(24B)	-77.0(3)
C(17B)-C(22B)-C(23B)-C(24B)	102.7(3)
C(21B)-C(22B)-C(23B)-C(25B)	47.0(3)
C(17B)-C(22B)-C(23B)-C(25B)	-133.4(2)

C(19B)-C(18B)-C(26B)-C(27B)	32.7(4)
C(17B)-C(18B)-C(26B)-C(27B)	-149.4(2)
C(19B)-C(18B)-C(26B)-C(28B)	-91.4(3)
C(17B)-C(18B)-C(26B)-C(28B)	86.5(3)
N(5B)-W(1B)-C(29B)-C(30B)	-1.5(3)
C(9B)-W(1B)-C(29B)-C(30B)	-99.7(3)
O(1B)-W(1B)-C(29B)-C(30B)	178.7(3)
C(1B)-W(1B)-C(29B)-C(30B)	97.3(3)
O(4B)-W(1B)-C(29B)-C(30B)	-179.8(2)
W(1B)-C(29B)-C(30B)-C(31B)	-111.6(3)
W(1B)-C(29B)-C(30B)-C(32B)	6.1(4)
W(1B)-C(29B)-C(30B)-C(33B)	128.9(3)
C(31B)-C(30B)-C(33B)-C(38B)	132.1(3)
C(32B)-C(30B)-C(33B)-C(38B)	15.1(3)
C(29B)-C(30B)-C(33B)-C(38B)	-108.6(3)
C(31B)-C(30B)-C(33B)-C(34B)	-50.2(3)
C(32B)-C(30B)-C(33B)-C(34B)	-167.2(3)
C(29B)-C(30B)-C(33B)-C(34B)	69.1(3)
C(38B)-C(33B)-C(34B)-C(35B)	0.3(4)
C(30B)-C(33B)-C(34B)-C(35B)	-177.5(3)
C(33B)-C(34B)-C(35B)-C(36B)	-0.4(5)
C(34B)-C(35B)-C(36B)-C(37B)	0.2(6)
C(35B)-C(36B)-C(37B)-C(38B)	0.0(5)
C(34B)-C(33B)-C(38B)-C(37B)	0.0(4)
C(30B)-C(33B)-C(38B)-C(37B)	177.8(3)
C(36B)-C(37B)-C(38B)-C(33B)	-0.1(5)
O(3B)-S(1B)-C(39B)-F(1B)	176.99(17)
O(2B)-S(1B)-C(39B)-F(1B)	53.8(2)
O(1B)-S(1B)-C(39B)-F(1B)	-64.44(19)
O(3B)-S(1B)-C(39B)-F(2B)	-62.5(2)
O(2B)-S(1B)-C(39B)-F(2B)	174.39(18)
O(1B)-S(1B)-C(39B)-F(2B)	56.1(2)
O(3B)-S(1B)-C(39B)-F(3B)	57.2(2)
O(2B)-S(1B)-C(39B)-F(3B)	-65.9(2)
O(1B)-S(1B)-C(39B)-F(3B)	175.81(17)
O(6B)-S(2B)-C(40B)-F(4B)	175.9(2)
O(5B)-S(2B)-C(40B)-F(4B)	53.8(2)
O(4B)-S(2B)-C(40B)-F(4B)	-64.5(2)
O(6B)-S(2B)-C(40B)-F(5B)	-63.8(2)
O(5B)-S(2B)-C(40B)-F(5B)	174.1(2)
O(4B)-S(2B)-C(40B)-F(5B)	55.8(2)
O(6B)-S(2B)-C(40B)-F(6B)	56.8(2)
O(5B)-S(2B)-C(40B)-F(6B)	-65.3(2)
O(4B)-S(2B)-C(40B)-F(6B)	176.4(2)