Electronic Supplementary Information for Dalton Transactions

‘Pincer’ dicarbene complexes of some early transition metals and uranium

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Electronic Supplementary Information

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Structural Data for 1a

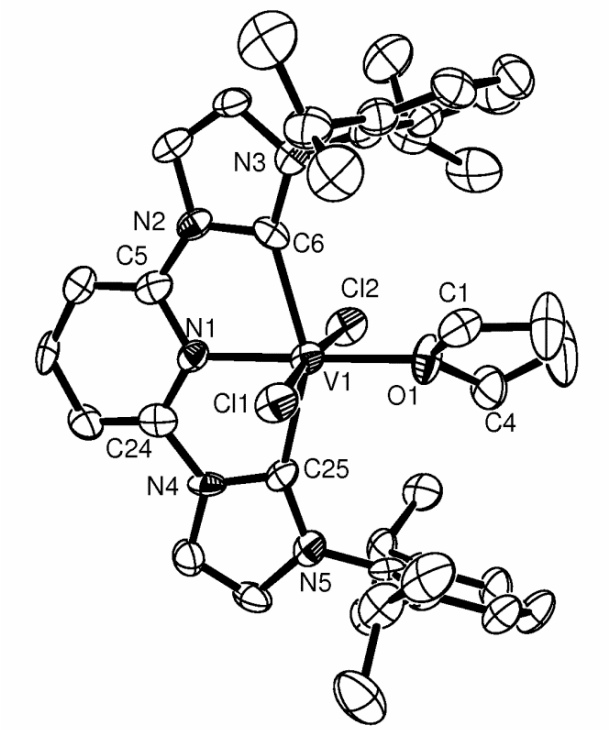

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Table 1. Crystal data and structure refinement for 1a.

Identification code	1a	
Empirical formula	C47 H65 Cl2 N5 O3 V	
Formula weight	869.88	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P n a 21	
Unit cell dimensions	a = 10.306(3) Å	α= 90°.
	b = 32.019(11) Å	β= 90°.
	c = 13.807(5) Å	γ = 90°.
Volume	4556(3) Å^3	
Z	4	
Density (calculated)	1.268 Mg/m^3	
Absorption coefficient	0.380 mm^{-1}	
F(000)	1852	
Crystal size	0.22 x 0.10 x 0.02 mm^3	
Theta range for data collection	3.21 to 24.20°.	
Index ranges	-11<=h<=11, -36<=k<=36, -14<=l<=15	
Reflections collected	21996	
Independent reflections	6436 [R(int) = 0.1892]	
Completeness to theta = 24.20°	95.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.988 and 0.955	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6436 / 1 / 531	
Goodness-of-fit on F^2	0.923	
Final R indices [I>2sigma(I)]	R1 = 0.0656, wR2 = 0.0915	
R indices (all data)	R1 = 0.1917, wR2 = 0.1215	
Absolute structure parameter	0.04(5)	
Largest diff. peak and hole	0.301 and -0.325 e.Å^{-3}	

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Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 1a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	7959(8)	1638(3)	5064(6)	45(2)
C(2)	7156(10)	2020(3)	5040(9)	82(4)
C(3)	5828(10)	1893(3)	5317(10)	95(5)
C(4)	5792(8)	1440(3)	5201(7)	49(3)
C(5)	9230(8)	12(3)	6687(6)	35(2)
C(6)	9123(8)	760(3)	6811(6)	30(2)
C(7)	10424(8)	819(3)	8153(6)	37(2)
C(8)	10388(8)	418(3)	7940(6)	38(2)
C(9)	9546(9)	1469(3)	7434(6)	37(2)
C(10)	10492(8)	1692(3)	6975(6)	40(2)
C(11)	10394(9)	2129(3)	6970(6)	47(3)
C(12)	9356(10)	2324(3)	7407(7)	55(3)
C(13)	8391(10)	2081(4)	7853(7)	58(3)
C(14)	8492(8)	1656(3)	7866(6)	41(2)
C(15)	7471(9)	1392(3)	8393(6)	47(3)
C(16)	7820(10)	1367(3)	9459(7)	73(3)
C(17)	6072(9)	1556(3)	8273(7)	75(3)
C(18)	11676(9)	1489(3)	6497(7)	53(3)
C(19)	12845(9)	1505(3)	7188(7)	75(3)
C(20)	12012(9)	1676(3)	5521(8)	71(3)
C(21)	9654(8)	-386(3)	6935(6)	38(2)
C(22)	9192(7)	-720(3)	6409(6)	39(2)
C(23)	8331(6)	-669(3)	5653(7)	40(2)
C(24)	7964(7)	-267(3)	5455(6)	32(2)
C(25)	6667(7)	260(3)	4659(6)	30(2)
C(26)	5617(8)	-184(3)	3613(7)	42(2)
C(27)	6453(8)	-421(3)	4106(7)	41(2)
C(28)	4900(8)	555(3)	3648(6)	34(2)
C(29)	3652(7)	577(3)	4028(6)	36(2)
C(30)	2851(9)	896(3)	3726(7)	47(3)

C(31)	3269(8)	1183(3)	3052(7)	48(3)
C(32)	4481(8)	1159(3)	2674(6)	46(3)
C(33)	5323(8)	844(3)	2946(7)	42(2)
C(34)	6599(8)	787(3)	2443(6)	49(3)
C(35)	6384(10)	573(3)	1463(7)	79(4)
C(36)	7298(9)	1191(3)	2292(7)	67(3)
C(37)	3175(7)	250(3)	4747(6)	40(2)
C(38)	2209(8)	-41(2)	4249(6)	46(2)
C(39)	2542(7)	449(2)	5628(7)	49(2)
C(40)	8967(13)	2114(5)	2237(12)	120(5)
C(41)	10181(10)	1915(3)	2599(8)	75(4)
C(42)	10267(17)	2632(4)	2721(13)	136(7)
C(43)	10773(14)	2253(4)	3186(10)	132(6)
C(44)	6811(11)	8298(4)	5167(9)	94(4)
C(45)	6678(14)	7839(4)	4959(9)	91(4)
C(46)	8061(12)	7701(4)	5084(9)	86(4)
C(47)	8802(12)	8065(5)	4705(10)	102(4)
Cl(1)	9350(2)	754(1)	4310(2)	43(1)
Cl(2)	6002(2)	634(1)	6764(2)	45(1)
N(1)	8393(6)	73(2)	5936(5)	29(2)
N(2)	9611(6)	374(2)	7126(5)	31(2)
N(3)	9665(6)	1027(2)	7455(5)	33(2)
N(4)	7068(6)	-150(2)	4737(5)	33(2)
N(5)	5750(6)	231(2)	3933(5)	35(2)
O(1)	7111(5)	1293(2)	5258(4)	44(2)
O(2)	9232(12)	2538(4)	2172(10)	175(5)
O(3)	7986(11)	8425(3)	4778(6)	122(4)
V(1)	7748(1)	672(1)	5600(1)	31(1)

Table 3. Bond lengths [Å] and angles [°] for 1a.

C(1)-O(1)	1.434(8)
C(1)-C(2)	1.478(11)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(2)-C(3)	1.478(12)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(4)	1.459(11)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-O(1)	1.441(8)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-N(1)	1.363(9)
C(5)-N(2)	1.365(10)
C(5)-C(21)	1.388(10)
C(6)-N(3)	1.354(9)
C(6)-N(2)	1.405(9)
C(6)-V(1)	2.209(9)
C(7)-C(8)	1.316(11)
C(7)-N(3)	1.409(10)
C(7)-H(7)	0.9500
C(8)-N(2)	1.387(9)
C(8)-H(8)	0.9500
C(9)-C(10)	1.366(11)
C(9)-C(14)	1.377(11)
C(9)-N(3)	1.420(10)
C(10)-C(11)	1.401(11)
C(10)-C(18)	1.533(12)
C(11)-C(12)	1.378(12)
C(11)-H(11)	0.9500
C(12)-C(13)	1.405(12)
C(12)-H(12)	0.9500

C(13)-C(14)	1.364(12)
C(13)-H(13)	0.9500
C(14)-C(15)	1.533(12)
C(15)-C(16)	1.517(12)
C(15)-C(17)	1.544(12)
C(15)-H(15)	1.0000
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-C(20)	1.514(12)
C(18)-C(19)	1.537(12)
C(18)-H(18)	1.0000
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-C(22)	1.377(11)
C(21)-H(21)	0.9500
C(22)-C(23)	1.380(11)
C(22)-H(22)	0.9500
C(23)-C(24)	1.369(11)
C(23)-H(23)	0.9500
C(24)-N(1)	1.348(9)
C(24)-N(4)	1.405(9)
C(25)-N(4)	1.378(10)
C(25)-N(5)	1.381(9)
C(25)-V(1)	2.162(9)
C(26)-C(27)	1.336(11)
C(26)-N(5)	1.406(10)
C(26)-H(26)	0.9500

C(27)-N(4)	1.384(9)
C(27)-H(27)	0.9500
C(28)-C(29)	1.392(11)
C(28)-C(33)	1.409(11)
C(28)-N(5)	1.414(10)
C(29)-C(30)	1.378(11)
C(29)-C(37)	1.525(11)
C(30)-C(31)	1.376(11)
C(30)-H(30)	0.9500
C(31)-C(32)	1.356(11)
C(31)-H(31)	0.9500
C(32)-C(33)	1.383(11)
C(32)-H(32)	0.9500
C(33)-C(34)	1.498(11)
C(34)-C(36)	1.496(12)
C(34)-C(35)	1.533(12)
C(34)-H(34)	1.0000
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
C(37)-C(39)	1.520(11)
C(37)-C(38)	1.527(10)
C(37)-H(37)	1.0000
C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800
C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
C(40)-O(2)	1.390(13)
C(40)-C(41)	1.490(14)
C(40)-H(40A)	0.9900

C(40)-H(40B)	0.9900
C(41)-C(43)	1.483(14)
C(41)-H(41A)	0.9900
C(41)-H(41B)	0.9900
C(42)-O(2)	1.343(15)
C(42)-C(43)	1.467(15)
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)-O(3)	1.386(12)
C(44)-C(45)	1.504(13)
C(44)-H(44A)	0.9900
C(44)-H(44B)	0.9900
C(45)-C(46)	1.502(14)
C(45)-H(45A)	0.9900
C(45)-H(45B)	0.9900
C(46)-C(47)	1.489(14)
C(46)-H(46A)	0.9900
C(46)-H(46B)	0.9900
C(47)-O(3)	1.428(13)
C(47)-H(47A)	0.9900
C(47)-H(47B)	0.9900
Cl(1)-V(1)	2.443(3)
Cl(2)-V(1)	2.416(3)
N(1)-V(1)	2.084(7)
O(1)-V(1)	2.145(5)

O(1)-C(1)-C(2)	107.5(7)
O(1)-C(1)-H(1A)	110.2
C(2)-C(1)-H(1A)	110.2
O(1)-C(1)-H(1B)	110.2
C(2)-C(1)-H(1B)	110.2
H(1A)-C(1)-H(1B)	108.5
C(1)-C(2)-C(3)	106.5(8)

C(1)-C(2)-H(2A)	110.4
C(3)-C(2)-H(2A)	110.4
C(1)-C(2)-H(2B)	110.4
C(3)-C(2)-H(2B)	110.4
H(2A)-C(2)-H(2B)	108.6
C(4)-C(3)-C(2)	105.6(8)
C(4)-C(3)-H(3A)	110.6
C(2)-C(3)-H(3A)	110.6
C(4)-C(3)-H(3B)	110.6
C(2)-C(3)-H(3B)	110.6
H(3A)-C(3)-H(3B)	108.7
O(1)-C(4)-C(3)	107.2(7)
O(1)-C(4)-H(4A)	110.3
C(3)-C(4)-H(4A)	110.3
O(1)-C(4)-H(4B)	110.3
C(3)-C(4)-H(4B)	110.3
H(4A)-C(4)-H(4B)	108.5
N(1)-C(5)-N(2)	113.4(8)
N(1)-C(5)-C(21)	121.2(8)
N(2)-C(5)-C(21)	125.3(8)
N(3)-C(6)-N(2)	101.8(7)
N(3)-C(6)-V(1)	147.3(7)
N(2)-C(6)-V(1)	110.6(5)
C(8)-C(7)-N(3)	107.0(8)
C(8)-C(7)-H(7)	126.5
N(3)-C(7)-H(7)	126.5
C(7)-C(8)-N(2)	107.4(8)
C(7)-C(8)-H(8)	126.3
N(2)-C(8)-H(8)	126.3
C(10)-C(9)-C(14)	122.4(9)
C(10)-C(9)-N(3)	118.1(9)
C(14)-C(9)-N(3)	119.5(8)
C(9)-C(10)-C(11)	118.3(9)
C(9)-C(10)-C(18)	123.0(9)
C(11)-C(10)-C(18)	118.6(8)

C(12)-C(11)-C(10)	120.4(9)
C(12)-C(11)-H(11)	119.8
C(10)-C(11)-H(11)	119.8
C(11)-C(12)-C(13)	119.4(9)
C(11)-C(12)-H(12)	120.3
C(13)-C(12)-H(12)	120.3
C(14)-C(13)-C(12)	120.3(9)
C(14)-C(13)-H(13)	119.9
C(12)-C(13)-H(13)	119.9
C(13)-C(14)-C(9)	119.3(9)
C(13)-C(14)-C(15)	120.3(9)
C(9)-C(14)-C(15)	120.4(9)
C(16)-C(15)-C(14)	109.1(7)
C(16)-C(15)-C(17)	110.0(8)
C(14)-C(15)-C(17)	113.7(8)
C(16)-C(15)-H(15)	108.0
C(14)-C(15)-H(15)	108.0
C(17)-C(15)-H(15)	108.0
C(15)-C(16)-H(16A)	109.5
C(15)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(15)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(15)-C(17)-H(17A)	109.5
C(15)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(15)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(20)-C(18)-C(10)	113.4(8)
C(20)-C(18)-C(19)	111.1(8)
C(10)-C(18)-C(19)	110.0(8)
C(20)-C(18)-H(18)	107.4
C(10)-C(18)-H(18)	107.4

C(19)-C(18)-H(18)	107.4
C(18)-C(19)-H(19A)	109.5
C(18)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(18)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(18)-C(20)-H(20A)	109.5
C(18)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(18)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(22)-C(21)-C(5)	118.2(8)
C(22)-C(21)-H(21)	120.9
C(5)-C(21)-H(21)	120.9
C(21)-C(22)-C(23)	122.0(8)
C(21)-C(22)-H(22)	119.0
C(23)-C(22)-H(22)	119.0
C(24)-C(23)-C(22)	116.0(8)
C(24)-C(23)-H(23)	122.0
C(22)-C(23)-H(23)	122.0
N(1)-C(24)-C(23)	124.7(8)
N(1)-C(24)-N(4)	110.4(8)
C(23)-C(24)-N(4)	124.9(8)
N(4)-C(25)-N(5)	101.5(7)
N(4)-C(25)-V(1)	112.3(6)
N(5)-C(25)-V(1)	146.1(7)
C(27)-C(26)-N(5)	108.3(8)
C(27)-C(26)-H(26)	125.9
N(5)-C(26)-H(26)	125.9
C(26)-C(27)-N(4)	105.1(8)
C(26)-C(27)-H(27)	127.5
N(4)-C(27)-H(27)	127.5
C(29)-C(28)-C(33)	120.8(8)

C(29)-C(28)-N(5)	120.3(8)
C(33)-C(28)-N(5)	118.8(8)
C(30)-C(29)-C(28)	118.5(8)
C(30)-C(29)-C(37)	120.9(8)
C(28)-C(29)-C(37)	120.6(8)
C(31)-C(30)-C(29)	120.8(8)
C(31)-C(30)-H(30)	119.6
C(29)-C(30)-H(30)	119.6
C(32)-C(31)-C(30)	120.7(9)
C(32)-C(31)-H(31)	119.7
C(30)-C(31)-H(31)	119.7
C(31)-C(32)-C(33)	121.0(9)
C(31)-C(32)-H(32)	119.5
C(33)-C(32)-H(32)	119.5
C(32)-C(33)-C(28)	118.1(8)
C(32)-C(33)-C(34)	120.9(9)
C(28)-C(33)-C(34)	120.8(8)
C(36)-C(34)-C(33)	112.5(8)
C(36)-C(34)-C(35)	109.4(8)
C(33)-C(34)-C(35)	109.7(8)
C(36)-C(34)-H(34)	108.4
C(33)-C(34)-H(34)	108.4
C(35)-C(34)-H(34)	108.4
C(34)-C(35)-H(35A)	109.5
C(34)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(34)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(34)-C(36)-H(36A)	109.5
C(34)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(34)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5

C(39)-C(37)-C(29)	111.8(7)
C(39)-C(37)-C(38)	109.7(6)
C(29)-C(37)-C(38)	109.7(7)
C(39)-C(37)-H(37)	108.6
C(29)-C(37)-H(37)	108.6
C(38)-C(37)-H(37)	108.6
C(37)-C(38)-H(38A)	109.5
C(37)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(37)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(37)-C(39)-H(39A)	109.5
C(37)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(37)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
O(2)-C(40)-C(41)	105.9(11)
O(2)-C(40)-H(40A)	110.5
C(41)-C(40)-H(40A)	110.5
O(2)-C(40)-H(40B)	110.5
C(41)-C(40)-H(40B)	110.5
H(40A)-C(40)-H(40B)	108.7
C(43)-C(41)-C(40)	102.5(10)
C(43)-C(41)-H(41A)	111.3
C(40)-C(41)-H(41A)	111.3
C(43)-C(41)-H(41B)	111.3
C(40)-C(41)-H(41B)	111.3
H(41A)-C(41)-H(41B)	109.2
O(2)-C(42)-C(43)	110.2(12)
O(2)-C(42)-H(42A)	109.6
C(43)-C(42)-H(42A)	109.6
O(2)-C(42)-H(42B)	109.6
C(43)-C(42)-H(42B)	109.6

H(42A)-C(42)-H(42B)	108.1
C(42)-C(43)-C(41)	102.6(10)
C(42)-C(43)-H(43A)	111.2
C(41)-C(43)-H(43A)	111.2
C(42)-C(43)-H(43B)	111.2
C(41)-C(43)-H(43B)	111.2
H(43A)-C(43)-H(43B)	109.2
O(3)-C(44)-C(45)	106.9(10)
O(3)-C(44)-H(44A)	110.3
C(45)-C(44)-H(44A)	110.3
O(3)-C(44)-H(44B)	110.3
C(45)-C(44)-H(44B)	110.3
H(44A)-C(44)-H(44B)	108.6
C(46)-C(45)-C(44)	100.3(10)
C(46)-C(45)-H(45A)	111.7
C(44)-C(45)-H(45A)	111.7
C(46)-C(45)-H(45B)	111.7
C(44)-C(45)-H(45B)	111.7
H(45A)-C(45)-H(45B)	109.5
C(47)-C(46)-C(45)	102.5(10)
C(47)-C(46)-H(46A)	111.3
C(45)-C(46)-H(46A)	111.3
C(47)-C(46)-H(46B)	111.3
C(45)-C(46)-H(46B)	111.3
H(46A)-C(46)-H(46B)	109.2
O(3)-C(47)-C(46)	107.7(10)
O(3)-C(47)-H(47A)	110.2
C(46)-C(47)-H(47A)	110.2
O(3)-C(47)-H(47B)	110.2
C(46)-C(47)-H(47B)	110.2
H(47A)-C(47)-H(47B)	108.5
C(24)-N(1)-C(5)	117.8(8)
C(24)-N(1)-V(1)	121.9(6)
C(5)-N(1)-V(1)	120.2(6)
C(5)-N(2)-C(8)	127.8(8)

C(5)-N(2)-C(6)	120.5(7)
C(8)-N(2)-C(6)	111.5(7)
C(6)-N(3)-C(7)	112.3(7)
C(6)-N(3)-C(9)	125.4(8)
C(7)-N(3)-C(9)	122.2(8)
C(25)-N(4)-C(27)	114.2(7)
C(25)-N(4)-C(24)	120.4(7)
C(27)-N(4)-C(24)	125.2(8)
C(25)-N(5)-C(26)	111.0(7)
C(25)-N(5)-C(28)	125.2(7)
C(26)-N(5)-C(28)	123.1(7)
C(1)-O(1)-C(4)	108.2(6)
C(1)-O(1)-V(1)	124.6(4)
C(4)-O(1)-V(1)	127.2(5)
C(42)-O(2)-C(40)	109.7(12)
C(44)-O(3)-C(47)	107.8(9)
N(1)-V(1)-O(1)	179.2(3)
N(1)-V(1)-C(25)	74.7(3)
O(1)-V(1)-C(25)	106.0(3)
N(1)-V(1)-C(6)	75.2(3)
O(1)-V(1)-C(6)	104.2(3)
C(25)-V(1)-C(6)	149.6(3)
N(1)-V(1)-Cl(2)	92.47(17)
O(1)-V(1)-Cl(2)	88.00(16)
C(25)-V(1)-Cl(2)	89.2(2)
C(6)-V(1)-Cl(2)	88.9(2)
N(1)-V(1)-Cl(1)	92.56(17)
O(1)-V(1)-Cl(1)	87.02(16)
C(25)-V(1)-Cl(1)	88.6(2)
C(6)-V(1)-Cl(1)	96.0(2)
Cl(2)-V(1)-Cl(1)	173.73(10)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for 1a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	41(6)	52(7)	40(6)	9(5)	-7(5)	-8(5)
C(2)	75(8)	47(8)	125(10)	19(7)	5(8)	21(7)
C(3)	58(7)	44(8)	183(15)	-1(8)	8(9)	17(6)
C(4)	33(5)	50(7)	63(7)	-6(5)	3(5)	8(4)
C(5)	22(5)	52(7)	30(6)	0(6)	3(5)	-2(5)
C(6)	33(5)	25(6)	31(5)	-4(5)	8(5)	-13(4)
C(7)	30(5)	48(7)	34(6)	-4(5)	-10(5)	-3(5)
C(8)	24(5)	61(8)	29(6)	8(5)	-3(5)	0(5)
C(9)	33(6)	36(7)	43(6)	4(5)	-9(5)	-4(5)
C(10)	42(6)	46(7)	33(6)	2(5)	-1(5)	-3(5)
C(11)	58(7)	41(7)	40(6)	-1(5)	3(5)	-13(5)
C(12)	69(8)	40(7)	57(7)	-6(6)	-1(6)	0(6)
C(13)	51(7)	75(10)	47(7)	-17(7)	2(6)	-1(6)
C(14)	40(6)	48(8)	36(6)	2(5)	-11(5)	5(5)
C(15)	44(6)	57(7)	41(6)	-9(5)	16(5)	-9(5)
C(16)	65(7)	92(9)	62(8)	18(6)	-3(6)	0(6)
C(17)	54(7)	114(10)	57(7)	-23(7)	18(6)	-1(7)
C(18)	39(6)	61(7)	58(7)	-4(6)	-5(6)	-11(5)
C(19)	46(6)	104(10)	76(8)	8(7)	13(7)	-6(6)
C(20)	65(7)	90(8)	58(7)	4(8)	13(7)	3(6)
C(21)	29(5)	43(7)	43(6)	6(5)	-3(5)	4(5)
C(22)	34(5)	25(6)	57(6)	15(5)	-3(5)	11(5)
C(23)	25(4)	37(6)	57(6)	-14(6)	-3(6)	-7(4)
C(24)	23(5)	51(7)	24(6)	-2(6)	13(5)	-7(5)
C(25)	18(5)	43(7)	29(5)	3(5)	1(4)	2(4)
C(26)	29(5)	52(7)	46(6)	-24(6)	-5(5)	-2(5)
C(27)	35(5)	38(6)	49(6)	-9(6)	-2(5)	6(5)
C(28)	37(6)	42(7)	25(5)	-8(5)	-15(5)	-2(5)
C(29)	22(5)	46(7)	41(6)	-8(5)	-4(5)	-2(4)
C(30)	31(5)	52(7)	57(7)	-1(6)	4(5)	14(5)

C(31)	24(5)	72(8)	48(6)	15(6)	-2(5)	12(5)
C(32)	43(6)	57(7)	37(6)	10(5)	-4(5)	5(6)
C(33)	31(6)	58(7)	39(6)	-8(6)	-11(5)	9(5)
C(34)	35(6)	70(8)	41(6)	13(6)	14(5)	0(5)
C(35)	101(9)	70(9)	65(8)	-19(7)	27(7)	4(7)
C(36)	34(6)	114(10)	53(7)	0(7)	7(6)	18(7)
C(37)	24(5)	45(6)	51(6)	-1(5)	-1(5)	10(4)
C(38)	41(5)	49(6)	48(6)	0(5)	12(5)	-5(5)
C(39)	27(5)	66(6)	54(5)	-8(7)	0(6)	1(4)
C(40)	105(12)	73(11)	181(16)	11(10)	12(11)	-15(9)
C(41)	50(7)	70(9)	104(10)	5(8)	-11(7)	3(7)
C(42)	170(17)	54(10)	183(17)	-9(11)	-84(14)	7(11)
C(43)	169(15)	71(11)	157(14)	-34(10)	-104(13)	-1(10)
C(44)	72(9)	111(12)	100(10)	-51(9)	-10(8)	22(8)
C(45)	112(12)	83(11)	79(9)	-7(8)	-11(8)	-8(9)
C(46)	105(12)	80(10)	74(9)	2(7)	-15(9)	-18(9)
C(47)	89(10)	108(12)	107(11)	-22(9)	36(8)	2(10)
Cl(1)	29(1)	64(2)	35(1)	0(1)	5(1)	3(1)
Cl(2)	37(1)	62(2)	36(2)	7(1)	6(1)	-4(1)
N(1)	23(4)	37(5)	28(5)	2(4)	0(4)	2(3)
N(2)	22(4)	39(5)	32(5)	5(4)	-4(4)	-6(4)
N(3)	25(4)	40(5)	35(5)	6(4)	4(4)	-2(4)
N(4)	23(4)	47(6)	28(4)	-11(4)	-6(4)	-9(4)
N(5)	25(4)	49(6)	30(5)	1(4)	7(4)	10(4)
O(1)	27(3)	37(4)	67(5)	16(3)	6(3)	6(3)
O(2)	158(10)	115(10)	252(16)	39(10)	-85(10)	0(8)
O(3)	154(10)	80(7)	133(8)	-32(6)	77(7)	-33(7)
V(1)	23(1)	40(1)	30(1)	0(1)	2(1)	0(1)

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Structural Data for 1b

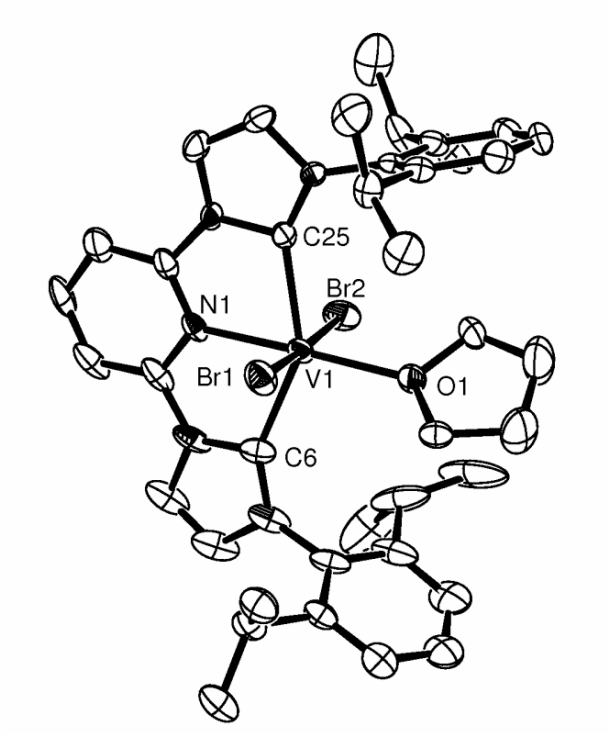

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Table 1. Crystal data and structure refinement for **1b**

Identification code	**1b**	
Empirical formula	C39 H49 Br2 N5 O V	
Formula weight	814.59	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 15.6919(15) Å	α= 90∞.
	b = 14.6332(15) Å	β= 102.828(7)∞.
	c = 17.1157(12) Å	γ = 90∞.
Volume	3832.1(6) $Å^3$	
Z	4	
Density (calculated)	1.412 Mg/m^3	
Absorption coefficient	2.381 mm^{-1}	
F(000)	1676	
Crystal size	0.20 x 0.10 x 0.02 mm^3	
Theta range for data collection	3.00 to 27.64∞.	
Index ranges	-20<=h<=20, -18<=k<=19, -22<=l<=20	
Reflections collected	36118	
Independent reflections	8801 [R(int) = 0.0883]	
Completeness to theta = 27.64∞	98.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9539 and 0.5780	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8801 / 4 / 445	
Goodness-of-fit on F^2	1.019	
Final R indices [I>2sigma(I)]	R1 = 0.0755, wR2 = 0.1573	
R indices (all data)	R1 = 0.1398, wR2 = 0.1831	
Largest diff. peak and hole	0.772 and -0.988 $e.Å^{-3}$	

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Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **1b**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1A)	3674(4)	4140(4)	3455(4)	42(2)
C(2A)	4300(30)	4679(17)	4068(18)	62(5)
C(3A)	4371(6)	5584(5)	3679(5)	72(3)
C(1B)	3674(4)	4140(4)	3455(4)	42(2)
C(2B)	4550(10)	4586(8)	3793(14)	62(5)
C(3B)	4371(6)	5584(5)	3679(5)	72(3)
C(4)	3604(4)	5667(4)	2987(4)	37(2)
C(5)	155(4)	4542(4)	1090(4)	34(2)
C(6)	1031(4)	5468(4)	2137(4)	30(1)
C(7)	-39(5)	6431(5)	2320(5)	47(2)
C(8)	-423(4)	5851(5)	1767(5)	46(2)
C(9)	1457(4)	6765(4)	3094(4)	35(2)
C(10)	1672(4)	7608(4)	2833(4)	32(1)
C(11)	2226(4)	8165(5)	3382(4)	38(2)
C(12)	2550(5)	7895(5)	4154(4)	48(2)
C(13)	2346(5)	7061(5)	4395(4)	53(2)
C(14)	1784(6)	6462(5)	3890(4)	51(2)
C(15)	1507(8)	5564(5)	4161(5)	82(4)
C(16A)	635(8)	5648(7)	4360(6)	110(5)
C(17)	2170(10)	5146(6)	4859(5)	129(6)
C(18)	1352(4)	7928(4)	1974(4)	35(2)
C(19)	2120(4)	7968(5)	1558(4)	41(2)
C(20)	886(4)	8852(5)	1924(4)	45(2)
C(21)	-610(4)	4316(5)	550(5)	43(2)
C(22)	-574(4)	3627(5)	15(4)	46(2)
C(23)	196(4)	3163(4)	16(4)	44(2)
C(24)	930(4)	3445(4)	586(4)	31(1)
C(25)	2407(3)	3240(4)	1345(3)	23(1)
C(26)	2838(4)	2159(4)	553(3)	31(1)
C(27)	2024(4)	2382(4)	195(4)	32(1)

C(28)	3878(4)	2573(3)	1837(3)	22(1)
C(29)	4609(4)	3011(4)	1697(3)	27(1)
C(30)	5397(4)	2877(4)	2267(4)	33(1)
C(31)	5422(4)	2337(4)	2924(4)	32(1)
C(32)	4683(4)	1896(4)	3034(3)	30(1)
C(33)	3886(4)	1996(4)	2492(3)	28(1)
C(34)	3078(4)	1499(5)	2606(4)	44(2)
C(35)	3058(5)	1340(5)	3479(5)	56(2)
C(36)	2992(6)	592(5)	2153(5)	70(3)
C(37)	4585(4)	3593(4)	965(3)	32(1)
C(38)	4974(5)	3065(5)	361(4)	47(2)
C(39)	5054(5)	4498(5)	1169(4)	48(2)
Br(1)	2668(1)	5400(1)	964(1)	37(1)
Br(2)	1508(1)	3371(1)	3002(1)	42(1)
N(1)	914(3)	4105(3)	1107(3)	26(1)
N(2)	230(3)	5249(3)	1649(3)	35(1)
N(3)	835(3)	6210(3)	2537(3)	37(1)
N(4)	1754(3)	3031(3)	680(3)	26(1)
N(5)	3062(3)	2678(3)	1259(3)	22(1)
O(1)	3141(3)	4801(3)	2934(2)	30(1)
V(1)	2031(1)	4441(1)	1990(1)	24(1)

Table 3. Bond lengths [Å] and angles [∞] for **1b**.

C(1A)-O(1)	1.448(7)
C(1A)-C(2A)	1.495(18)
C(1A)-H(1A1)	0.9900
C(1A)-H(1A2)	0.9900
C(2A)-C(3A)	1.497(19)
C(2A)-H(2A1)	0.9900
C(2A)-H(2A2)	0.9900
C(3A)-C(4)	1.494(10)
C(3A)-H(3A1)	0.9900
C(3A)-H(3A2)	0.9900
C(2B)-H(2B1)	0.9900
C(2B)-H(2B2)	0.9900
C(4)-O(1)	1.453(7)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-N(1)	1.347(7)
C(5)-C(21)	1.383(9)
C(5)-N(2)	1.396(8)
C(6)-N(3)	1.355(8)
C(6)-N(2)	1.383(8)
C(6)-V(1)	2.227(6)
C(7)-C(8)	1.314(10)
C(7)-N(3)	1.378(8)
C(7)-H(7)	0.9500
C(8)-N(2)	1.399(8)
C(8)-H(8)	0.9500
C(9)-C(10)	1.378(8)
C(9)-C(14)	1.418(9)
C(9)-N(3)	1.452(8)
C(10)-C(11)	1.394(9)
C(10)-C(18)	1.518(8)
C(11)-C(12)	1.365(9)
C(11)-H(11)	0.9500

C(12)-C(13)	1.349(10)
C(12)-H(12)	0.9500
C(13)-C(14)	1.397(11)
C(13)-H(13)	0.9500
C(14)-C(15)	1.489(10)
C(15)-C(16A)	1.487(15)
C(15)-C(17)	1.528(14)
C(15)-H(15)	1.0000
C(16A)-H(16A)	0.9800
C(16A)-H(16B)	0.9800
C(16A)-H(16C)	0.9800
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-C(19)	1.531(8)
C(18)-C(20)	1.532(9)
C(18)-H(18)	1.0000
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-C(22)	1.372(10)
C(21)-H(21)	0.9500
C(22)-C(23)	1.384(10)
C(22)-H(22)	0.9500
C(23)-C(24)	1.398(8)
C(23)-H(23)	0.9500
C(24)-N(1)	1.319(8)
C(24)-N(4)	1.403(7)
C(25)-N(5)	1.350(7)
C(25)-N(4)	1.386(7)
C(25)-V(1)	2.224(6)
C(26)-C(27)	1.329(8)

C(26)-N(5)	1.404(7)
C(26)-H(26)	0.9500
C(27)-N(4)	1.389(8)
C(27)-H(27)	0.9500
C(28)-C(29)	1.380(8)
C(28)-C(33)	1.401(8)
C(28)-N(5)	1.443(7)
C(29)-C(30)	1.408(8)
C(29)-C(37)	1.510(8)
C(30)-C(31)	1.368(8)
C(30)-H(30)	0.9500
C(31)-C(32)	1.376(8)
C(31)-H(31)	0.9500
C(32)-C(33)	1.389(8)
C(32)-H(32)	0.9500
C(33)-C(34)	1.512(8)
C(34)-C(35)	1.520(9)
C(34)-C(36)	1.528(11)
C(34)-H(34)	1.0000
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
C(37)-C(39)	1.517(9)
C(37)-C(38)	1.523(9)
C(37)-H(37)	1.0000
C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800
C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
Br(1)-V(1)	2.6142(11)

Br(2)-V(1)	2.5997(11)
N(1)-V(1)	2.103(5)
O(1)-V(1)	2.162(4)

O(1)-C(1A)-C(2A)	106.3(12)
O(1)-C(1A)-H(1A1)	110.5
C(2A)-C(1A)-H(1A1)	110.5
O(1)-C(1A)-H(1A2)	110.5
C(2A)-C(1A)-H(1A2)	110.5
H(1A1)-C(1A)-H(1A2)	108.7
C(1A)-C(2A)-C(3A)	104.8(14)
C(1A)-C(2A)-H(2A1)	110.8
C(3A)-C(2A)-H(2A1)	110.8
C(1A)-C(2A)-H(2A2)	110.8
C(3A)-C(2A)-H(2A2)	110.8
H(2A1)-C(2A)-H(2A2)	108.9
C(4)-C(3A)-C(2A)	107.4(11)
C(4)-C(3A)-H(3A1)	110.2
C(2A)-C(3A)-H(3A1)	110.2
C(4)-C(3A)-H(3A2)	110.2
C(2A)-C(3A)-H(3A2)	110.2
H(3A1)-C(3A)-H(3A2)	108.5
H(2B1)-C(2B)-H(2B2)	109.0
O(1)-C(4)-C(3A)	106.4(5)
O(1)-C(4)-H(4A)	110.4
C(3A)-C(4)-H(4A)	110.4
O(1)-C(4)-H(4B)	110.4
C(3A)-C(4)-H(4B)	110.4
H(4A)-C(4)-H(4B)	108.6
N(1)-C(5)-C(21)	122.2(6)
N(1)-C(5)-N(2)	113.4(5)
C(21)-C(5)-N(2)	124.3(6)
N(3)-C(6)-N(2)	102.3(5)
N(3)-C(6)-V(1)	147.4(5)
N(2)-C(6)-V(1)	110.2(4)

C(8)-C(7)-N(3)	108.2(6)
C(8)-C(7)-H(7)	125.9
N(3)-C(7)-H(7)	125.9
C(7)-C(8)-N(2)	106.1(6)
C(7)-C(8)-H(8)	127.0
N(2)-C(8)-H(8)	127.0
C(10)-C(9)-C(14)	122.0(7)
C(10)-C(9)-N(3)	117.7(6)
C(14)-C(9)-N(3)	120.2(6)
C(9)-C(10)-C(11)	117.8(6)
C(9)-C(10)-C(18)	122.5(6)
C(11)-C(10)-C(18)	119.7(5)
C(12)-C(11)-C(10)	121.7(7)
C(12)-C(11)-H(11)	119.1
C(10)-C(11)-H(11)	119.1
C(13)-C(12)-C(11)	119.7(7)
C(13)-C(12)-H(12)	120.1
C(11)-C(12)-H(12)	120.1
C(12)-C(13)-C(14)	122.5(7)
C(12)-C(13)-H(13)	118.7
C(14)-C(13)-H(13)	118.7
C(13)-C(14)-C(9)	116.2(6)
C(13)-C(14)-C(15)	123.3(7)
C(9)-C(14)-C(15)	120.5(8)
C(16A)-C(15)-C(14)	110.2(7)
C(16A)-C(15)-C(17)	110.8(8)
C(14)-C(15)-C(17)	113.7(10)
C(16A)-C(15)-H(15)	107.3
C(14)-C(15)-H(15)	107.3
C(17)-C(15)-H(15)	107.3
C(15)-C(16A)-H(16A)	109.5
C(15)-C(16A)-H(16B)	109.5
H(16A)-C(16A)-H(16B)	109.5
C(15)-C(16A)-H(16C)	109.5
H(16A)-C(16A)-H(16C)	109.5

H(16B)-C(16A)-H(16C)	109.5
C(15)-C(17)-H(17A)	109.5
C(15)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(15)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(10)-C(18)-C(19)	109.7(5)
C(10)-C(18)-C(20)	112.1(5)
C(19)-C(18)-C(20)	110.8(5)
C(10)-C(18)-H(18)	108.0
C(19)-C(18)-H(18)	108.0
C(20)-C(18)-H(18)	108.0
C(18)-C(19)-H(19A)	109.5
C(18)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(18)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(18)-C(20)-H(20A)	109.5
C(18)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(18)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(22)-C(21)-C(5)	117.6(6)
C(22)-C(21)-H(21)	121.2
C(5)-C(21)-H(21)	121.2
C(21)-C(22)-C(23)	121.7(6)
C(21)-C(22)-H(22)	119.2
C(23)-C(22)-H(22)	119.2
C(22)-C(23)-C(24)	116.1(7)
C(22)-C(23)-H(23)	121.9
C(24)-C(23)-H(23)	121.9
N(1)-C(24)-C(23)	123.5(6)

N(1)-C(24)-N(4)	113.2(5)
C(23)-C(24)-N(4)	123.3(6)
N(5)-C(25)-N(4)	102.6(5)
N(5)-C(25)-V(1)	145.9(4)
N(4)-C(25)-V(1)	110.6(4)
C(27)-C(26)-N(5)	107.2(5)
C(27)-C(26)-H(26)	126.4
N(5)-C(26)-H(26)	126.4
C(26)-C(27)-N(4)	106.4(5)
C(26)-C(27)-H(27)	126.8
N(4)-C(27)-H(27)	126.8
C(29)-C(28)-C(33)	124.0(5)
C(29)-C(28)-N(5)	118.5(5)
C(33)-C(28)-N(5)	117.5(5)
C(28)-C(29)-C(30)	116.8(5)
C(28)-C(29)-C(37)	122.5(5)
C(30)-C(29)-C(37)	120.7(5)
C(31)-C(30)-C(29)	120.6(6)
C(31)-C(30)-H(30)	119.7
C(29)-C(30)-H(30)	119.7
C(30)-C(31)-C(32)	120.8(6)
C(30)-C(31)-H(31)	119.6
C(32)-C(31)-H(31)	119.6
C(31)-C(32)-C(33)	121.4(5)
C(31)-C(32)-H(32)	119.3
C(33)-C(32)-H(32)	119.3
C(32)-C(33)-C(28)	116.3(5)
C(32)-C(33)-C(34)	121.3(5)
C(28)-C(33)-C(34)	122.3(5)
C(33)-C(34)-C(35)	113.7(6)
C(33)-C(34)-C(36)	109.5(6)
C(35)-C(34)-C(36)	110.4(6)
C(33)-C(34)-H(34)	107.7
C(35)-C(34)-H(34)	107.7
C(36)-C(34)-H(34)	107.7

C(34)-C(35)-H(35A)	109.5
C(34)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(34)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(34)-C(36)-H(36A)	109.5
C(34)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(34)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
C(29)-C(37)-C(39)	112.4(5)
C(29)-C(37)-C(38)	109.7(5)
C(39)-C(37)-C(38)	110.6(5)
C(29)-C(37)-H(37)	108.0
C(39)-C(37)-H(37)	108.0
C(38)-C(37)-H(37)	108.0
C(37)-C(38)-H(38A)	109.5
C(37)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(37)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(37)-C(39)-H(39A)	109.5
C(37)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(37)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(24)-N(1)-C(5)	118.9(5)
C(24)-N(1)-V(1)	121.2(4)
C(5)-N(1)-V(1)	119.8(4)
C(6)-N(2)-C(5)	120.8(5)
C(6)-N(2)-C(8)	111.4(6)

C(5)-N(2)-C(8)	127.7(6)
C(6)-N(3)-C(7)	112.1(6)
C(6)-N(3)-C(9)	125.9(5)
C(7)-N(3)-C(9)	122.0(5)
C(25)-N(4)-C(27)	111.9(5)
C(25)-N(4)-C(24)	119.6(5)
C(27)-N(4)-C(24)	128.5(5)
C(25)-N(5)-C(26)	111.8(5)
C(25)-N(5)-C(28)	124.8(4)
C(26)-N(5)-C(28)	123.2(5)
C(1A)-O(1)-C(4)	109.3(4)
C(1A)-O(1)-V(1)	123.8(3)
C(4)-O(1)-V(1)	124.6(3)
N(1)-V(1)-O(1)	177.41(18)
N(1)-V(1)-C(25)	74.28(19)
O(1)-V(1)-C(25)	107.79(18)
N(1)-V(1)-C(6)	75.1(2)
O(1)-V(1)-C(6)	102.8(2)
C(25)-V(1)-C(6)	149.4(2)
N(1)-V(1)-Br(2)	90.13(12)
O(1)-V(1)-Br(2)	88.31(11)
C(25)-V(1)-Br(2)	90.74(14)
C(6)-V(1)-Br(2)	89.83(14)
N(1)-V(1)-Br(1)	91.37(12)
O(1)-V(1)-Br(1)	90.38(11)
C(25)-V(1)-Br(1)	84.67(14)
C(6)-V(1)-Br(1)	95.57(14)
Br(2)-V(1)-Br(1)	174.60(5)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **1b**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1A)	42(4)	31(4)	45(4)	6(3)	-11(3)	6(3)
C(2A)	58(9)	49(6)	63(11)	-9(6)	-23(7)	4(6)
C(3A)	71(6)	45(5)	81(6)	10(4)	-20(5)	-25(4)
C(1B)	42(4)	31(4)	45(4)	6(3)	-11(3)	6(3)
C(2B)	58(9)	49(6)	63(11)	-9(6)	-23(7)	4(6)
C(3B)	71(6)	45(5)	81(6)	10(4)	-20(5)	-25(4)
C(4)	45(4)	17(3)	45(4)	3(3)	2(3)	-2(3)
C(5)	20(3)	27(3)	56(4)	24(3)	7(3)	-1(3)
C(6)	39(4)	16(3)	41(4)	9(3)	20(3)	-3(3)
C(7)	40(4)	29(4)	86(6)	12(4)	41(4)	2(3)
C(8)	28(4)	34(4)	83(6)	24(4)	30(4)	7(3)
C(9)	39(4)	22(3)	53(4)	4(3)	29(3)	9(3)
C(10)	27(3)	30(3)	41(4)	7(3)	14(3)	9(3)
C(11)	31(4)	42(4)	44(4)	6(3)	17(3)	3(3)
C(12)	61(5)	49(5)	39(4)	-6(3)	20(4)	17(4)
C(13)	81(6)	53(5)	33(4)	-4(4)	27(4)	21(4)
C(14)	87(6)	31(4)	46(4)	12(3)	38(4)	24(4)
C(15)	193(12)	23(4)	44(5)	1(3)	60(6)	-2(5)
C(16A)	171(12)	101(8)	73(7)	-18(6)	60(7)	-103(8)
C(17)	306(19)	37(5)	57(6)	22(4)	69(9)	62(8)
C(18)	34(4)	23(3)	47(4)	10(3)	8(3)	-3(3)
C(19)	47(4)	39(4)	41(4)	11(3)	16(3)	5(3)
C(20)	34(4)	41(4)	64(5)	18(3)	15(3)	10(3)
C(21)	19(3)	32(4)	77(5)	25(4)	5(3)	1(3)
C(22)	20(3)	39(4)	65(5)	22(4)	-18(3)	-9(3)
C(23)	41(4)	27(3)	53(4)	8(3)	-11(3)	-6(3)
C(24)	24(3)	21(3)	40(4)	11(3)	-7(3)	-5(2)
C(25)	19(3)	18(3)	30(3)	2(2)	-1(2)	-4(2)
C(26)	39(4)	23(3)	30(3)	-7(2)	7(3)	-5(3)
C(27)	33(4)	25(3)	33(3)	-3(3)	-4(3)	-10(3)

C(28)	28(3)	14(3)	24(3)	-2(2)	4(2)	4(2)
C(29)	30(3)	20(3)	32(3)	0(2)	9(3)	1(2)
C(30)	26(3)	33(3)	42(4)	-1(3)	8(3)	-4(3)
C(31)	22(3)	35(3)	34(3)	2(3)	-4(3)	5(3)
C(32)	34(4)	28(3)	28(3)	5(2)	6(3)	9(3)
C(33)	27(3)	19(3)	38(3)	2(2)	8(3)	1(2)
C(34)	23(3)	47(4)	59(5)	27(3)	3(3)	2(3)
C(35)	40(4)	56(5)	78(6)	36(4)	28(4)	18(4)
C(36)	79(6)	54(5)	67(5)	20(4)	-6(5)	-38(5)
C(37)	32(3)	36(4)	26(3)	6(3)	4(3)	-7(3)
C(38)	62(5)	49(4)	30(4)	5(3)	13(3)	-4(4)
C(39)	59(5)	39(4)	43(4)	9(3)	9(4)	-13(4)
Br(1)	34(1)	33(1)	42(1)	10(1)	4(1)	0(1)
Br(2)	45(1)	28(1)	55(1)	6(1)	17(1)	-2(1)
N(1)	17(2)	19(2)	39(3)	11(2)	0(2)	-3(2)
N(2)	28(3)	18(3)	63(4)	16(2)	19(3)	2(2)
N(3)	34(3)	25(3)	62(4)	14(3)	32(3)	6(2)
N(4)	24(3)	20(2)	28(3)	-1(2)	-7(2)	-5(2)
N(5)	23(3)	16(2)	26(2)	-2(2)	2(2)	-3(2)
O(1)	33(2)	23(2)	32(2)	5(2)	1(2)	-2(2)
V(1)	23(1)	17(1)	31(1)	4(1)	3(1)	0(1)

Electronic Supplementary Information for Dalton Transactions

Electronic Supplementary Information for Dalton Transactions

Structural Data for 2b

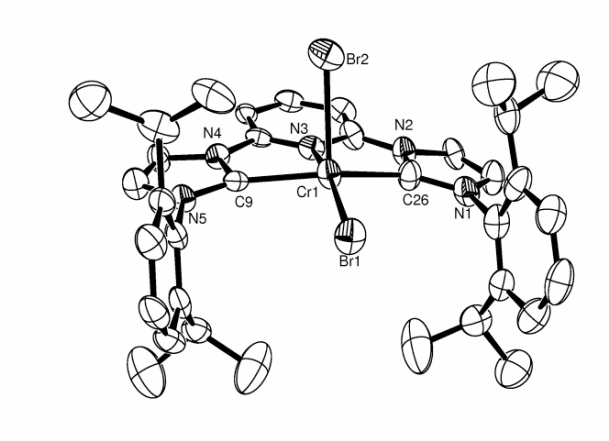


Table 5. Crystal data and structure refinement for **2b**.

Identification code	2b	
Empirical formula	C82 H106 Br4 Cl0 Cr2 N10 O3	
Formula weight	1703.41	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Trigonal	
Space group	R -3	
Unit cell dimensions	a = 34.5630(7) Å	α= 90∞.
	b = 34.5630(7) Å	β= 90∞.
	c = 41.0813(15) Å	γ = 120∞.
Volume	42501(2) Å^3	
Z	18	
Density (calculated)	1.198 Mg/m^3	
Absorption coefficient	1.968 mm^{-1}	
F(000)	15840	
Crystal size	0.20 x 0.08 x 0.04 mm^3	
Theta range for data collection	2.98 to 24.69∞.	
Index ranges	-40<=h<=36, -40<=k<=31, -48<=l<=48	
Reflections collected	82975	
Independent reflections	15994 [R(int) = 0.1702]	
Completeness to theta = 24.69∞	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9254 and 0.6943	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	15994 / 0 / 885	
Goodness-of-fit on F^2	1.038	
Final R indices [I>2sigma(I)]	R1 = 0.0998, wR2 = 0.1998	
R indices (all data)	R1 = 0.2029, wR2 = 0.2395	
Largest diff. peak and hole	1.669 and -0.556 e.Å^{-3}	

Table 6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **2b**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(2)	1906(4)	3874(4)	3098(3)	57(3)
C(3)	1804(4)	4547(4)	3162(3)	68(4)
C(1)	1170(3)	4181(3)	1827(2)	25(2)
C(4)	2491(3)	4836(3)	2512(2)	27(2)
C(5)	820(3)	4224(3)	1706(2)	30(2)
C(6)	499(3)	3876(3)	1519(2)	31(2)
C(7)	1561(3)	4880(3)	2163(2)	28(2)
C(8)	1925(3)	5051(3)	2348(2)	29(2)
C(9)	8(3)	3375(3)	225(2)	34(2)
C(10)	-900(4)	3072(3)	-651(2)	39(3)
C(11)	1843(3)	4402(3)	2129(2)	28(2)
C(12)	-1178(4)	2791(4)	372(3)	52(3)
C(13)	344(4)	1737(4)	22(3)	45(3)
C(14)	129(3)	4042(3)	443(2)	38(3)
C(15)	676(3)	3774(3)	557(2)	31(2)
C(16)	899(3)	2470(4)	1491(2)	40(3)
C(17)	-244(3)	3870(3)	261(2)	42(3)
C(18)	2409(3)	4609(3)	2806(2)	33(2)
C(19)	1336(3)	4089(3)	861(2)	39(3)
C(20)	1887(4)	2585(3)	1603(2)	40(3)
C(21)	2910(3)	5156(3)	2403(2)	30(2)
C(22)	966(3)	4112(3)	761(2)	29(2)
C(23)	1144(4)	2415(4)	2340(3)	62(3)
C(24)	-1320(4)	2759(4)	-544(3)	46(3)
C(25)	1107(3)	3438(3)	552(3)	38(3)
C(26)	770(3)	2777(3)	218(2)	39(3)
C(27)	-1413(4)	2663(3)	-221(3)	44(3)
C(28)	1348(3)	2631(4)	211(3)	45(3)
C(29)	2192(5)	2480(4)	1740(3)	70(4)
C(30)	1479(3)	2990(3)	402(3)	38(3)

C(31)	1525(4)	2459(4)	2134(3)	45(3)
C(32)	885(3)	3483(3)	1592(2)	27(2)
C(33)	1580(3)	2597(3)	1808(2)	37(3)
C(34)	1411(3)	3747(3)	761(2)	38(3)
C(35)	-1282(4)	2319(4)	452(3)	68(4)
C(36)	2781(4)	4715(3)	2996(2)	42(3)
C(37)	698(4)	2704(3)	1423(2)	42(3)
C(38)	-557(3)	3307(3)	-437(2)	37(3)
C(39)	3312(4)	5352(4)	1878(3)	69(4)
C(40)	250(3)	1693(4)	375(3)	49(3)
C(41)	102(4)	1377(4)	-189(3)	55(3)
C(42)	-1075(4)	2895(3)	14(2)	38(3)
C(43)	3207(4)	5032(4)	2894(3)	46(3)
C(44)	666(3)	2134(3)	-121(3)	41(3)
C(45)	525(3)	3494(3)	1460(2)	31(2)
C(46)	1328(3)	3142(3)	1730(2)	31(2)
C(47)	750(3)	2204(3)	-450(3)	42(3)
C(48)	2985(3)	5399(4)	2082(2)	45(3)
C(49)	3131(4)	5894(4)	2136(3)	65(4)
C(50)	2361(4)	3077(4)	1147(3)	76(4)
C(51)	-654(3)	3211(3)	-104(2)	32(2)
C(52)	-97(4)	3634(3)	-552(2)	42(3)
C(53)	504(4)	1835(4)	-652(3)	52(3)
C(54)	191(4)	1432(4)	-520(3)	57(3)
C(55)	521(4)	1539(5)	550(3)	86(4)
C(56)	1912(4)	2698(4)	1240(2)	46(3)
C(57)	-238(4)	1404(4)	458(3)	73(4)
C(58)	1835(5)	2355(5)	2257(3)	76(4)
C(59)	1305(5)	2660(5)	2662(3)	84(4)
C(60)	1777(4)	2284(4)	1036(3)	64(4)
C(61)	-1558(4)	2866(4)	486(3)	67(4)
C(62)	2159(5)	2359(5)	2061(3)	80(4)
C(63)	1947(3)	4297(4)	2929(2)	43(3)
C(64)	95(5)	3424(4)	-773(4)	97(5)
C(65)	-82(4)	4032(4)	-741(4)	91(5)

C(66)	1085(4)	2650(4)	-598(3)	51(3)
C(67)	3256(3)	5244(3)	2605(2)	34(2)
C(68)	1366(4)	2630(4)	-871(3)	76(4)
C(69)	848(5)	2895(5)	-713(4)	110(6)
C(70)	805(6)	1925(6)	2402(5)	154(9)
C(71)	3687(6)	4487(5)	3594(4)	116(6)
C(72)	4065(5)	4877(5)	3440(4)	85(4)
C(73)	3587(9)	4662(7)	3871(5)	177(11)
C(74)	3764(8)	5126(7)	3815(5)	165(10)
C(75)	2727(5)	5892(5)	3059(4)	94(5)
C(76)	2654(6)	5894(6)	3415(4)	117(6)
C(77)	2253(6)	5931(8)	3454(5)	164(11)
C(78)	2045(6)	5831(5)	3144(4)	98(5)
C(79)	9394(8)	2653(7)	1703(5)	153(8)
C(80)	9312(12)	2033(11)	1922(8)	225(13)
C(81)	8926(11)	1911(11)	1796(8)	232(13)
C(82)	8929(10)	2342(10)	1629(7)	216(12)
N(1)	914(3)	2502(3)	98(2)	40(2)
N(2)	1125(3)	3078(3)	408(2)	38(2)
N(3)	736(3)	3440(2)	457(2)	31(2)
N(4)	285(3)	3745(2)	423(2)	32(2)
N(5)	-306(2)	3470(2)	131(2)	31(2)
N(6)	1203(2)	3818(2)	1768(2)	26(2)
N(7)	1512(2)	4490(2)	2027(2)	25(2)
N(8)	965(2)	3120(2)	1568(2)	29(2)
N(9)	2095(2)	4757(2)	2326(2)	27(2)
N(10)	1274(3)	2733(3)	1677(2)	38(2)
O(1)	2335(3)	5810(3)	2904(2)	88(3)
O(2)	4035(3)	5259(3)	3534(2)	82(3)
O(3)	9657(8)	2422(9)	1799(6)	255(9)
Cr(1)	227(1)	2900(1)	215(1)	34(1)
Cr(2)	1763(1)	3802(1)	1921(1)	28(1)
Br(1)	-277(1)	2375(1)	-196(1)	47(1)
Br(2)	-125(1)	2560(1)	793(1)	50(1)
Br(3)	2205(1)	4189(1)	1385(1)	40(1)

Br(4)	2318(1)	3703(1)	2220(1)	47(1)

Table 7. Bond lengths [Å] and angles [∞] for **2b**.

C(2)-C(63)	1.559(14)
C(3)-C(63)	1.526(15)
C(1)-N(6)	1.339(11)
C(1)-C(5)	1.384(12)
C(1)-N(7)	1.396(11)
C(4)-C(21)	1.384(12)
C(4)-C(18)	1.393(12)
C(4)-N(9)	1.466(11)
C(5)-C(6)	1.392(12)
C(6)-C(45)	1.389(12)
C(7)-C(8)	1.330(12)
C(7)-N(7)	1.391(11)
C(8)-N(9)	1.408(11)
C(9)-N(5)	1.340(11)
C(9)-N(4)	1.409(12)
C(9)-Cr(1)	2.125(10)
C(10)-C(38)	1.369(13)
C(10)-C(24)	1.377(14)
C(11)-N(9)	1.361(11)
C(11)-N(7)	1.386(11)
C(11)-Cr(2)	2.129(9)
C(12)-C(42)	1.512(14)
C(12)-C(35)	1.520(15)
C(12)-C(61)	1.534(15)
C(13)-C(44)	1.392(14)
C(13)-C(41)	1.400(15)
C(13)-C(40)	1.475(15)
C(14)-C(17)	1.343(13)
C(14)-N(4)	1.380(11)
C(15)-N(3)	1.336(11)
C(15)-C(22)	1.377(12)
C(15)-N(4)	1.417(11)
C(16)-C(37)	1.334(13)

C(16)-N(10)	1.382(12)
C(17)-N(5)	1.392(11)
C(18)-C(36)	1.387(13)
C(18)-C(63)	1.499(13)
C(19)-C(22)	1.382(13)
C(19)-C(34)	1.394(13)
C(20)-C(33)	1.371(13)
C(20)-C(29)	1.394(15)
C(20)-C(56)	1.532(13)
C(21)-C(67)	1.359(13)
C(21)-C(48)	1.516(13)
C(23)-C(31)	1.509(15)
C(23)-C(59)	1.515(16)
C(23)-C(70)	1.525(19)
C(24)-C(27)	1.368(14)
C(25)-N(3)	1.343(11)
C(25)-C(34)	1.363(13)
C(25)-N(2)	1.407(12)
C(26)-N(1)	1.367(12)
C(26)-N(2)	1.387(12)
C(26)-Cr(1)	2.122(10)
C(27)-C(42)	1.415(13)
C(28)-C(30)	1.339(13)
C(28)-N(1)	1.410(12)
C(29)-C(62)	1.370(16)
C(30)-N(2)	1.401(12)
C(31)-C(58)	1.384(15)
C(31)-C(33)	1.404(13)
C(32)-N(6)	1.342(11)
C(32)-C(45)	1.375(12)
C(32)-N(8)	1.415(11)
C(33)-N(10)	1.455(12)
C(36)-C(43)	1.389(14)
C(37)-N(8)	1.394(12)
C(38)-C(51)	1.409(13)

C(38)-C(52)	1.492(14)
C(39)-C(48)	1.482(14)
C(40)-C(55)	1.477(15)
C(40)-C(57)	1.507(15)
C(41)-C(54)	1.387(16)
C(42)-C(51)	1.399(13)
C(43)-C(67)	1.360(13)
C(44)-C(47)	1.378(14)
C(44)-N(1)	1.440(12)
C(46)-N(10)	1.348(11)
C(46)-N(8)	1.391(11)
C(46)-Cr(2)	2.156(10)
C(47)-C(53)	1.397(14)
C(47)-C(66)	1.518(14)
C(48)-C(49)	1.537(15)
C(50)-C(56)	1.495(15)
C(51)-N(5)	1.452(11)
C(52)-C(64)	1.509(15)
C(52)-C(65)	1.557(15)
C(53)-C(54)	1.378(15)
C(56)-C(60)	1.516(15)
C(58)-C(62)	1.375(17)
C(66)-C(68)	1.508(15)
C(66)-C(69)	1.516(16)
C(71)-C(73)	1.41(2)
C(71)-C(72)	1.472(19)
C(72)-O(2)	1.430(15)
C(73)-C(74)	1.42(2)
C(74)-O(2)	1.410(16)
C(75)-O(1)	1.389(16)
C(75)-C(76)	1.48(2)
C(76)-C(77)	1.46(2)
C(77)-C(78)	1.41(2)
C(78)-O(1)	1.434(16)
C(79)-C(82)	1.45(3)

C(79)-O(3)	1.53(3)
C(80)-C(81)	1.29(3)
C(80)-O(3)	1.37(3)
C(81)-C(82)	1.63(3)
N(3)-Cr(1)	2.070(7)
N(6)-Cr(2)	2.059(7)
Cr(1)-Br(1)	2.4516(18)
Cr(1)-Br(2)	2.657(2)
Cr(2)-Br(4)	2.4421(17)
Cr(2)-Br(3)	2.6312(17)

N(6)-C(1)-C(5)	121.8(8)
N(6)-C(1)-N(7)	112.7(7)
C(5)-C(1)-N(7)	125.5(9)
C(21)-C(4)-C(18)	124.3(8)
C(21)-C(4)-N(9)	119.3(8)
C(18)-C(4)-N(9)	116.1(8)
C(1)-C(5)-C(6)	117.8(9)
C(45)-C(6)-C(5)	121.0(9)
C(8)-C(7)-N(7)	106.8(8)
C(7)-C(8)-N(9)	106.7(8)
N(5)-C(9)-N(4)	102.1(8)
N(5)-C(9)-Cr(1)	146.0(7)
N(4)-C(9)-Cr(1)	111.7(6)
C(38)-C(10)-C(24)	121.6(10)
N(9)-C(11)-N(7)	102.1(7)
N(9)-C(11)-Cr(2)	146.0(7)
N(7)-C(11)-Cr(2)	111.9(6)
C(42)-C(12)-C(35)	111.6(9)
C(42)-C(12)-C(61)	112.1(9)
C(35)-C(12)-C(61)	110.6(10)
C(44)-C(13)-C(41)	116.2(10)
C(44)-C(13)-C(40)	122.9(10)
C(41)-C(13)-C(40)	120.9(11)
C(17)-C(14)-N(4)	106.4(9)

N(3)-C(15)-C(22)	124.0(9)
N(3)-C(15)-N(4)	111.9(8)
C(22)-C(15)-N(4)	124.1(9)
C(37)-C(16)-N(10)	108.7(9)
C(14)-C(17)-N(5)	107.0(9)
C(36)-C(18)-C(4)	116.1(9)
C(36)-C(18)-C(63)	121.0(9)
C(4)-C(18)-C(63)	122.7(8)
C(22)-C(19)-C(34)	122.1(9)
C(33)-C(20)-C(29)	117.2(9)
C(33)-C(20)-C(56)	122.4(9)
C(29)-C(20)-C(56)	120.4(9)
C(67)-C(21)-C(4)	115.9(8)
C(67)-C(21)-C(48)	121.2(9)
C(4)-C(21)-C(48)	122.9(8)
C(15)-C(22)-C(19)	115.7(9)
C(31)-C(23)-C(59)	112.0(11)
C(31)-C(23)-C(70)	110.6(11)
C(59)-C(23)-C(70)	109.9(12)
C(27)-C(24)-C(10)	121.9(10)
N(3)-C(25)-C(34)	122.9(9)
N(3)-C(25)-N(2)	110.3(8)
C(34)-C(25)-N(2)	126.8(9)
N(1)-C(26)-N(2)	103.4(8)
N(1)-C(26)-Cr(1)	143.6(7)
N(2)-C(26)-Cr(1)	113.0(7)
C(24)-C(27)-C(42)	119.8(10)
C(30)-C(28)-N(1)	107.5(9)
C(62)-C(29)-C(20)	120.7(11)
C(28)-C(30)-N(2)	106.5(9)
C(58)-C(31)-C(33)	116.4(10)
C(58)-C(31)-C(23)	121.3(10)
C(33)-C(31)-C(23)	122.3(9)
N(6)-C(32)-C(45)	123.5(8)
N(6)-C(32)-N(8)	111.3(8)

C(45)-C(32)-N(8)	125.2(8)
C(20)-C(33)-C(31)	123.5(9)
C(20)-C(33)-N(10)	118.7(9)
C(31)-C(33)-N(10)	117.7(9)
C(25)-C(34)-C(19)	116.9(10)
C(18)-C(36)-C(43)	121.0(9)
C(16)-C(37)-N(8)	105.0(9)
C(10)-C(38)-C(51)	116.5(10)
C(10)-C(38)-C(52)	121.8(10)
C(51)-C(38)-C(52)	121.6(9)
C(13)-C(40)-C(55)	111.5(9)
C(13)-C(40)-C(57)	114.2(10)
C(55)-C(40)-C(57)	110.5(10)
C(54)-C(41)-C(13)	119.6(11)
C(51)-C(42)-C(27)	116.5(9)
C(51)-C(42)-C(12)	123.6(9)
C(27)-C(42)-C(12)	119.9(10)
C(67)-C(43)-C(36)	119.1(9)
C(47)-C(44)-C(13)	125.6(10)
C(47)-C(44)-N(1)	118.5(10)
C(13)-C(44)-N(1)	115.8(10)
C(32)-C(45)-C(6)	116.6(9)
N(10)-C(46)-N(8)	102.7(8)
N(10)-C(46)-Cr(2)	145.8(7)
N(8)-C(46)-Cr(2)	111.2(6)
C(44)-C(47)-C(53)	116.3(10)
C(44)-C(47)-C(66)	123.9(10)
C(53)-C(47)-C(66)	119.8(10)
C(39)-C(48)-C(21)	111.1(9)
C(39)-C(48)-C(49)	111.1(9)
C(21)-C(48)-C(49)	111.3(9)
C(42)-C(51)-C(38)	123.7(9)
C(42)-C(51)-N(5)	117.8(8)
C(38)-C(51)-N(5)	118.3(9)
C(38)-C(52)-C(64)	112.5(9)

C(38)-C(52)-C(65)	112.3(9)
C(64)-C(52)-C(65)	107.2(10)
C(54)-C(53)-C(47)	120.1(11)
C(53)-C(54)-C(41)	122.1(11)
C(50)-C(56)-C(60)	112.5(10)
C(50)-C(56)-C(20)	111.9(10)
C(60)-C(56)-C(20)	110.2(9)
C(62)-C(58)-C(31)	121.1(11)
C(29)-C(62)-C(58)	120.6(11)
C(18)-C(63)-C(3)	109.5(9)
C(18)-C(63)-C(2)	112.9(9)
C(3)-C(63)-C(2)	110.4(8)
C(68)-C(66)-C(47)	115.6(10)
C(68)-C(66)-C(69)	109.6(11)
C(47)-C(66)-C(69)	110.0(9)
C(21)-C(67)-C(43)	123.5(9)
C(73)-C(71)-C(72)	104.5(14)
O(2)-C(72)-C(71)	106.7(12)
C(74)-C(73)-C(71)	107.1(16)
O(2)-C(74)-C(73)	110.1(15)
O(1)-C(75)-C(76)	107.5(13)
C(77)-C(76)-C(75)	106.1(15)
C(78)-C(77)-C(76)	105.6(15)
C(77)-C(78)-O(1)	110.4(15)
C(82)-C(79)-O(3)	113(2)
C(81)-C(80)-O(3)	115(3)
C(80)-C(81)-C(82)	110(3)
C(79)-C(82)-C(81)	95(2)
C(26)-N(1)-C(28)	111.1(8)
C(26)-N(1)-C(44)	125.1(8)
C(28)-N(1)-C(44)	123.8(8)
C(26)-N(2)-C(30)	111.5(8)
C(26)-N(2)-C(25)	119.2(8)
C(30)-N(2)-C(25)	129.0(8)
C(15)-N(3)-C(25)	118.4(8)

C(15)-N(3)-Cr(1)	119.9(6)
C(25)-N(3)-Cr(1)	121.2(6)
C(14)-N(4)-C(9)	111.6(8)
C(14)-N(4)-C(15)	129.6(8)
C(9)-N(4)-C(15)	118.7(8)
C(9)-N(5)-C(17)	112.9(8)
C(9)-N(5)-C(51)	124.4(8)
C(17)-N(5)-C(51)	122.6(8)
C(1)-N(6)-C(32)	119.2(8)
C(1)-N(6)-Cr(2)	119.5(6)
C(32)-N(6)-Cr(2)	121.1(6)
C(11)-N(7)-C(7)	112.2(7)
C(11)-N(7)-C(1)	119.1(7)
C(7)-N(7)-C(1)	128.6(8)
C(46)-N(8)-C(37)	111.9(8)
C(46)-N(8)-C(32)	119.4(8)
C(37)-N(8)-C(32)	128.4(8)
C(11)-N(9)-C(8)	112.2(7)
C(11)-N(9)-C(4)	126.6(7)
C(8)-N(9)-C(4)	121.1(7)
C(46)-N(10)-C(16)	111.7(8)
C(46)-N(10)-C(33)	122.4(8)
C(16)-N(10)-C(33)	125.9(8)
C(75)-O(1)-C(78)	108.0(12)
C(74)-O(2)-C(72)	105.2(12)
C(80)-O(3)-C(79)	99(2)
N(3)-Cr(1)-C(26)	74.9(4)
N(3)-Cr(1)-C(9)	76.3(4)
C(26)-Cr(1)-C(9)	147.9(4)
N(3)-Cr(1)-Br(1)	165.1(2)
C(26)-Cr(1)-Br(1)	103.1(3)
C(9)-Cr(1)-Br(1)	101.0(3)
N(3)-Cr(1)-Br(2)	88.0(2)
C(26)-Cr(1)-Br(2)	99.3(3)
C(9)-Cr(1)-Br(2)	93.7(2)

Br(1)-Cr(1)-Br(2)	106.82(7)
N(6)-Cr(2)-C(11)	76.2(3)
N(6)-Cr(2)-C(46)	75.6(3)
C(11)-Cr(2)-C(46)	149.2(3)
N(6)-Cr(2)-Br(4)	166.1(2)
C(11)-Cr(2)-Br(4)	101.9(3)
C(46)-Cr(2)-Br(4)	102.4(2)
N(6)-Cr(2)-Br(3)	92.7(2)
C(11)-Cr(2)-Br(3)	94.6(2)
C(46)-Cr(2)-Br(3)	98.9(2)
Br(4)-Cr(2)-Br(3)	101.26(6)

Symmetry transformations used to generate equivalent atoms:

Table 8. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **2b** The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

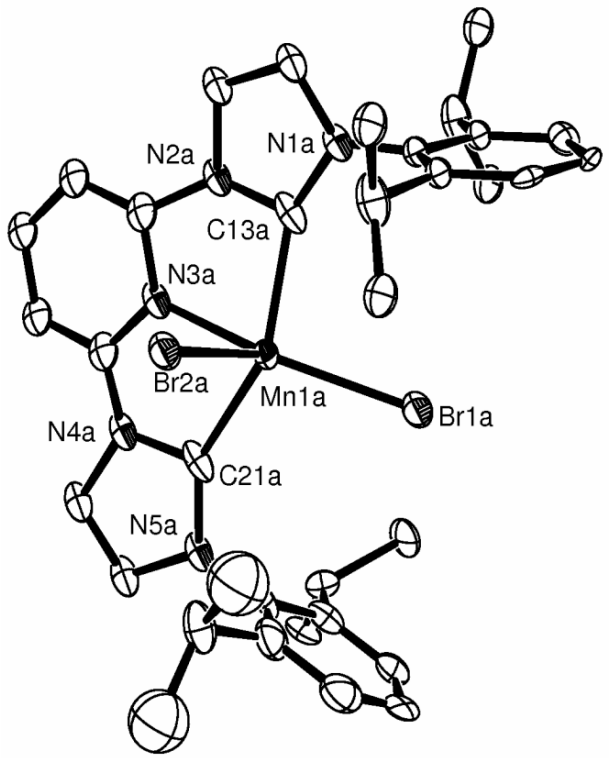
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(2)	80(9)	58(8)	40(7)	9(6)	21(6)	40(7)
C(3)	52(8)	58(8)	94(10)	35(7)	30(7)	28(7)
C(1)	12(5)	33(6)	26(5)	5(4)	5(4)	8(5)
C(4)	34(6)	26(5)	23(5)	-4(4)	-6(5)	15(5)
C(5)	26(6)	33(6)	33(6)	-6(5)	4(5)	15(5)
C(6)	28(6)	29(6)	34(6)	10(5)	-1(5)	12(5)
C(7)	28(6)	36(6)	25(5)	2(5)	0(4)	19(5)
C(8)	35(6)	20(5)	31(5)	-6(4)	-4(5)	14(5)
C(9)	41(6)	47(7)	22(5)	7(5)	5(5)	27(6)
C(10)	46(7)	42(7)	29(6)	1(5)	-10(5)	21(6)
C(11)	26(5)	37(6)	17(5)	3(5)	6(4)	14(5)
C(12)	41(7)	54(8)	41(7)	-7(6)	-25(6)	10(6)
C(13)	36(7)	57(8)	50(7)	-17(6)	-7(6)	30(6)
C(14)	48(7)	31(6)	42(6)	-9(5)	-14(5)	25(6)
C(15)	32(6)	36(6)	19(5)	0(5)	-9(4)	13(5)
C(16)	36(6)	36(6)	41(6)	-11(5)	-11(5)	12(6)
C(17)	48(7)	40(7)	43(6)	-20(5)	-22(6)	25(6)
C(18)	28(6)	32(6)	33(6)	-2(5)	-4(5)	11(5)
C(19)	43(7)	32(6)	30(6)	0(5)	-7(5)	8(5)
C(20)	66(8)	51(7)	30(6)	-2(5)	3(5)	49(6)
C(21)	25(6)	34(6)	28(5)	2(5)	0(5)	12(5)
C(22)	39(6)	27(6)	23(5)	-3(4)	-5(5)	17(5)
C(23)	90(10)	76(9)	40(7)	13(7)	8(7)	57(9)
C(24)	67(9)	41(7)	40(7)	-16(5)	-29(6)	35(7)
C(25)	27(6)	34(6)	50(7)	0(5)	-11(5)	13(5)
C(26)	41(7)	38(6)	44(6)	-13(5)	-13(5)	24(6)
C(27)	49(7)	32(6)	50(7)	-6(5)	-13(6)	20(6)
C(28)	32(6)	47(7)	64(8)	-12(6)	-13(6)	26(6)
C(29)	101(11)	87(10)	60(9)	18(7)	26(8)	75(9)
C(30)	24(6)	34(6)	59(7)	2(6)	-10(5)	16(5)

C(31)	66(8)	57(8)	35(6)	5(5)	9(6)	48(7)
C(32)	27(6)	24(6)	30(5)	5(4)	-3(5)	11(5)
C(33)	46(7)	37(6)	38(6)	-4(5)	-4(5)	29(6)
C(34)	31(6)	35(6)	40(6)	-1(5)	-12(5)	9(5)
C(35)	74(9)	80(10)	52(8)	16(7)	-12(7)	39(8)
C(36)	48(7)	44(7)	31(6)	7(5)	-9(5)	21(6)
C(37)	42(7)	41(7)	43(7)	-10(5)	-10(5)	22(6)
C(38)	42(7)	32(6)	45(7)	-6(5)	-16(5)	25(6)
C(39)	75(9)	80(9)	45(7)	3(7)	24(7)	34(8)
C(40)	35(7)	47(7)	76(9)	3(6)	-2(6)	28(6)
C(41)	49(8)	53(8)	69(9)	-3(7)	7(7)	30(7)
C(42)	49(7)	49(7)	30(6)	-10(5)	-15(5)	34(6)
C(43)	41(7)	46(7)	48(7)	-6(6)	-23(6)	21(6)
C(44)	31(6)	33(7)	57(8)	-12(6)	-13(6)	15(6)
C(45)	25(6)	24(6)	36(6)	4(5)	-4(5)	6(5)
C(46)	37(6)	47(7)	22(5)	7(5)	0(5)	31(5)
C(47)	39(7)	41(7)	49(7)	-7(6)	-3(6)	24(6)
C(48)	32(6)	57(8)	37(6)	9(5)	7(5)	16(6)
C(49)	84(10)	54(8)	60(8)	5(7)	8(7)	36(7)
C(50)	84(10)	63(9)	61(9)	11(7)	2(8)	22(8)
C(51)	38(6)	29(6)	36(6)	-7(5)	-14(5)	22(5)
C(52)	51(7)	42(7)	32(6)	-3(5)	-9(5)	24(6)
C(53)	41(7)	59(8)	56(8)	-13(7)	1(6)	25(7)
C(54)	44(8)	37(7)	88(10)	-25(7)	-6(7)	17(6)
C(55)	70(10)	107(12)	88(11)	12(9)	17(8)	49(9)
C(56)	60(8)	59(8)	38(6)	10(6)	6(6)	45(7)
C(57)	42(8)	92(10)	83(10)	1(8)	0(7)	31(8)
C(58)	111(12)	104(11)	49(8)	21(8)	3(8)	80(10)
C(59)	104(12)	104(12)	65(9)	1(8)	22(8)	68(10)
C(60)	82(10)	67(9)	42(7)	6(6)	6(7)	35(8)
C(61)	65(9)	74(9)	58(8)	-11(7)	-7(7)	31(8)
C(62)	116(12)	125(13)	58(9)	25(8)	11(9)	105(11)
C(63)	40(7)	54(7)	32(6)	6(5)	-4(5)	22(6)
C(64)	88(11)	66(10)	134(14)	1(9)	52(10)	37(9)
C(65)	51(9)	72(10)	142(14)	26(10)	-6(9)	25(8)

C(66)	50(7)	43(7)	52(7)	-2(6)	1(6)	17(6)
C(67)	25(6)	31(6)	40(6)	-7(5)	0(5)	9(5)
C(68)	64(9)	82(10)	80(10)	2(8)	21(8)	34(8)
C(69)	90(11)	88(11)	178(17)	68(11)	81(12)	64(10)
C(70)	107(14)	116(16)	170(20)	-17(14)	86(14)	7(12)
C(71)	144(16)	66(11)	122(15)	-14(10)	38(13)	40(12)
C(72)	69(10)	74(11)	113(13)	-21(10)	-7(9)	36(9)
C(73)	300(30)	117(17)	160(20)	48(15)	130(20)	130(20)
C(74)	250(30)	127(17)	136(17)	56(14)	140(19)	111(18)
C(75)	42(9)	72(10)	137(16)	-28(10)	6(10)	5(8)
C(76)	114(16)	139(16)	68(12)	-18(11)	-10(11)	40(13)
C(77)	65(12)	220(20)	129(19)	-74(17)	26(12)	8(14)
C(78)	134(15)	86(12)	105(13)	13(10)	25(13)	77(12)
N(1)	37(5)	44(5)	44(5)	-8(4)	-18(4)	23(5)
N(2)	36(5)	34(5)	47(5)	-7(4)	-13(4)	19(4)
N(3)	31(5)	21(5)	30(5)	-5(4)	-7(4)	5(4)
N(4)	38(5)	30(5)	28(4)	-14(4)	-13(4)	17(4)
N(5)	31(5)	32(5)	31(5)	-12(4)	-18(4)	17(4)
N(6)	19(4)	30(5)	30(4)	-2(4)	-1(4)	12(4)
N(7)	27(5)	28(5)	24(4)	-4(4)	-4(4)	16(4)
N(8)	34(5)	29(5)	24(4)	1(4)	-2(4)	15(4)
N(9)	31(5)	28(5)	21(4)	10(4)	10(4)	15(4)
N(10)	52(6)	36(5)	34(5)	4(4)	1(4)	28(5)
O(1)	78(7)	83(7)	83(7)	-29(6)	-4(6)	26(6)
O(2)	97(7)	71(6)	75(7)	-5(5)	-7(6)	41(6)
Cr(1)	32(1)	31(1)	41(1)	-11(1)	-16(1)	17(1)
Cr(2)	27(1)	36(1)	25(1)	1(1)	0(1)	19(1)
Br(1)	40(1)	42(1)	53(1)	-18(1)	-16(1)	18(1)
Br(2)	46(1)	46(1)	46(1)	0(1)	-13(1)	14(1)
Br(3)	26(1)	63(1)	26(1)	7(1)	0(1)	19(1)
Br(4)	45(1)	72(1)	37(1)	4(1)	-2(1)	40(1)

Electronic Supplementary Information for Dalton Transactions

Structural Data for 3



Electronic Supplementary Information for Dalton Transactions

Table 1. Crystal data and structure refinement for 3.

Identification code	3	
Empirical formula	C39 H49 Br2 Mn N5 O	
Formula weight	818.59	
Temperature	95(2) K	
Wavelength	0.71073 ≈	
Crystal system	Monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 10.6948(8) ≈	α= 90∞.
	b = 18.7188(14) ≈	β= 93.796(9)∞.
	c = 19.2039(19) ≈	γ = 90∞.
Volume	3836.1(6) ≈^{3}	
Z	4	
Density (calculated)	1.417 Mg/m^3	
Absorption coefficient	2.464 mm^{-1}	
F(000)	1684	
Crystal size	0.25 x 0.25 x 0.25 mm^3	
Theta range for data collection	2.97 to 25.03∞.	
Index ranges	-12<=h<=12, -22<=k<=22, -22<=l<=19	
Reflections collected	26916	
Independent reflections	6754 [R(int) = 0.0661]	
Completeness to theta = 25.03∞	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.5779 and 0.5779	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6754 / 1413 / 415	
Goodness-of-fit on F^2	1.059	
Final R indices [I>2sigma(I)]	R1 = 0.0874, wR2 = 0.2042	
R indices (all data)	R1 = 0.1373, wR2 = 0.2333	
Largest diff. peak and hole	2.097 and -1.073 e.≈$^{-3}$	

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

	x	y	z	U(eq)
O(1A)	8290(4)	5786(2)	1033(2)	60(1)
C(41A)	10469(5)	6081(3)	1011(2)	68(1)
C(40A)	10004(5)	6230(3)	1745(3)	68(1)
C(43A)	9017(6)	5565(3)	1701(4)	68(1)
C(42A)	9289(5)	5797(3)	568(4)	68(1)
O(1B)	8849(4)	5963(2)	1715(2)	60(1)
C(41B)	10729(4)	5714(2)	1035(3)	68(1)
C(40B)	9942(5)	6328(3)	1331(3)	68(1)
C(43B)	9275(5)	5228(3)	1793(3)	68(1)
C(42B)	9836(5)	5098(3)	1114(3)	68(1)
Mn(1A)	3339(1)	3154(1)	991(1)	20(1)
Br(1A)	3078(1)	2378(1)	2060(1)	29(1)
Br(2A)	1956(1)	4236(1)	643(1)	29(1)
N(1A)	5507(2)	4177(1)	1936(1)	26(1)
C(14A)	6368(2)	4675(1)	1680(1)	31(1)
C(15A)	6420(3)	4559(2)	952(1)	31(1)
N(2A)	5593(3)	3989(1)	758(1)	26(1)
C(13A)	5028(2)	3753(1)	1366(1)	28(1)
N(3A)	4325(1)	3419(1)	20(1)	26(1)
C(16A)	5212(2)	3963(1)	62(1)	28(1)
C(17A)	5784(2)	4177(1)	-533(1)	28(1)
C(18A)	5470(2)	3848(2)	-1169(1)	28(1)
C(19A)	4584(2)	3304(1)	-1211(1)	28(1)
C(20A)	4011(2)	3090(1)	-617(1)	28(1)
C(1A)	5444(1)	3953(1)	2546(1)	20(1)
C(2A)	4439(2)	4234(1)	2880(1)	20(1)
C(3A)	4316(2)	4089(2)	3582(1)	18(1)
C(5A)	5196(3)	3664(2)	3950(1)	21(1)
C(4A)	6201(2)	3384(1)	3616(1)	25(1)
C(6A)	6325(2)	3529(1)	2914(1)	20(1)

N(4A)	2975(2)	2712(1)	-519(1)	26(1)
C(22A)	2274(2)	2349(1)	-1064(1)	31(1)
C(23A)	1396(2)	1898(1)	-756(2)	31(1)
N(5A)	1554(2)	1983(1)	-21(2)	26(1)
C(21A)	2530(2)	2486(1)	126(1)	28(1)
C(24A)	1044(1)	1576(1)	462(1)	34(1)
C(25A)	1488(1)	930(1)	734(1)	35(1)
C(26A)	857(1)	587(1)	1249(1)	43(1)
C(27A)	-218(1)	891(1)	1491(1)	39(1)
C(28A)	-662(1)	1537(1)	1219(1)	49(1)
C(29A)	-31(1)	1880(1)	704(1)	40(1)
C(7A)	7399(4)	3164(2)	2557(2)	38(1)
C(11A)	3388(4)	5436(2)	2800(2)	32(1)
C(12A)	2106(4)	4374(2)	2535(2)	32(1)
C(10A)	3381(4)	4663(2)	2529(2)	38(1)
C(9A)	8644(4)	3504(2)	2842(2)	32(1)
C(8A)	7333(4)	2382(2)	2576(2)	32(1)
C(30A)	2571(4)	589(2)	512(2)	37(1)
C(31A)	2559(4)	-44(3)	71(2)	42(1)
C(32A)	3564(4)	372(3)	1179(2)	47(2)
C(33A)	-598(1)	2577(1)	395(1)	38(1)
C(34A)	-680(2)	3137(1)	976(1)	88(1)
C(35A)	-1928(1)	2440(1)	64(1)	88(1)
Mn(1B)	3748(1)	2715(1)	1102(1)	20(1)
Br(1B)	2510(1)	2362(1)	2115(1)	29(1)
Br(2B)	5639(1)	1938(1)	974(1)	29(1)
N(1B)	5493(2)	4020(1)	1948(1)	26(1)
C(14B)	6396(2)	4548(1)	1809(1)	31(1)
C(15B)	6381(3)	4642(2)	1075(1)	31(1)
N(2B)	5469(3)	4171(1)	760(1)	26(1)
C(13B)	4920(2)	3787(1)	1299(1)	28(1)
N(3B)	4270(2)	3332(1)	111(1)	26(1)
C(16B)	5299(2)	3787(1)	158(1)	28(1)
C(17B)	5828(2)	4016(2)	-446(1)	28(1)
C(18B)	5328(3)	3790(2)	-1095(1)	28(1)

C(19B)	4299(3)	3335(1)	-1141(1)	28(1)
C(20B)	3770(2)	3106(1)	-538(1)	28(1)
C(1B)	5188(2)	3891(1)	2667(1)	20(1)
C(2B)	4179(2)	4173(1)	2996(1)	20(1)
C(3B)	4050(2)	4033(2)	3699(1)	23(1)
C(4B)	4929(3)	3612(2)	4072(1)	28(1)
C(5B)	5938(3)	3330(2)	3743(1)	24(1)
C(6B)	6067(2)	3469(1)	3041(1)	20(1)
N(4B)	2975(2)	2557(1)	-528(1)	26(1)
C(22B)	2230(2)	2198(1)	-1059(1)	31(1)
C(23B)	1361(2)	1758(1)	-731(2)	31(1)
N(5B)	1570(3)	1845(1)	2(2)	26(1)
C(21B)	2567(2)	2338(1)	128(1)	28(1)
C(7B)	7208(4)	3152(3)	2695(2)	38(1)
C(11B)	3404(4)	5439(3)	2800(2)	32(1)
C(24B)	912(1)	1548(1)	478(1)	27(1)
C(25B)	1410(1)	895(1)	701(1)	33(1)
C(26B)	768(1)	470(1)	1152(1)	39(1)
C(27B)	-372(2)	699(1)	1380(1)	40(1)
C(28B)	-870(1)	1352(1)	1157(1)	41(1)
C(29B)	-228(1)	1777(1)	706(1)	40(1)
C(12B)	1907(4)	4358(3)	2691(2)	32(1)
C(10B)	3212(5)	4677(3)	2563(3)	38(1)
C(9B)	8416(4)	3425(3)	2989(2)	32(1)
C(8B)	7217(4)	2304(2)	2817(2)	32(1)
C(30B)	2728(4)	604(3)	410(3)	33(1)
C(31B)	2279(5)	-157(2)	59(3)	42(2)
C(32B)	3705(5)	606(2)	962(3)	44(2)
C(33B)	-674(1)	2535(1)	502(1)	38(1)
C(34B)	-739(6)	3070(3)	997(2)	88(1)
C(35B)	-1490(5)	2592(3)	-170(2)	88(1)

Table 3. Bond lengths [≈] and angles [∞] for 3.

O(1A)-C(42A)	1.437(7)
O(1A)-C(43A)	1.513(7)
C(41A)-C(40A)	1.549(7)
C(41A)-C(42A)	1.567(8)
C(41A)-H(41A)	0.9900
C(41A)-H(41B)	0.9900
C(40A)-C(43A)	1.630(8)
C(40A)-H(40A)	0.9900
C(40A)-H(40B)	0.9900
C(43A)-H(43A)	0.9900
C(43A)-H(43B)	0.9900
C(42A)-H(42A)	0.9900
C(42A)-H(42B)	0.9900
O(1B)-C(43B)	1.454(7)
O(1B)-C(40B)	1.579(7)
C(41B)-C(42B)	1.512(6)
C(41B)-C(40B)	1.553(7)
C(41B)-H(41C)	0.9900
C(41B)-H(41D)	0.9900
C(40B)-H(40C)	0.9900
C(40B)-H(40D)	0.9900
C(43B)-C(42B)	1.491(7)
C(43B)-H(43C)	0.9900
C(43B)-H(43D)	0.9900
C(42B)-H(42C)	0.9900
C(42B)-H(42D)	0.9900
Mn(1A)-C(13A)	2.206(2)
Mn(1A)-C(21A)	2.210(2)
Mn(1A)-N(3A)	2.2574(16)
Mn(1A)-Br(1A)	2.5458(7)
Mn(1A)-Br(2A)	2.5708(7)
N(1A)-C(1A)	1.250(2)
N(1A)-C(14A)	1.4200

N(1A)-C(13A)	1.4200
C(14A)-C(15A)	1.4200
C(14A)-H(14A)	0.9500
C(15A)-N(2A)	1.4200
C(15A)-H(15A)	0.9500
N(2A)-C(16A)	1.372(2)
N(2A)-C(13A)	1.4200
N(3A)-C(16A)	1.3900
N(3A)-C(20A)	1.3900
C(16A)-C(17A)	1.3900
C(17A)-C(18A)	1.3900
C(17A)-H(17A)	0.9500
C(18A)-C(19A)	1.3900
C(18A)-H(18A)	0.9500
C(19A)-C(20A)	1.3900
C(19A)-H(19A)	0.9500
C(20A)-N(4A)	1.338(2)
C(1A)-C(2A)	1.3900
C(1A)-C(6A)	1.3900
C(2A)-C(3A)	1.3900
C(2A)-C(10A)	1.510(5)
C(3A)-C(5A)	1.3900
C(3A)-H(3A)	0.9500
C(5A)-C(4A)	1.3900
C(5A)-H(5A)	0.9500
C(4A)-C(6A)	1.3900
C(4A)-H(4A)	0.9500
C(6A)-C(7A)	1.536(5)
N(4A)-C(22A)	1.4200
N(4A)-C(21A)	1.4200
C(22A)-C(23A)	1.4200
C(22A)-H(22A)	0.9500
C(23A)-N(5A)	1.4200
C(23A)-H(23A)	0.9500
N(5A)-C(24A)	1.343(2)

N(5A)-C(21A)	1.4200
C(24A)-C(25A)	1.3900
C(24A)-C(29A)	1.3900
C(25A)-C(26A)	1.3900
C(25A)-C(30A)	1.413(5)
C(26A)-C(27A)	1.3900
C(26A)-H(26A)	0.9500
C(27A)-C(28A)	1.3900
C(27A)-H(27A)	0.9500
C(28A)-C(29A)	1.3900
C(28A)-H(28A)	0.9500
C(29A)-C(33A)	1.5401
C(7A)-C(8A)	1.465(6)
C(7A)-C(9A)	1.543(6)
C(7A)-H(7A)	1.0000
C(11A)-C(10A)	1.537(6)
C(11A)-H(11A)	0.9800
C(11A)-H(11B)	0.9800
C(11A)-H(11C)	0.9800
C(12A)-C(10A)	1.469(6)
C(12A)-H(12A)	0.9800
C(12A)-H(12B)	0.9800
C(12A)-H(12C)	0.9800
C(10A)-H(10A)	1.0000
C(9A)-H(9A1)	0.9800
C(9A)-H(9A2)	0.9800
C(9A)-H(9A3)	0.9800
C(8A)-H(8A1)	0.9800
C(8A)-H(8A2)	0.9800
C(8A)-H(8A3)	0.9800
C(30A)-C(31A)	1.456(6)
C(30A)-C(32A)	1.660(6)
C(30A)-H(30A)	1.0000
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(35A)	1.5398(6)
C(33A)-C(34A)	1.5399(6)
C(33A)-H(33A)	1.0000
C(34A)-H(34A)	0.9800
C(34A)-H(34B)	0.9800
C(34A)-H(34C)	0.9800
C(35A)-H(35A)	0.9800
C(35A)-H(35B)	0.9800
C(35A)-H(35C)	0.9800
Mn(1B)-C(21B)	2.298(2)
Mn(1B)-N(3B)	2.3257(16)
Mn(1B)-C(13B)	2.384(2)
Mn(1B)-Br(1B)	2.5126(8)
Mn(1B)-Br(2B)	2.5151(7)
N(1B)-C(13B)	1.4200
N(1B)-C(14B)	1.4200
N(1B)-C(1B)	1.460(2)
C(14B)-C(15B)	1.4200
C(14B)-H(14B)	0.9500
C(15B)-N(2B)	1.4200
C(15B)-H(15B)	0.9500
N(2B)-C(16B)	1.364(3)
N(2B)-C(13B)	1.4200
N(3B)-C(16B)	1.3900
N(3B)-C(20B)	1.3900
C(16B)-C(17B)	1.3900
C(17B)-C(18B)	1.3900
C(17B)-H(17B)	0.9500
C(18B)-C(19B)	1.3900
C(18B)-H(18B)	0.9500
C(19B)-C(20B)	1.3900

C(19B)-H(19B)	0.9500
C(20B)-N(4B)	1.334(2)
C(1B)-C(2B)	1.3900
C(1B)-C(6B)	1.3900
C(2B)-C(3B)	1.3900
C(2B)-C(10B)	1.593(5)
C(3B)-C(4B)	1.3900
C(3B)-H(3B)	0.9500
C(4B)-C(5B)	1.3900
C(4B)-H(4B)	0.9500
C(5B)-C(6B)	1.3900
C(5B)-H(5B)	0.9500
C(6B)-C(7B)	1.546(5)
N(4B)-C(22B)	1.4200
N(4B)-C(21B)	1.4200
C(22B)-C(23B)	1.4200
C(22B)-H(22B)	0.9500
C(23B)-N(5B)	1.4200
C(23B)-H(23B)	0.9500
N(5B)-C(24B)	1.312(2)
N(5B)-C(21B)	1.4200
C(7B)-C(9B)	1.467(6)
C(7B)-C(8B)	1.604(7)
C(7B)-H(7B)	1.0000
C(11B)-C(10B)	1.507(7)
C(11B)-H(11D)	0.9800
C(11B)-H(11E)	0.9800
C(11B)-H(11F)	0.9800
C(24B)-C(25B)	1.3900
C(24B)-C(29B)	1.3900
C(25B)-C(26B)	1.3900
C(25B)-C(30B)	1.643(5)
C(26B)-C(27B)	1.3900
C(26B)-H(26B)	0.9500
C(27B)-C(28B)	1.3900

C(27B)-H(27B)	0.9500
C(28B)-C(29B)	1.3900
C(28B)-H(28B)	0.9500
C(29B)-C(33B)	1.5401
C(12B)-C(10B)	1.553(7)
C(12B)-H(12D)	0.9800
C(12B)-H(12E)	0.9800
C(12B)-H(12F)	0.9800
C(10B)-H(10B)	1.0000
C(9B)-H(9B1)	0.9800
C(9B)-H(9B2)	0.9800
C(9B)-H(9B3)	0.9800
C(8B)-H(8B1)	0.9800
C(8B)-H(8B2)	0.9800
C(8B)-H(8B3)	0.9800
C(30B)-C(32B)	1.439(7)
C(30B)-C(31B)	1.635(7)
C(30B)-H(30B)	1.0000
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(34B)	1.386(5)
C(33B)-C(35B)	1.514(4)
C(33B)-H(33B)	1.0000
C(34B)-H(34D)	0.9800
C(34B)-H(34E)	0.9800
C(34B)-H(34F)	0.9800
C(35B)-H(35D)	0.9800
C(35B)-H(35E)	0.9800
C(35B)-H(35F)	0.9800

C(42A)-O(1A)-C(43A)	99.7(4)

C(40A)-C(41A)-C(42A)	105.0(5)
C(40A)-C(41A)-H(41A)	110.7
C(42A)-C(41A)-H(41A)	110.7
C(40A)-C(41A)-H(41B)	110.7
C(42A)-C(41A)-H(41B)	110.7
H(41A)-C(41A)-H(41B)	108.8
C(41A)-C(40A)-C(43A)	93.6(4)
C(41A)-C(40A)-H(40A)	113.0
C(43A)-C(40A)-H(40A)	113.0
C(41A)-C(40A)-H(40B)	113.0
C(43A)-C(40A)-H(40B)	113.0
H(40A)-C(40A)-H(40B)	110.4
O(1A)-C(43A)-C(40A)	97.5(4)
O(1A)-C(43A)-H(43A)	112.3
C(40A)-C(43A)-H(43A)	112.3
O(1A)-C(43A)-H(43B)	112.3
C(40A)-C(43A)-H(43B)	112.3
H(43A)-C(43A)-H(43B)	109.9
O(1A)-C(42A)-C(41A)	105.8(5)
O(1A)-C(42A)-H(42A)	110.6
C(41A)-C(42A)-H(42A)	110.6
O(1A)-C(42A)-H(42B)	110.6
C(41A)-C(42A)-H(42B)	110.6
H(42A)-C(42A)-H(42B)	108.7
C(43B)-O(1B)-C(40B)	102.7(4)
C(42B)-C(41B)-C(40B)	99.6(4)
C(42B)-C(41B)-H(41C)	111.8
C(40B)-C(41B)-H(41C)	111.8
C(42B)-C(41B)-H(41D)	111.8
C(40B)-C(41B)-H(41D)	111.8
H(41C)-C(41B)-H(41D)	109.6
C(41B)-C(40B)-O(1B)	106.7(4)
C(41B)-C(40B)-H(40C)	110.4
O(1B)-C(40B)-H(40C)	110.4
C(41B)-C(40B)-H(40D)	110.4

O(1B)-C(40B)-H(40D)	110.4
H(40C)-C(40B)-H(40D)	108.6
O(1B)-C(43B)-C(42B)	101.9(4)
O(1B)-C(43B)-H(43C)	111.4
C(42B)-C(43B)-H(43C)	111.4
O(1B)-C(43B)-H(43D)	111.4
C(42B)-C(43B)-H(43D)	111.4
H(43C)-C(43B)-H(43D)	109.3
C(43B)-C(42B)-C(41B)	104.8(4)
C(43B)-C(42B)-H(42C)	110.8
C(41B)-C(42B)-H(42C)	110.8
C(43B)-C(42B)-H(42D)	110.8
C(41B)-C(42B)-H(42D)	110.8
H(42C)-C(42B)-H(42D)	108.9
C(13A)-Mn(1A)-C(21A)	143.58(8)
C(13A)-Mn(1A)-N(3A)	74.99(7)
C(21A)-Mn(1A)-N(3A)	71.60(6)
C(13A)-Mn(1A)-Br(1A)	99.12(6)
C(21A)-Mn(1A)-Br(1A)	102.96(5)
N(3A)-Mn(1A)-Br(1A)	150.91(5)
C(13A)-Mn(1A)-Br(2A)	97.41(6)
C(21A)-Mn(1A)-Br(2A)	93.48(6)
N(3A)-Mn(1A)-Br(2A)	84.52(4)
Br(1A)-Mn(1A)-Br(2A)	124.57(3)
C(1A)-N(1A)-C(14A)	128.35(12)
C(1A)-N(1A)-C(13A)	119.75(12)
C(14A)-N(1A)-C(13A)	108.0
N(1A)-C(14A)-C(15A)	108.0
N(1A)-C(14A)-H(14A)	126.0
C(15A)-C(14A)-H(14A)	126.0
N(2A)-C(15A)-C(14A)	108.0
N(2A)-C(15A)-H(15A)	126.0
C(14A)-C(15A)-H(15A)	126.0
C(16A)-N(2A)-C(15A)	115.05(17)
C(16A)-N(2A)-C(13A)	132.42(18)

C(15A)-N(2A)-C(13A)	108.0
N(2A)-C(13A)-N(1A)	108.0
N(2A)-C(13A)-Mn(1A)	105.86(10)
N(1A)-C(13A)-Mn(1A)	141.39(11)
C(16A)-N(3A)-C(20A)	120.0
C(16A)-N(3A)-Mn(1A)	117.82(7)
C(20A)-N(3A)-Mn(1A)	122.04(7)
N(2A)-C(16A)-N(3A)	103.95(15)
N(2A)-C(16A)-C(17A)	132.11(15)
N(3A)-C(16A)-C(17A)	120.0
C(18A)-C(17A)-C(16A)	120.0
C(18A)-C(17A)-H(17A)	120.0
C(16A)-C(17A)-H(17A)	120.0
C(19A)-C(18A)-C(17A)	120.0
C(19A)-C(18A)-H(18A)	120.0
C(17A)-C(18A)-H(18A)	120.0
C(18A)-C(19A)-C(20A)	120.0
C(18A)-C(19A)-H(19A)	120.0
C(20A)-C(19A)-H(19A)	120.0
N(4A)-C(20A)-C(19A)	133.05(12)
N(4A)-C(20A)-N(3A)	105.31(12)
C(19A)-C(20A)-N(3A)	120.0
N(1A)-C(1A)-C(2A)	113.39(12)
N(1A)-C(1A)-C(6A)	126.28(12)
C(2A)-C(1A)-C(6A)	120.0
C(3A)-C(2A)-C(1A)	120.0
C(3A)-C(2A)-C(10A)	114.8(2)
C(1A)-C(2A)-C(10A)	125.1(2)
C(2A)-C(3A)-C(5A)	120.0
C(2A)-C(3A)-H(3A)	120.0
C(5A)-C(3A)-H(3A)	120.0
C(4A)-C(5A)-C(3A)	120.0
C(4A)-C(5A)-H(5A)	120.0
C(3A)-C(5A)-H(5A)	120.0
C(5A)-C(4A)-C(6A)	120.0

C(5A)-C(4A)-H(4A)	120.0
C(6A)-C(4A)-H(4A)	120.0
C(4A)-C(6A)-C(1A)	120.0
C(4A)-C(6A)-C(7A)	117.93(19)
C(1A)-C(6A)-C(7A)	121.94(19)
C(20A)-N(4A)-C(22A)	123.38(12)
C(20A)-N(4A)-C(21A)	127.53(12)
C(22A)-N(4A)-C(21A)	108.0
C(23A)-C(22A)-N(4A)	108.0
C(23A)-C(22A)-H(22A)	126.0
N(4A)-C(22A)-H(22A)	126.0
N(5A)-C(23A)-C(22A)	108.0
N(5A)-C(23A)-H(23A)	126.0
C(22A)-C(23A)-H(23A)	126.0
C(24A)-N(5A)-C(23A)	126.63(19)
C(24A)-N(5A)-C(21A)	124.42(19)
C(23A)-N(5A)-C(21A)	108.0
N(5A)-C(21A)-N(4A)	108.0
N(5A)-C(21A)-Mn(1A)	140.44(10)
N(4A)-C(21A)-Mn(1A)	110.42(10)
N(5A)-C(24A)-C(25A)	127.52(13)
N(5A)-C(24A)-C(29A)	112.46(13)
C(25A)-C(24A)-C(29A)	120.0
C(26A)-C(25A)-C(24A)	120.0
C(26A)-C(25A)-C(30A)	116.90(19)
C(24A)-C(25A)-C(30A)	123.10(19)
C(25A)-C(26A)-C(27A)	120.0
C(25A)-C(26A)-H(26A)	120.0
C(27A)-C(26A)-H(26A)	120.0
C(26A)-C(27A)-C(28A)	120.0
C(26A)-C(27A)-H(27A)	120.0
C(28A)-C(27A)-H(27A)	120.0
C(29A)-C(28A)-C(27A)	120.0
C(29A)-C(28A)-H(28A)	120.0
C(27A)-C(28A)-H(28A)	120.0

C(28A)-C(29A)-C(24A)	120.0
C(28A)-C(29A)-C(33A)	117.90(5)
C(24A)-C(29A)-C(33A)	122.03(5)
C(8A)-C(7A)-C(6A)	113.2(4)
C(8A)-C(7A)-C(9A)	116.4(4)
C(6A)-C(7A)-C(9A)	108.2(3)
C(8A)-C(7A)-H(7A)	106.1
C(6A)-C(7A)-H(7A)	106.1
C(9A)-C(7A)-H(7A)	106.1
C(12A)-C(10A)-C(2A)	118.0(4)
C(12A)-C(10A)-C(11A)	109.2(4)
C(2A)-C(10A)-C(11A)	111.4(3)
C(12A)-C(10A)-H(10A)	105.8
C(2A)-C(10A)-H(10A)	105.8
C(11A)-C(10A)-H(10A)	105.8
C(25A)-C(30A)-C(31A)	124.6(4)
C(25A)-C(30A)-C(32A)	111.9(3)
C(31A)-C(30A)-C(32A)	103.3(4)
C(25A)-C(30A)-H(30A)	105.1
C(31A)-C(30A)-H(30A)	105.1
C(32A)-C(30A)-H(30A)	105.1
C(35A)-C(33A)-C(34A)	108.42(11)
C(35A)-C(33A)-C(29A)	110.34(8)
C(34A)-C(33A)-C(29A)	109.69(6)
C(35A)-C(33A)-H(33A)	109.5
C(34A)-C(33A)-H(33A)	109.5
C(29A)-C(33A)-H(33A)	109.5
C(21B)-Mn(1B)-N(3B)	68.56(6)
C(21B)-Mn(1B)-C(13B)	129.95(7)
N(3B)-Mn(1B)-C(13B)	63.85(6)
C(21B)-Mn(1B)-Br(1B)	105.11(6)
N(3B)-Mn(1B)-Br(1B)	158.65(5)
C(13B)-Mn(1B)-Br(1B)	113.40(6)
C(21B)-Mn(1B)-Br(2B)	98.34(7)
N(3B)-Mn(1B)-Br(2B)	88.20(5)

C(13B)-Mn(1B)-Br(2B)	94.84(7)
Br(1B)-Mn(1B)-Br(2B)	113.10(3)
C(13B)-N(1B)-C(14B)	108.0
C(13B)-N(1B)-C(1B)	131.94(12)
C(14B)-N(1B)-C(1B)	119.34(12)
C(15B)-C(14B)-N(1B)	108.0
C(15B)-C(14B)-H(14B)	126.0
N(1B)-C(14B)-H(14B)	126.0
N(2B)-C(15B)-C(14B)	108.0
N(2B)-C(15B)-H(15B)	126.0
C(14B)-C(15B)-H(15B)	126.0
C(16B)-N(2B)-C(15B)	137.55(19)
C(16B)-N(2B)-C(13B)	108.23(17)
C(15B)-N(2B)-C(13B)	108.0
N(2B)-C(13B)-N(1B)	108.0
N(2B)-C(13B)-Mn(1B)	123.34(9)
N(1B)-C(13B)-Mn(1B)	126.13(9)
C(16B)-N(3B)-C(20B)	120.0
C(16B)-N(3B)-Mn(1B)	118.96(7)
C(20B)-N(3B)-Mn(1B)	118.94(7)
N(2B)-C(16B)-N(3B)	115.98(16)
N(2B)-C(16B)-C(17B)	120.33(15)
N(3B)-C(16B)-C(17B)	120.0
C(16B)-C(17B)-C(18B)	120.0
C(16B)-C(17B)-H(17B)	120.0
C(18B)-C(17B)-H(17B)	120.0
C(17B)-C(18B)-C(19B)	120.0
C(17B)-C(18B)-H(18B)	120.0
C(19B)-C(18B)-H(18B)	120.0
C(20B)-C(19B)-C(18B)	120.0
C(20B)-C(19B)-H(19B)	120.0
C(18B)-C(19B)-H(19B)	120.0
N(4B)-C(20B)-C(19B)	122.96(13)
N(4B)-C(20B)-N(3B)	115.43(13)
C(19B)-C(20B)-N(3B)	120.0

C(2B)-C(1B)-C(6B)	120.0
C(2B)-C(1B)-N(1B)	126.56(12)
C(6B)-C(1B)-N(1B)	113.35(12)
C(1B)-C(2B)-C(3B)	120.0
C(1B)-C(2B)-C(10B)	119.0(2)
C(3B)-C(2B)-C(10B)	121.0(2)
C(2B)-C(3B)-C(4B)	120.0
C(2B)-C(3B)-H(3B)	120.0
C(4B)-C(3B)-H(3B)	120.0
C(5B)-C(4B)-C(3B)	120.0
C(5B)-C(4B)-H(4B)	120.0
C(3B)-C(4B)-H(4B)	120.0
C(6B)-C(5B)-C(4B)	120.0
C(6B)-C(5B)-H(5B)	120.0
C(4B)-C(5B)-H(5B)	120.0
C(5B)-C(6B)-C(1B)	120.0
C(5B)-C(6B)-C(7B)	118.5(2)
C(1B)-C(6B)-C(7B)	121.5(2)
C(20B)-N(4B)-C(22B)	132.98(13)
C(20B)-N(4B)-C(21B)	117.90(14)
C(22B)-N(4B)-C(21B)	108.0
C(23B)-C(22B)-N(4B)	108.0
C(23B)-C(22B)-H(22B)	126.0
N(4B)-C(22B)-H(22B)	126.0
N(5B)-C(23B)-C(22B)	108.0
N(5B)-C(23B)-H(23B)	126.0
C(22B)-C(23B)-H(23B)	126.0
C(24B)-N(5B)-C(23B)	125.8(2)
C(24B)-N(5B)-C(21B)	126.1(2)
C(23B)-N(5B)-C(21B)	108.0
N(5B)-C(21B)-N(4B)	108.0
N(5B)-C(21B)-Mn(1B)	134.70(11)
N(4B)-C(21B)-Mn(1B)	116.72(11)
C(9B)-C(7B)-C(6B)	113.6(4)
C(9B)-C(7B)-C(8B)	107.0(4)

C(6B)-C(7B)-C(8B)	108.3(3)
C(9B)-C(7B)-H(7B)	109.3
C(6B)-C(7B)-H(7B)	109.3
C(8B)-C(7B)-H(7B)	109.3
N(5B)-C(24B)-C(25B)	112.04(14)
N(5B)-C(24B)-C(29B)	127.60(14)
C(25B)-C(24B)-C(29B)	120.0
C(26B)-C(25B)-C(24B)	120.0
C(26B)-C(25B)-C(30B)	119.54(18)
C(24B)-C(25B)-C(30B)	120.42(18)
C(27B)-C(26B)-C(25B)	120.0
C(27B)-C(26B)-H(26B)	120.0
C(25B)-C(26B)-H(26B)	120.0
C(28B)-C(27B)-C(26B)	120.0
C(28B)-C(27B)-H(27B)	120.0
C(26B)-C(27B)-H(27B)	120.0
C(27B)-C(28B)-C(29B)	120.0
C(27B)-C(28B)-H(28B)	120.0
C(29B)-C(28B)-H(28B)	120.0
C(28B)-C(29B)-C(24B)	120.0
C(28B)-C(29B)-C(33B)	121.82(8)
C(24B)-C(29B)-C(33B)	117.90(8)
C(11B)-C(10B)-C(12B)	115.0(4)
C(11B)-C(10B)-C(2B)	109.5(3)
C(12B)-C(10B)-C(2B)	104.4(3)
C(11B)-C(10B)-H(10B)	109.3
C(12B)-C(10B)-H(10B)	109.3
C(2B)-C(10B)-H(10B)	109.3
C(32B)-C(30B)-C(31B)	119.0(4)
C(32B)-C(30B)-C(25B)	110.3(4)
C(31B)-C(30B)-C(25B)	101.2(3)
C(32B)-C(30B)-H(30B)	108.6
C(31B)-C(30B)-H(30B)	108.6
C(25B)-C(30B)-H(30B)	108.6
C(34B)-C(33B)-C(35B)	118.8(3)

C(34B)-C(33B)-C(29B)	121.4(2)
C(35B)-C(33B)-C(29B)	115.7(2)
C(34B)-C(33B)-H(33B)	96.8
C(35B)-C(33B)-H(33B)	96.8
C(29B)-C(33B)-H(33B)	96.8

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\approx^2$x 10^3)for 3. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1A)	62(2)	39(1)	79(2)	16(1)	-3(1)	5(1)
C(41A)	62(1)	60(1)	82(1)	9(1)	9(1)	-9(1)
C(40A)	62(1)	60(1)	82(1)	9(1)	9(1)	-9(1)
C(43A)	62(1)	60(1)	82(1)	9(1)	9(1)	-9(1)
C(42A)	62(1)	60(1)	82(1)	9(1)	9(1)	-9(1)
O(1B)	62(2)	39(1)	79(2)	16(1)	-3(1)	5(1)
C(41B)	62(1)	60(1)	82(1)	9(1)	9(1)	-9(1)
C(40B)	62(1)	60(1)	82(1)	9(1)	9(1)	-9(1)
C(43B)	62(1)	60(1)	82(1)	9(1)	9(1)	-9(1)
C(42B)	62(1)	60(1)	82(1)	9(1)	9(1)	-9(1)
Mn(1A)	24(1)	22(1)	14(1)	-1(1)	0(1)	-1(1)
Br(1A)	32(1)	32(1)	23(1)	0(1)	-3(1)	0(1)
Br(2A)	32(1)	32(1)	23(1)	0(1)	-3(1)	0(1)
N(1A)	44(1)	9(1)	23(1)	-4(1)	-12(1)	10(1)
C(14A)	54(1)	13(1)	24(1)	-4(1)	-14(1)	7(1)
C(15A)	54(1)	13(1)	24(1)	-4(1)	-14(1)	7(1)
N(2A)	44(1)	9(1)	23(1)	-4(1)	-12(1)	10(1)
C(13A)	35(1)	22(1)	23(1)	-9(1)	-12(1)	18(1)
N(3A)	44(1)	9(1)	23(1)	-4(1)	-12(1)	10(1)
C(16A)	38(1)	18(1)	28(1)	2(1)	-2(1)	9(1)
C(17A)	38(1)	18(1)	28(1)	2(1)	-2(1)	9(1)
C(18A)	38(1)	18(1)	28(1)	2(1)	-2(1)	9(1)
C(19A)	38(1)	18(1)	28(1)	2(1)	-2(1)	9(1)
C(20A)	38(1)	18(1)	28(1)	2(1)	-2(1)	9(1)
C(1A)	23(1)	22(1)	15(1)	-2(1)	2(1)	-2(1)
C(2A)	23(1)	22(1)	15(1)	-2(1)	2(1)	-2(1)
C(3A)	19(2)	12(2)	23(2)	-7(2)	11(1)	-7(1)
C(5A)	28(2)	22(2)	12(2)	4(2)	2(2)	-14(2)
C(4A)	30(2)	21(2)	25(2)	-3(2)	-4(2)	3(2)
C(6A)	23(1)	22(1)	15(1)	-2(1)	2(1)	-2(1)

N(4A)	44(1)	9(1)	23(1)	-4(1)	-12(1)	10(1)
C(22A)	54(1)	13(1)	24(1)	-4(1)	-14(1)	7(1)
C(23A)	54(1)	13(1)	24(1)	-4(1)	-14(1)	7(1)
N(5A)	44(1)	9(1)	23(1)	-4(1)	-12(1)	10(1)
C(21A)	35(1)	22(1)	23(1)	-9(1)	-12(1)	18(1)
C(24A)	41(2)	44(2)	14(2)	2(2)	-13(2)	-9(2)
C(25A)	24(2)	44(2)	34(2)	-4(2)	-11(2)	0(2)
C(26A)	52(2)	47(2)	28(2)	-2(2)	-15(2)	-23(2)
C(27A)	43(2)	60(2)	14(2)	-16(2)	-2(2)	-33(2)
C(28A)	36(2)	79(3)	30(2)	-11(2)	3(2)	-14(2)
C(29A)	38(2)	61(3)	20(2)	-2(2)	-1(2)	-2(2)
C(7A)	45(1)	48(1)	23(1)	-1(1)	2(1)	19(1)
C(11A)	37(1)	36(1)	23(1)	2(1)	8(1)	1(1)
C(12A)	37(1)	36(1)	23(1)	2(1)	8(1)	1(1)
C(10A)	45(1)	48(1)	23(1)	-1(1)	2(1)	19(1)
C(9A)	37(1)	36(1)	23(1)	2(1)	8(1)	1(1)
C(8A)	37(1)	36(1)	23(1)	2(1)	8(1)	1(1)
C(30A)	39(2)	33(2)	36(2)	4(2)	-4(2)	-17(2)
C(31A)	39(2)	52(3)	33(2)	-8(2)	-14(2)	-19(2)
C(32A)	49(3)	43(3)	46(3)	22(2)	-27(2)	-3(2)
C(33A)	45(1)	48(1)	23(1)	-1(1)	2(1)	19(1)
C(34A)	89(1)	88(1)	88(1)	0(1)	5(1)	0(1)
C(35A)	89(1)	88(1)	88(1)	0(1)	5(1)	0(1)
Mn(1B)	24(1)	22(1)	14(1)	-1(1)	0(1)	-1(1)
Br(1B)	32(1)	32(1)	23(1)	0(1)	-3(1)	0(1)
Br(2B)	32(1)	32(1)	23(1)	0(1)	-3(1)	0(1)
N(1B)	44(1)	9(1)	23(1)	-4(1)	-12(1)	10(1)
C(14B)	54(1)	13(1)	24(1)	-4(1)	-14(1)	7(1)
C(15B)	54(1)	13(1)	24(1)	-4(1)	-14(1)	7(1)
N(2B)	44(1)	9(1)	23(1)	-4(1)	-12(1)	10(1)
C(13B)	35(1)	22(1)	23(1)	-9(1)	-12(1)	18(1)
N(3B)	44(1)	9(1)	23(1)	-4(1)	-12(1)	10(1)
C(16B)	38(1)	18(1)	28(1)	2(1)	-2(1)	9(1)
C(17B)	38(1)	18(1)	28(1)	2(1)	-2(1)	9(1)
C(18B)	38(1)	18(1)	28(1)	2(1)	-2(1)	9(1)

C(19B)	38(1)	18(1)	28(1)	2(1)	-2(1)	9(1)
C(20B)	38(1)	18(1)	28(1)	2(1)	-2(1)	9(1)
C(1B)	23(1)	22(1)	15(1)	-2(1)	2(1)	-2(1)
C(2B)	23(1)	22(1)	15(1)	-2(1)	2(1)	-2(1)
C(3B)	26(2)	31(2)	12(2)	7(2)	9(2)	-10(2)
C(4B)	34(2)	30(2)	22(2)	5(2)	8(2)	-11(2)
C(5B)	25(2)	33(2)	12(2)	12(2)	1(2)	-10(2)
C(6B)	23(1)	22(1)	15(1)	-2(1)	2(1)	-2(1)
N(4B)	44(1)	9(1)	23(1)	-4(1)	-12(1)	10(1)
C(22B)	54(1)	13(1)	24(1)	-4(1)	-14(1)	7(1)
C(23B)	54(1)	13(1)	24(1)	-4(1)	-14(1)	7(1)
N(5B)	44(1)	9(1)	23(1)	-4(1)	-12(1)	10(1)
C(21B)	35(1)	22(1)	23(1)	-9(1)	-12(1)	18(1)
C(7B)	45(1)	48(1)	23(1)	-1(1)	2(1)	19(1)
C(11B)	37(1)	36(1)	23(1)	2(1)	8(1)	1(1)
C(24B)	14(2)	39(2)	27(2)	-4(2)	4(2)	-4(2)
C(25B)	35(2)	30(2)	33(2)	-11(2)	-7(2)	-14(2)
C(26B)	35(2)	44(2)	36(2)	-16(2)	-13(2)	-19(2)
C(27B)	42(2)	46(2)	30(2)	-27(2)	-11(2)	-15(2)
C(28B)	40(2)	55(3)	29(2)	-26(2)	6(2)	7(2)
C(29B)	30(2)	68(3)	21(2)	-13(2)	-3(2)	22(2)
C(12B)	37(1)	36(1)	23(1)	2(1)	8(1)	1(1)
C(10B)	45(1)	48(1)	23(1)	-1(1)	2(1)	19(1)
C(9B)	37(1)	36(1)	23(1)	2(1)	8(1)	1(1)
C(8B)	37(1)	36(1)	23(1)	2(1)	8(1)	1(1)
C(30B)	21(2)	37(2)	41(2)	-6(2)	6(2)	12(2)
C(31B)	56(3)	14(2)	54(3)	-10(2)	-15(3)	-7(2)
C(32B)	63(3)	20(2)	47(3)	8(2)	-6(3)	21(2)
C(33B)	45(1)	48(1)	23(1)	-1(1)	2(1)	19(1)
C(34B)	89(1)	88(1)	88(1)	0(1)	5(1)	0(1)
C(35B)	89(1)	88(1)	88(1)	0(1)	5(1)	0(1)

Electronic Supplementary Information for Dalton Transactions

Structural Data for 4

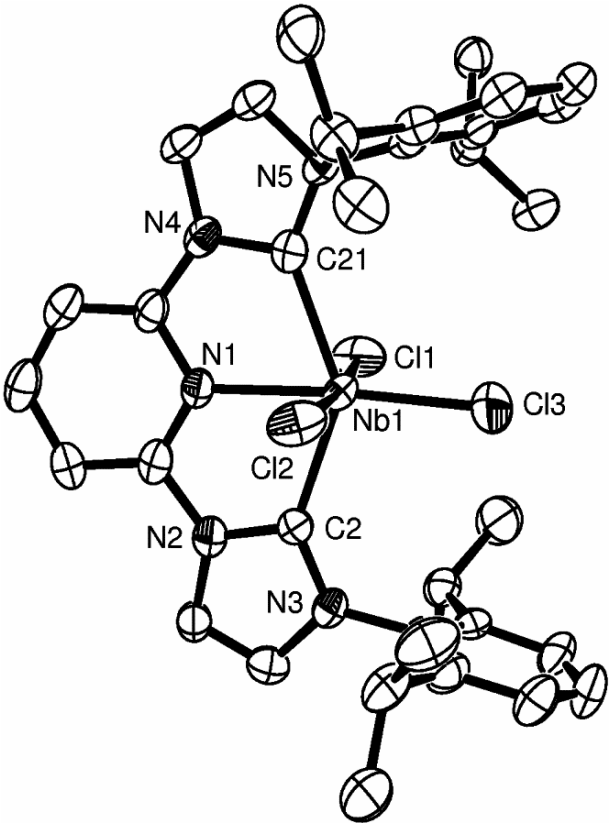

Table 9. Crystal data and structure refinement for **4**.

Identification code	4	
Empirical formula	C39 H49 Cl3 N5 Nb O	
Formula weight	803.09	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 10.803(7) Å	α= 90∞.
	b = 18.707(11) Å	β= 92.61(6)∞.
	c = 18.838(17) Å	γ = 90∞.
Volume	3803(5) Å^3	
Z	4	
Density (calculated)	1.403 Mg/m^3	
Absorption coefficient	0.565 mm^{-1}	
F(000)	1672	
Crystal size	0.06 x 0.04 x 0.01 mm^3	
Theta range for data collection	3.77 to 27.56∞.	
Index ranges	-13<=h<=14, -23<=k<=24, -24<=l<=18	
Reflections collected	26634	
Independent reflections	8730 [R(int) = 0.1325]	
Completeness to theta = 27.56∞	99.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9944 and 0.6249	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8730 / 8 / 460	
Goodness-of-fit on F^2	1.012	
Final R indices [I>2sigma(I)]	R1 = 0.0902, wR2 = 0.1446	
R indices (all data)	R1 = 0.1973, wR2 = 0.1774	
Largest diff. peak and hole	1.069 and -0.512 e.≈$^{-3}$	

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

	x	y	z	U(eq)
C(1)	4103(5)	1845(3)	-613(4)	33(2)
C(2)	2707(5)	2503(3)	75(3)	27(1)
C(3)	1594(6)	3075(3)	-796(4)	38(2)
C(4)	2439(6)	2688(3)	-1114(4)	35(2)
C(5)	1022(5)	3315(3)	459(3)	33(2)
C(6)	-102(5)	2993(3)	619(3)	38(2)
C(7)	-833(7)	3366(4)	1090(4)	53(2)
C(8)	-447(7)	4006(4)	1375(4)	62(2)
C(9)	666(7)	4298(3)	1203(4)	53(2)
C(10)	1428(6)	3970(3)	725(4)	43(2)
C(11)	2624(6)	4325(3)	529(4)	47(2)
C(12)	3419(7)	4515(4)	1189(5)	62(2)
C(13)	2348(7)	4990(3)	73(4)	57(2)
C(14)	-558(6)	2300(3)	302(4)	40(2)
C(15)	-990(7)	1780(4)	860(5)	65(2)
C(16)	-1604(7)	2454(4)	-241(4)	59(2)
C(17)	4630(6)	1661(3)	-1245(4)	39(2)
C(18)	5575(6)	1156(3)	-1192(4)	45(2)
C(19)	5931(6)	858(3)	-551(4)	41(2)
C(20)	5342(5)	1087(3)	43(4)	34(2)
C(21)	4999(5)	1156(3)	1275(4)	31(2)
C(22)	6347(5)	307(3)	1674(4)	36(2)
C(23)	6425(5)	320(3)	979(4)	36(2)
C(24)	5302(5)	1013(3)	2595(3)	32(2)
C(25)	4281(5)	743(3)	2946(4)	34(2)
C(26)	4205(6)	908(3)	3654(4)	40(2)
C(27)	5070(6)	1329(3)	4006(4)	39(2)
C(28)	6064(6)	1596(3)	3643(4)	38(2)
C(29)	6197(5)	1448(3)	2930(4)	33(2)
C(30)	7298(6)	1740(3)	2549(4)	41(2)

C(31)	7407(6)	2551(3)	2651(4)	50(2)
C(32)	8498(6)	1364(4)	2819(4)	52(2)
C(33)	3312(5)	259(3)	2590(4)	33(2)
C(34)	3459(6)	-498(3)	2884(4)	39(2)
C(35)	1991(5)	536(3)	2691(4)	42(2)
C(36A)	1040(20)	4040(20)	3054(14)	47(4)
C(37A)	-18(9)	3661(4)	3390(6)	98(4)
C(38A)	-535(7)	4229(4)	3849(5)	70(3)
C(39A)	645(14)	4501(11)	4182(13)	62(4)
C(36B)	1246(12)	3894(8)	3207(9)	47(4)
C(37B)	-18(9)	3661(4)	3390(6)	98(4)
C(38B)	-535(7)	4229(4)	3849(5)	70(3)
C(39B)	358(10)	4862(6)	3718(7)	62(4)
Cl(1)	2114(1)	966(1)	822(1)	53(1)
Cl(2)	5260(2)	2905(1)	1087(1)	49(1)
Cl(3)	2635(2)	2458(1)	2000(1)	81(1)
N(1)	4454(4)	1592(2)	23(3)	30(1)
N(2)	3126(4)	2340(2)	-580(3)	31(1)
N(3)	1759(4)	2965(2)	-70(3)	31(1)
N(4)	5596(4)	844(2)	725(3)	33(1)
N(5)	5478(4)	821(2)	1865(3)	31(1)
Nb(1)	3608(1)	1989(1)	1018(1)	33(1)
O(1A)	1608(12)	4171(7)	3771(10)	66(2)
O(1B)	1064(7)	4653(4)	3113(5)	66(2)

Table 11. Bond lengths [Å] and angles [∞] for 04neo008.

C(1)-N(1)	1.329(8)
C(1)-C(17)	1.386(8)
C(1)-N(2)	1.406(7)
C(2)-N(3)	1.359(7)
C(2)-N(2)	1.370(7)
C(2)-Nb(1)	2.206(6)
C(3)-C(4)	1.329(8)
C(3)-N(3)	1.387(8)
C(3)-H(3)	0.9500
C(4)-N(2)	1.386(8)
C(4)-H(4)	0.9500
C(5)-C(10)	1.387(8)
C(5)-C(6)	1.401(8)
C(5)-N(3)	1.458(7)
C(6)-C(7)	1.401(8)
C(6)-C(14)	1.501(9)
C(7)-C(8)	1.370(10)
C(7)-H(7)	0.9500
C(8)-C(9)	1.372(10)
C(8)-H(8)	0.9500
C(9)-C(10)	1.390(9)
C(9)-H(9)	0.9500
C(10)-C(11)	1.514(9)
C(11)-C(12)	1.520(11)
C(11)-C(13)	1.532(10)
C(11)-H(11)	1.0000
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-C(16)	1.516(10)

C(14)-C(15)	1.521(9)
C(14)-H(14)	1.0000
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)	1.391(9)
C(17)-H(17)	0.9500
C(18)-C(19)	1.369(10)
C(18)-H(18)	0.9500
C(19)-C(20)	1.381(8)
C(19)-H(19)	0.9500
C(20)-N(1)	1.345(7)
C(20)-N(4)	1.378(8)
C(21)-N(5)	1.358(8)
C(21)-N(4)	1.376(7)
C(21)-Nb(1)	2.203(6)
C(22)-C(23)	1.316(9)
C(22)-N(5)	1.402(7)
C(22)-H(22)	0.9500
C(23)-N(4)	1.398(7)
C(23)-H(23)	0.9500
C(24)-C(29)	1.394(8)
C(24)-C(25)	1.406(8)
C(24)-N(5)	1.442(8)
C(25)-C(26)	1.375(9)
C(25)-C(33)	1.517(9)
C(26)-C(27)	1.370(9)
C(26)-H(26)	0.9500
C(27)-C(28)	1.392(8)
C(27)-H(27)	0.9500
C(28)-C(29)	1.384(9)
C(28)-H(28)	0.9500

C(29)-C(30)	1.518(8)
C(30)-C(31)	1.535(8)
C(30)-C(32)	1.541(9)
C(30)-H(30)	1.0000
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-C(34)	1.527(8)
C(33)-C(35)	1.539(8)
C(33)-H(33)	1.0000
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(36A)-O(1A)	1.48(2)
C(36A)-C(37A)	1.508(19)
C(36A)-H(36A)	0.9900
C(36A)-H(36B)	0.9900
C(37A)-C(38A)	1.493(11)
C(37A)-H(37A)	0.9900
C(37A)-H(37B)	0.9900
C(38A)-C(39A)	1.485(15)
C(38A)-H(38A)	0.9900
C(38A)-H(38B)	0.9900
C(39A)-O(1A)	1.462(16)
C(39A)-H(39A)	0.9900
C(39A)-H(39B)	0.9900
C(36B)-O(1B)	1.444(15)
C(36B)-H(36C)	0.9900
C(36B)-H(36D)	0.9900

C(39B)-O(1B)	1.454(11)
C(39B)-H(39C)	0.9900
C(39B)-H(39D)	0.9900
Cl(1)-Nb(1)	2.520(2)
Cl(2)-Nb(1)	2.473(2)
Cl(3)-Nb(1)	2.341(3)
N(1)-Nb(1)	2.248(5)

N(1)-C(1)-C(17)	125.1(6)
N(1)-C(1)-N(2)	112.2(5)
C(17)-C(1)-N(2)	122.7(6)
N(3)-C(2)-N(2)	103.8(5)
N(3)-C(2)-Nb(1)	137.8(4)
N(2)-C(2)-Nb(1)	118.4(4)
C(4)-C(3)-N(3)	107.8(6)
C(4)-C(3)-H(3)	126.1
N(3)-C(3)-H(3)	126.1
C(3)-C(4)-N(2)	106.5(6)
C(3)-C(4)-H(4)	126.7
N(2)-C(4)-H(4)	126.7
C(10)-C(5)-C(6)	124.4(6)
C(10)-C(5)-N(3)	118.0(5)
C(6)-C(5)-N(3)	117.4(5)
C(5)-C(6)-C(7)	116.2(6)
C(5)-C(6)-C(14)	123.9(5)
C(7)-C(6)-C(14)	119.9(6)
C(8)-C(7)-C(6)	120.8(7)
C(8)-C(7)-H(7)	119.6
C(6)-C(7)-H(7)	119.6
C(7)-C(8)-C(9)	120.7(6)
C(7)-C(8)-H(8)	119.7
C(9)-C(8)-H(8)	119.7
C(8)-C(9)-C(10)	121.9(7)
C(8)-C(9)-H(9)	119.1
C(10)-C(9)-H(9)	119.1

C(5)-C(10)-C(9)	116.0(6)
C(5)-C(10)-C(11)	124.0(6)
C(9)-C(10)-C(11)	120.0(6)
C(10)-C(11)-C(12)	111.1(6)
C(10)-C(11)-C(13)	110.3(6)
C(12)-C(11)-C(13)	110.9(6)
C(10)-C(11)-H(11)	108.1
C(12)-C(11)-H(11)	108.1
C(13)-C(11)-H(11)	108.1
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(11)-C(13)-H(13A)	109.5
C(11)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(11)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(6)-C(14)-C(16)	109.0(5)
C(6)-C(14)-C(15)	112.4(6)
C(16)-C(14)-C(15)	110.2(6)
C(6)-C(14)-H(14)	108.4
C(16)-C(14)-H(14)	108.4
C(15)-C(14)-H(14)	108.4
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(1)-C(17)-C(18)	115.9(7)
C(1)-C(17)-H(17)	122.1
C(18)-C(17)-H(17)	122.1
C(19)-C(18)-C(17)	121.0(6)
C(19)-C(18)-H(18)	119.5
C(17)-C(18)-H(18)	119.5
C(18)-C(19)-C(20)	117.9(6)
C(18)-C(19)-H(19)	121.1
C(20)-C(19)-H(19)	121.1
N(1)-C(20)-N(4)	111.7(5)
N(1)-C(20)-C(19)	123.3(7)
N(4)-C(20)-C(19)	125.0(6)
N(5)-C(21)-N(4)	104.3(5)
N(5)-C(21)-Nb(1)	137.5(4)
N(4)-C(21)-Nb(1)	118.2(5)
C(23)-C(22)-N(5)	108.5(6)
C(23)-C(22)-H(22)	125.8
N(5)-C(22)-H(22)	125.8
C(22)-C(23)-N(4)	106.5(5)
C(22)-C(23)-H(23)	126.7
N(4)-C(23)-H(23)	126.7
C(29)-C(24)-C(25)	122.6(6)
C(29)-C(24)-N(5)	117.4(5)
C(25)-C(24)-N(5)	120.0(6)
C(26)-C(25)-C(24)	117.3(6)
C(26)-C(25)-C(33)	119.6(5)
C(24)-C(25)-C(33)	123.1(6)
C(27)-C(26)-C(25)	122.0(6)
C(27)-C(26)-H(26)	119.0
C(25)-C(26)-H(26)	119.0
C(26)-C(27)-C(28)	119.5(7)

C(26)-C(27)-H(27)	120.2
C(28)-C(27)-H(27)	120.2
C(29)-C(28)-C(27)	121.5(6)
C(29)-C(28)-H(28)	119.3
C(27)-C(28)-H(28)	119.3
C(28)-C(29)-C(24)	117.1(5)
C(28)-C(29)-C(30)	120.4(6)
C(24)-C(29)-C(30)	122.5(6)
C(29)-C(30)-C(31)	110.7(5)
C(29)-C(30)-C(32)	110.2(5)
C(31)-C(30)-C(32)	110.6(6)
C(29)-C(30)-H(30)	108.4
C(31)-C(30)-H(30)	108.4
C(32)-C(30)-H(30)	108.4
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(30)-C(32)-H(32A)	109.5
C(30)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(30)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(25)-C(33)-C(34)	109.6(5)
C(25)-C(33)-C(35)	111.7(5)
C(34)-C(33)-C(35)	110.4(5)
C(25)-C(33)-H(33)	108.4
C(34)-C(33)-H(33)	108.4
C(35)-C(33)-H(33)	108.4
C(33)-C(34)-H(34A)	109.5
C(33)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5

C(33)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(33)-C(35)-H(35A)	109.5
C(33)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(33)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
O(1A)-C(36A)-C(37A)	89.2(14)
O(1A)-C(36A)-H(36A)	113.8
C(37A)-C(36A)-H(36A)	113.8
O(1A)-C(36A)-H(36B)	113.8
C(37A)-C(36A)-H(36B)	113.8
H(36A)-C(36A)-H(36B)	111.0
C(38A)-C(37A)-C(36A)	102.8(16)
C(38A)-C(37A)-H(37A)	111.2
C(36A)-C(37A)-H(37A)	111.2
C(38A)-C(37A)-H(37B)	111.2
C(36A)-C(37A)-H(37B)	111.2
H(37A)-C(37A)-H(37B)	109.1
C(39A)-C(38A)-C(37A)	98.7(9)
C(39A)-C(38A)-H(38A)	112.0
C(37A)-C(38A)-H(38A)	112.0
C(39A)-C(38A)-H(38B)	112.0
C(37A)-C(38A)-H(38B)	112.0
H(38A)-C(38A)-H(38B)	109.7
O(1A)-C(39A)-C(38A)	104.4(13)
O(1A)-C(39A)-H(39A)	110.9
C(38A)-C(39A)-H(39A)	110.9
O(1A)-C(39A)-H(39B)	110.9
C(38A)-C(39A)-H(39B)	110.9
H(39A)-C(39A)-H(39B)	108.9
O(1B)-C(36B)-H(36C)	111.5
O(1B)-C(36B)-H(36D)	111.5

H(36C)-C(36B)-H(36D)	109.3
O(1B)-C(39B)-H(39C)	110.6
O(1B)-C(39B)-H(39D)	110.6
H(39C)-C(39B)-H(39D)	108.7
C(1)-N(1)-C(20)	116.7(5)
C(1)-N(1)-Nb(1)	121.6(4)
C(20)-N(1)-Nb(1)	121.7(5)
C(2)-N(2)-C(4)	111.2(5)
C(2)-N(2)-C(1)	117.8(5)
C(4)-N(2)-C(1)	131.0(5)
C(2)-N(3)-C(3)	110.7(5)
C(2)-N(3)-C(5)	125.3(5)
C(3)-N(3)-C(5)	124.0(5)
C(21)-N(4)-C(20)	118.8(5)
C(21)-N(4)-C(23)	110.7(6)
C(20)-N(4)-C(23)	130.4(5)
C(21)-N(5)-C(22)	110.0(5)
C(21)-N(5)-C(24)	127.1(5)
C(22)-N(5)-C(24)	122.3(6)
C(21)-Nb(1)-C(2)	139.2(2)
C(21)-Nb(1)-N(1)	69.5(2)
C(2)-Nb(1)-N(1)	69.8(2)
C(21)-Nb(1)-Cl(3)	114.66(18)
C(2)-Nb(1)-Cl(3)	105.98(16)
N(1)-Nb(1)-Cl(3)	175.79(15)
C(21)-Nb(1)-Cl(2)	89.73(15)
C(2)-Nb(1)-Cl(2)	91.79(15)
N(1)-Nb(1)-Cl(2)	87.35(13)
Cl(3)-Nb(1)-Cl(2)	92.73(9)
C(21)-Nb(1)-Cl(1)	85.47(15)
C(2)-Nb(1)-Cl(1)	87.54(15)
N(1)-Nb(1)-Cl(1)	84.75(13)
Cl(3)-Nb(1)-Cl(1)	95.30(9)
Cl(2)-Nb(1)-Cl(1)	171.81(6)
C(39A)-O(1A)-C(36A)	106.2(19)

C(36B)-O(1B)-C(39B)	104.0(10)

Symmetry transformations used to generate equivalent atoms:

Table 12. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **4**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	29(3)	29(3)	41(5)	-7(3)	9(3)	-8(3)
C(2)	24(3)	24(3)	34(4)	1(3)	2(3)	-5(2)
C(3)	40(4)	35(3)	37(5)	3(3)	-5(3)	-1(3)
C(4)	35(3)	39(3)	32(4)	-1(3)	5(3)	2(3)
C(5)	29(3)	34(3)	36(4)	-1(3)	0(3)	12(3)
C(6)	32(3)	44(4)	38(4)	11(3)	2(3)	17(3)
C(7)	45(4)	53(4)	64(6)	7(4)	24(4)	21(4)
C(8)	61(5)	69(5)	57(6)	-10(4)	23(5)	24(4)
C(9)	59(5)	38(4)	63(6)	-16(4)	8(4)	8(4)
C(10)	49(4)	36(4)	42(5)	-9(3)	-6(4)	12(3)
C(11)	39(4)	40(4)	60(6)	-14(4)	-3(4)	6(3)
C(12)	61(5)	39(4)	86(7)	-13(4)	-12(5)	2(4)
C(13)	59(5)	48(4)	64(6)	-10(4)	2(4)	4(4)
C(14)	33(3)	41(4)	47(5)	5(3)	9(3)	4(3)
C(15)	60(5)	56(5)	80(7)	14(4)	24(5)	0(4)
C(16)	46(4)	63(5)	68(6)	1(4)	0(4)	-4(4)
C(17)	42(4)	43(4)	31(4)	-2(3)	9(3)	-8(3)
C(18)	45(4)	38(4)	55(6)	-18(4)	17(4)	-2(3)
C(19)	30(3)	34(3)	59(6)	-6(4)	11(4)	1(3)
C(20)	30(3)	28(3)	45(5)	-1(3)	13(3)	-4(3)
C(21)	25(3)	31(3)	36(4)	-3(3)	3(3)	-8(3)
C(22)	26(3)	30(3)	53(5)	1(3)	2(3)	2(3)
C(23)	24(3)	29(3)	54(5)	2(3)	5(3)	3(3)
C(24)	29(3)	26(3)	39(5)	3(3)	1(3)	8(3)
C(25)	30(3)	25(3)	48(5)	5(3)	7(3)	10(3)
C(26)	29(3)	33(3)	57(5)	3(3)	1(4)	2(3)
C(27)	36(4)	40(4)	41(5)	-1(3)	4(3)	7(3)
C(28)	32(3)	33(3)	50(5)	-3(3)	0(3)	-2(3)
C(29)	28(3)	28(3)	43(5)	2(3)	-2(3)	-1(3)
C(30)	34(3)	50(4)	40(5)	1(3)	-5(3)	-11(3)

C(31)	46(4)	47(4)	55(5)	2(4)	-1(4)	-18(3)
C(32)	36(4)	65(5)	55(5)	1(4)	8(4)	-5(4)
C(33)	33(3)	26(3)	40(4)	4(3)	11(3)	0(3)
C(34)	41(4)	36(3)	41(5)	0(3)	8(3)	-1(3)
C(35)	30(3)	34(3)	64(5)	5(3)	3(3)	-2(3)
C(36A)	53(7)	35(9)	52(9)	7(6)	-10(6)	5(6)
C(37A)	100(7)	54(5)	142(10)	-19(6)	40(7)	-33(5)
C(38A)	63(5)	54(5)	93(8)	17(5)	17(5)	-6(4)
C(39A)	43(6)	51(7)	90(12)	-13(6)	-8(7)	5(5)
C(36B)	53(7)	35(9)	52(9)	7(6)	-10(6)	5(6)
C(37B)	100(7)	54(5)	142(10)	-19(6)	40(7)	-33(5)
C(38B)	63(5)	54(5)	93(8)	17(5)	17(5)	-6(4)
C(39B)	43(6)	51(7)	90(12)	-13(6)	-8(7)	5(5)
Cl(1)	29(1)	52(1)	77(2)	24(1)	-2(1)	-8(1)
Cl(2)	47(1)	29(1)	69(1)	-6(1)	-15(1)	-4(1)
Cl(3)	124(2)	70(1)	53(2)	11(1)	36(1)	40(1)
N(1)	29(3)	29(3)	33(4)	-3(2)	8(3)	-1(2)
N(2)	32(3)	27(2)	35(4)	-5(2)	6(3)	-5(2)
N(3)	28(3)	27(2)	37(4)	-6(3)	3(2)	-2(2)
N(4)	25(3)	26(3)	47(4)	0(3)	9(3)	-2(2)
N(5)	24(3)	27(3)	41(4)	-1(2)	5(3)	1(2)
Nb(1)	30(1)	32(1)	37(1)	-1(1)	5(1)	8(1)
O(1A)	52(4)	39(4)	108(7)	-1(4)	11(5)	-2(3)
O(1B)	52(4)	39(4)	108(7)	-1(4)	11(5)	-2(3)

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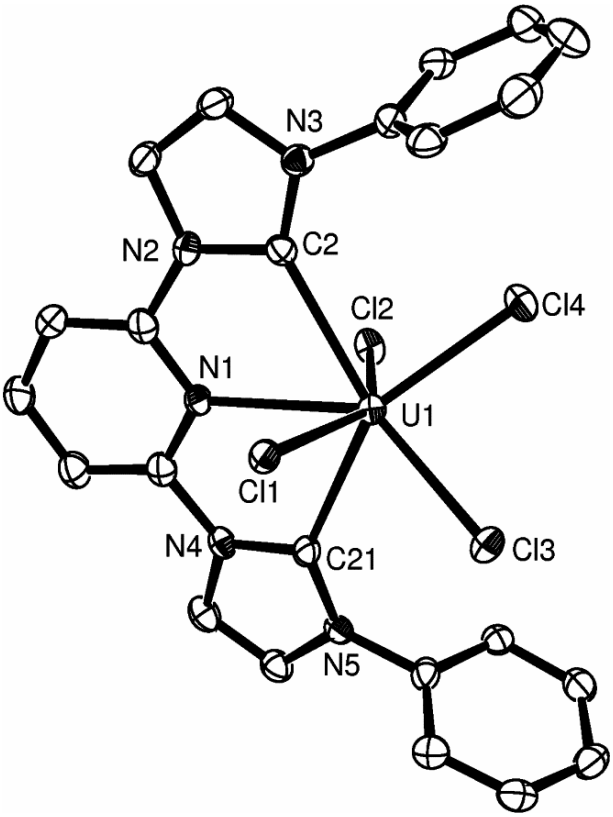
Structural Data for 5



Electronic Supplementary Information for Dalton Transactions

Table 1. Crystal data and structure refinement for **5**.

Identification code	**5**	
Empirical formula	C39 H49 Cl4 N5 O U	
Formula weight	983.66	
Temperature	120(2) K	
Wavelength	0.71073 ≈	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 10.7146(8) ≈	α= 90∞.
	b = 18.384(2) ≈	β= 93.628(10)∞.
	c = 20.229(4) ≈	γ = 90∞.
Volume	3976.7(9) ≈^{3}	
Z	4	
Density (calculated)	1.643 Mg/m^3	
Absorption coefficient	4.388 mm^{-1}	
F(000)	1944	
Crystal size	0.20 x 0.20 x 0.20 mm^3	
Theta range for data collection	3.05 to 26.15∞.	
Index ranges	-11<=h<=13, -22<=k<=22, -25<=l<=25	
Reflections collected	37286	
Independent reflections	7713 [R(int) = 0.0447]	
Completeness to theta = 26.15∞	97.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.4171 and 0.2835	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7713 / 0 / 459	
Goodness-of-fit on F^2	1.021	
Final R indices [I>2sigma(I)]	R1 = 0.0370, wR2 = 0.0715	
R indices (all data)	R1 = 0.0561, wR2 = 0.0771	
Largest diff. peak and hole	1.052 and -1.111 e.≈$^{-3}$	

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Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (≈^{2}x 10^3) for **5**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	9415(5)	1763(3)	5447(2)	21(1)
C(2)	7811(5)	2512(3)	4862(2)	18(1)
C(3)	6981(5)	3004(3)	5754(2)	24(1)
C(4)	7920(5)	2584(3)	5995(3)	24(1)
C(5)	5980(5)	3331(3)	4656(2)	23(1)
C(6)	6284(5)	3999(3)	4380(3)	26(1)
C(7)	5320(6)	4347(3)	3999(3)	36(2)
C(8)	4152(6)	4044(3)	3909(3)	38(2)
C(9)	3893(5)	3383(3)	4187(3)	34(1)
C(10)	4802(5)	3009(3)	4575(3)	26(1)
C(11)	4503(5)	2276(3)	4869(3)	30(1)
C(12)	3978(6)	1738(3)	4339(3)	40(2)
C(13)	3574(6)	2377(4)	5405(3)	45(2)
C(14)	7570(5)	4338(3)	4457(3)	31(1)
C(15)	7558(6)	5027(3)	4877(3)	42(2)
C(16)	8080(6)	4489(3)	3778(3)	42(2)
C(17)	9996(5)	1516(3)	6032(3)	24(1)
C(18)	10893(5)	987(3)	5988(3)	28(1)
C(19)	11202(5)	729(3)	5375(3)	26(1)
C(20)	10591(5)	1031(3)	4825(2)	20(1)
C(21)	10386(5)	1172(3)	3619(2)	20(1)
C(22)	11633(5)	234(3)	3354(3)	24(1)
C(23)	11633(5)	236(3)	4015(3)	24(1)
C(24)	10740(5)	985(3)	2415(2)	22(1)
C(25)	9683(5)	732(3)	2049(2)	21(1)
C(26)	9597(5)	907(3)	1376(3)	26(1)
C(27)	10494(5)	1312(3)	1092(3)	28(1)
C(28)	11524(5)	1558(3)	1474(3)	28(1)
C(29)	11679(5)	1396(3)	2146(3)	24(1)
C(30)	12834(5)	1662(3)	2548(3)	29(1)

C(31)	12949(6)	2488(3)	2528(3)	42(2)
C(32)	14021(5)	1308(4)	2311(3)	43(2)
C(33)	8677(5)	281(3)	2344(3)	25(1)
C(34)	8820(6)	-517(3)	2165(3)	32(1)
C(35)	7366(5)	567(3)	2139(3)	32(1)
C(36)	6262(6)	3646(3)	1808(3)	39(2)
C(37)	5349(6)	4090(3)	2161(3)	41(2)
C(38)	4471(7)	4325(5)	1593(4)	61(2)
C(39)	5337(6)	4414(4)	1024(3)	49(2)
Cl(1)	10359(1)	3077(1)	4251(1)	19(1)
Cl(2)	7449(1)	902(1)	3953(1)	21(1)
Cl(3)	9425(1)	2607(1)	2613(1)	26(1)
Cl(4)	6520(1)	2563(1)	3226(1)	28(1)
N(1)	9707(4)	1538(2)	4844(2)	17(1)
N(2)	8429(4)	2278(2)	5439(2)	18(1)
N(3)	6930(4)	2959(2)	5071(2)	20(1)
N(4)	10856(4)	812(2)	4174(2)	18(1)
N(5)	10885(4)	806(2)	3117(2)	19(1)
O(1)	6426(4)	3992(2)	1192(2)	42(1)
U(1)	8671(1)	2142(1)	3751(1)	18(1)

Table 3. Bond lengths [≈] and angles [∞] for **5**.

C(1)-N(1)	1.344(6)
C(1)-C(17)	1.380(7)
C(1)-N(2)	1.417(6)
C(2)-N(3)	1.340(6)
C(2)-N(2)	1.375(6)
C(2)-U(1)	2.573(5)
C(3)-C(4)	1.336(7)
C(3)-N(3)	1.382(6)
C(3)-H(3)	0.9500
C(4)-N(2)	1.398(6)
C(4)-H(4)	0.9500
C(5)-C(10)	1.395(7)
C(5)-C(6)	1.396(7)
C(5)-N(3)	1.448(6)
C(6)-C(7)	1.403(8)
C(6)-C(14)	1.512(8)
C(7)-C(8)	1.371(9)
C(7)-H(7)	0.9500
C(8)-C(9)	1.375(9)
C(8)-H(8)	0.9500
C(9)-C(10)	1.394(8)
C(9)-H(9)	0.9500
C(10)-C(11)	1.514(8)
C(11)-C(13)	1.529(8)
C(11)-C(12)	1.539(8)
C(11)-H(11)	1.0000
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-C(15)	1.527(8)

C(14)-C(16)	1.536(8)
C(14)-H(14)	1.0000
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)	1.374(7)
C(17)-H(17)	0.9500
C(18)-C(19)	1.388(7)
C(18)-H(18)	0.9500
C(19)-C(20)	1.372(7)
C(19)-H(19)	0.9500
C(20)-N(1)	1.331(6)
C(20)-N(4)	1.422(6)
C(21)-N(5)	1.356(6)
C(21)-N(4)	1.371(6)
C(21)-U(1)	2.587(5)
C(22)-C(23)	1.336(7)
C(22)-N(5)	1.390(6)
C(22)-H(22)	0.9500
C(23)-N(4)	1.397(6)
C(23)-H(23)	0.9500
C(24)-C(25)	1.395(7)
C(24)-C(29)	1.397(7)
C(24)-N(5)	1.455(6)
C(25)-C(26)	1.396(7)
C(25)-C(33)	1.512(7)
C(26)-C(27)	1.371(7)
C(26)-H(26)	0.9500
C(27)-C(28)	1.382(8)
C(27)-H(27)	0.9500
C(28)-C(29)	1.391(7)
C(28)-H(28)	0.9500

C(29)-C(30)	1.517(7)
C(30)-C(31)	1.524(8)
C(30)-C(32)	1.532(8)
C(30)-H(30)	1.0000
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-C(34)	1.521(7)
C(33)-C(35)	1.533(7)
C(33)-H(33)	1.0000
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(36)-O(1)	1.420(7)
C(36)-C(37)	1.492(8)
C(36)-H(36A)	0.9900
C(36)-H(36B)	0.9900
C(37)-C(38)	1.501(9)
C(37)-H(37A)	0.9900
C(37)-H(37B)	0.9900
C(38)-C(39)	1.533(10)
C(38)-H(38A)	0.9900
C(38)-H(38B)	0.9900
C(39)-O(1)	1.424(8)
C(39)-H(39A)	0.9900
C(39)-H(39B)	0.9900
Cl(1)-U(1)	2.6486(12)
Cl(2)-U(1)	2.6725(12)
Cl(3)-U(1)	2.6314(13)

Cl(4)-U(1)	2.5936(13)
N(1)-U(1)	2.653(4)

N(1)-C(1)-C(17)	124.0(5)
N(1)-C(1)-N(2)	114.4(4)
C(17)-C(1)-N(2)	121.7(5)
N(3)-C(2)-N(2)	103.6(4)
N(3)-C(2)-U(1)	137.4(3)
N(2)-C(2)-U(1)	118.6(3)
C(4)-C(3)-N(3)	108.1(4)
C(4)-C(3)-H(3)	126.0
N(3)-C(3)-H(3)	126.0
C(3)-C(4)-N(2)	105.2(4)
C(3)-C(4)-H(4)	127.4
N(2)-C(4)-H(4)	127.4
C(10)-C(5)-C(6)	124.0(5)
C(10)-C(5)-N(3)	117.7(5)
C(6)-C(5)-N(3)	118.3(5)
C(5)-C(6)-C(7)	116.0(5)
C(5)-C(6)-C(14)	123.7(5)
C(7)-C(6)-C(14)	120.2(5)
C(8)-C(7)-C(6)	121.5(6)
C(8)-C(7)-H(7)	119.2
C(6)-C(7)-H(7)	119.2
C(7)-C(8)-C(9)	120.7(6)
C(7)-C(8)-H(8)	119.7
C(9)-C(8)-H(8)	119.7
C(8)-C(9)-C(10)	121.0(6)
C(8)-C(9)-H(9)	119.5
C(10)-C(9)-H(9)	119.5
C(9)-C(10)-C(5)	116.9(5)
C(9)-C(10)-C(11)	120.2(5)
C(5)-C(10)-C(11)	122.9(5)
C(10)-C(11)-C(13)	109.5(5)
C(10)-C(11)-C(12)	112.0(5)

C(13)-C(11)-C(12)	110.3(5)
C(10)-C(11)-H(11)	108.3
C(13)-C(11)-H(11)	108.3
C(12)-C(11)-H(11)	108.3
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(11)-C(13)-H(13A)	109.5
C(11)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(11)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(6)-C(14)-C(15)	111.0(5)
C(6)-C(14)-C(16)	110.9(5)
C(15)-C(14)-C(16)	111.3(5)
C(6)-C(14)-H(14)	107.8
C(15)-C(14)-H(14)	107.8
C(16)-C(14)-H(14)	107.8
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(1)	117.2(5)

C(18)-C(17)-H(17)	121.4
C(1)-C(17)-H(17)	121.4
C(17)-C(18)-C(19)	120.5(5)
C(17)-C(18)-H(18)	119.8
C(19)-C(18)-H(18)	119.8
C(20)-C(19)-C(18)	117.3(5)
C(20)-C(19)-H(19)	121.4
C(18)-C(19)-H(19)	121.4
N(1)-C(20)-C(19)	124.3(5)
N(1)-C(20)-N(4)	114.1(4)
C(19)-C(20)-N(4)	121.6(5)
N(5)-C(21)-N(4)	103.5(4)
N(5)-C(21)-U(1)	137.4(3)
N(4)-C(21)-U(1)	118.3(3)
C(23)-C(22)-N(5)	107.8(5)
C(23)-C(22)-H(22)	126.1
N(5)-C(22)-H(22)	126.1
C(22)-C(23)-N(4)	105.7(5)
C(22)-C(23)-H(23)	127.1
N(4)-C(23)-H(23)	127.1
C(25)-C(24)-C(29)	123.6(5)
C(25)-C(24)-N(5)	118.4(4)
C(29)-C(24)-N(5)	117.9(4)
C(24)-C(25)-C(26)	116.3(5)
C(24)-C(25)-C(33)	123.2(5)
C(26)-C(25)-C(33)	120.4(5)
C(27)-C(26)-C(25)	122.0(5)
C(27)-C(26)-H(26)	119.0
C(25)-C(26)-H(26)	119.0
C(26)-C(27)-C(28)	119.9(5)
C(26)-C(27)-H(27)	120.0
C(28)-C(27)-H(27)	120.0
C(27)-C(28)-C(29)	121.2(5)
C(27)-C(28)-H(28)	119.4
C(29)-C(28)-H(28)	119.4

C(28)-C(29)-C(24)	116.9(5)
C(28)-C(29)-C(30)	119.9(5)
C(24)-C(29)-C(30)	123.2(5)
C(29)-C(30)-C(31)	111.8(5)
C(29)-C(30)-C(32)	111.1(5)
C(31)-C(30)-C(32)	110.1(5)
C(29)-C(30)-H(30)	107.9
C(31)-C(30)-H(30)	107.9
C(32)-C(30)-H(30)	107.9
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(30)-C(32)-H(32A)	109.5
C(30)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(30)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(25)-C(33)-C(34)	110.5(4)
C(25)-C(33)-C(35)	111.7(4)
C(34)-C(33)-C(35)	111.8(5)
C(25)-C(33)-H(33)	107.6
C(34)-C(33)-H(33)	107.6
C(35)-C(33)-H(33)	107.6
C(33)-C(34)-H(34A)	109.5
C(33)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(33)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(33)-C(35)-H(35A)	109.5
C(33)-C(35)-H(35B)	109.5

H(35A)-C(35)-H(35B)	109.5
C(33)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
O(1)-C(36)-C(37)	107.3(5)
O(1)-C(36)-H(36A)	110.3
C(37)-C(36)-H(36A)	110.3
O(1)-C(36)-H(36B)	110.3
C(37)-C(36)-H(36B)	110.3
H(36A)-C(36)-H(36B)	108.5
C(36)-C(37)-C(38)	100.9(5)
C(36)-C(37)-H(37A)	111.6
C(38)-C(37)-H(37A)	111.6
C(36)-C(37)-H(37B)	111.6
C(38)-C(37)-H(37B)	111.6
H(37A)-C(37)-H(37B)	109.4
C(37)-C(38)-C(39)	103.1(6)
C(37)-C(38)-H(38A)	111.1
C(39)-C(38)-H(38A)	111.1
C(37)-C(38)-H(38B)	111.1
C(39)-C(38)-H(38B)	111.1
H(38A)-C(38)-H(38B)	109.1
O(1)-C(39)-C(38)	106.8(5)
O(1)-C(39)-H(39A)	110.4
C(38)-C(39)-H(39A)	110.4
O(1)-C(39)-H(39B)	110.4
C(38)-C(39)-H(39B)	110.4
H(39A)-C(39)-H(39B)	108.6
C(20)-N(1)-C(1)	116.7(4)
C(20)-N(1)-U(1)	122.0(3)
C(1)-N(1)-U(1)	121.2(3)
C(2)-N(2)-C(4)	111.5(4)
C(2)-N(2)-C(1)	122.5(4)
C(4)-N(2)-C(1)	126.0(4)
C(2)-N(3)-C(3)	111.6(4)

C(2)-N(3)-C(5)	126.1(4)
C(3)-N(3)-C(5)	122.2(4)
C(21)-N(4)-C(23)	111.7(4)
C(21)-N(4)-C(20)	122.5(4)
C(23)-N(4)-C(20)	125.8(4)
C(21)-N(5)-C(22)	111.2(4)
C(21)-N(5)-C(24)	126.5(4)
C(22)-N(5)-C(24)	122.2(4)
C(36)-O(1)-C(39)	108.0(5)
C(2)-U(1)-C(21)	124.68(15)
C(2)-U(1)-Cl(4)	85.44(11)
C(21)-U(1)-Cl(4)	141.43(11)
C(2)-U(1)-Cl(3)	145.58(11)
C(21)-U(1)-Cl(3)	82.76(11)
Cl(4)-U(1)-Cl(3)	81.86(4)
C(2)-U(1)-Cl(1)	76.65(11)
C(21)-U(1)-Cl(1)	90.81(11)
Cl(4)-U(1)-Cl(1)	122.03(4)
Cl(3)-U(1)-Cl(1)	83.28(4)
C(2)-U(1)-N(1)	62.47(14)
C(21)-U(1)-N(1)	62.30(14)
Cl(4)-U(1)-N(1)	141.27(9)
Cl(3)-U(1)-N(1)	136.87(9)
Cl(1)-U(1)-N(1)	73.40(9)
C(2)-U(1)-Cl(2)	83.50(11)
C(21)-U(1)-Cl(2)	77.64(11)
Cl(4)-U(1)-Cl(2)	83.44(4)
Cl(3)-U(1)-Cl(2)	126.22(4)
Cl(1)-U(1)-Cl(2)	145.55(4)
N(1)-U(1)-Cl(2)	72.50(9)

Symmetry transformations used to generate equivalent atoms:

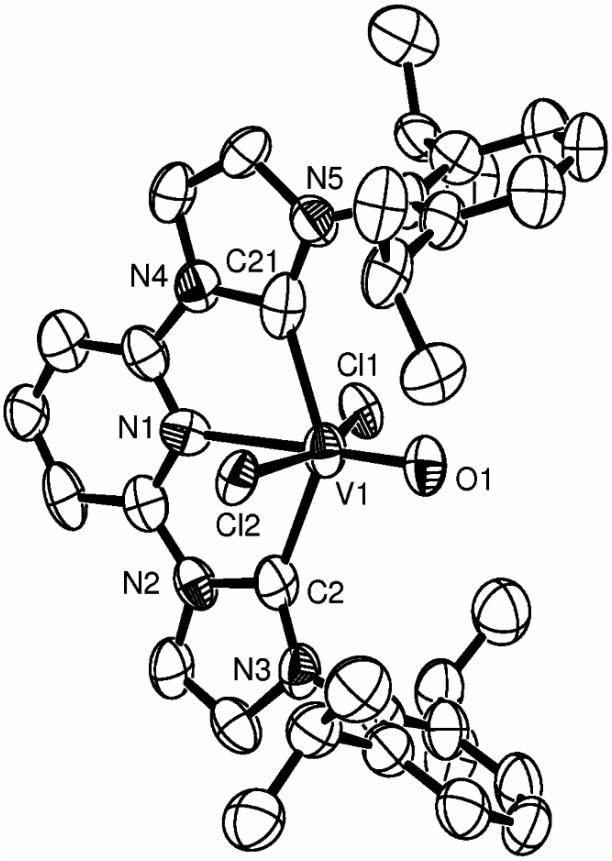
Table 4. Anisotropic displacement parameters ($\approx^2$x 10^3)for **5**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	18(3)	21(3)	23(3)	4(2)	-1(2)	-6(2)
C(2)	16(3)	18(3)	20(3)	4(2)	2(2)	-1(2)
C(3)	24(3)	28(3)	20(3)	-3(2)	6(2)	0(2)
C(4)	25(3)	31(3)	16(3)	-1(2)	3(2)	-2(2)
C(5)	24(3)	26(3)	19(3)	-1(2)	0(2)	7(2)
C(6)	30(3)	24(3)	25(3)	-2(2)	7(2)	7(2)
C(7)	47(4)	32(3)	30(3)	3(3)	7(3)	11(3)
C(8)	30(4)	42(4)	41(4)	1(3)	2(3)	19(3)
C(9)	20(3)	53(4)	29(3)	-8(3)	-1(2)	4(3)
C(10)	20(3)	35(3)	23(3)	-3(2)	5(2)	1(2)
C(11)	20(3)	41(4)	28(3)	-2(3)	3(2)	-4(3)
C(12)	35(4)	42(4)	43(4)	-7(3)	2(3)	-9(3)
C(13)	38(4)	64(5)	33(4)	2(3)	13(3)	-3(3)
C(14)	33(3)	20(3)	40(3)	4(2)	7(3)	-1(3)
C(15)	51(4)	33(4)	42(4)	0(3)	9(3)	-3(3)
C(16)	45(4)	35(4)	46(4)	1(3)	17(3)	-5(3)
C(17)	25(3)	29(3)	18(3)	0(2)	2(2)	2(2)
C(18)	27(3)	33(3)	24(3)	8(2)	-3(2)	4(3)
C(19)	24(3)	26(3)	27(3)	5(2)	-1(2)	1(2)
C(20)	19(3)	20(3)	22(3)	3(2)	-1(2)	-5(2)
C(21)	17(3)	26(3)	16(3)	-1(2)	0(2)	-4(2)
C(22)	21(3)	23(3)	27(3)	-3(2)	1(2)	4(2)
C(23)	22(3)	20(3)	30(3)	1(2)	-2(2)	4(2)
C(24)	24(3)	24(3)	17(3)	-3(2)	-1(2)	6(2)
C(25)	22(3)	19(3)	21(3)	-5(2)	3(2)	4(2)
C(26)	22(3)	28(3)	27(3)	-5(2)	-1(2)	2(2)
C(27)	34(3)	31(3)	21(3)	1(2)	7(2)	4(3)
C(28)	23(3)	27(3)	33(3)	2(2)	8(2)	1(2)
C(29)	23(3)	22(3)	27(3)	-2(2)	4(2)	-2(2)
C(30)	28(3)	30(3)	30(3)	-2(3)	4(3)	-5(3)

C(31)	31(4)	33(4)	60(4)	-6(3)	-4(3)	-1(3)
C(32)	28(3)	42(4)	59(4)	-8(3)	-4(3)	4(3)
C(33)	23(3)	27(3)	25(3)	1(2)	1(2)	-3(2)
C(34)	36(4)	27(3)	34(3)	-2(3)	3(3)	-1(3)
C(35)	21(3)	39(4)	34(3)	-3(3)	3(3)	-3(3)
C(36)	36(4)	36(4)	46(4)	5(3)	7(3)	4(3)
C(37)	46(4)	37(4)	40(4)	-1(3)	7(3)	2(3)
C(38)	56(5)	68(5)	58(5)	-1(4)	-1(4)	25(4)
C(39)	44(4)	53(4)	49(4)	12(4)	-7(3)	-4(4)
Cl(1)	18(1)	23(1)	17(1)	-1(1)	1(1)	-7(1)
Cl(2)	21(1)	13(1)	27(1)	1(1)	-4(1)	-3(1)
Cl(3)	29(1)	32(1)	18(1)	4(1)	4(1)	2(1)
Cl(4)	19(1)	35(1)	30(1)	3(1)	-2(1)	4(1)
N(1)	18(2)	17(2)	17(2)	2(2)	0(2)	3(2)
N(2)	21(2)	18(2)	16(2)	2(2)	-1(2)	-1(2)
N(3)	21(2)	19(2)	20(2)	1(2)	3(2)	1(2)
N(4)	17(2)	17(2)	21(2)	1(2)	-2(2)	2(2)
N(5)	15(2)	20(2)	21(2)	-1(2)	1(2)	2(2)
O(1)	44(3)	39(2)	44(3)	5(2)	9(2)	-1(2)
U(1)	17(1)	20(1)	17(1)	1(1)	1(1)	1(1)

Electronic Supplementary Information for Dalton Transactions

Structural Data for **6**



Electronic Supplementary Information for Dalton Transactions

Table 1. Crystal data and structure refinement for **6**.

Identification code	**6**	
Empirical formula	C35 H41 Cl2 N5 O V	
Formula weight	669.57	
Temperature	120(2) K	
Wavelength	0.6868 ≈	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 16.699(5) ≈	α= 90∞.
	b = 19.125(5) ≈	β= 97.012(4)∞.
	c = 22.226(6) ≈	γ = 90∞.
Volume	7045(3) ≈^{3}	
Z	8	
Density (calculated)	1.263 Mg/m^3	
Absorption coefficient	0.467 mm^{-1}	
F(000)	2808	
Crystal size	0.10 x 0.03 x 0.03 mm^3	
Theta range for data collection	2.06 to 20.08∞.	
Index ranges	-16<=h<=16, -19<=k<=19, -22<=l<=22	
Reflections collected	34114	
Independent reflections	7369 [R(int) = 0.1383]	
Completeness to theta = 20.08∞	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9861 and 0.621243	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7369 / 0 / 809	
Goodness-of-fit on F^2	0.969	
Final R indices [I>2sigma(I)]	R1 = 0.0763, wR2 = 0.1795	
R indices (all data)	R1 = 0.1342, wR2 = 0.2073	
Largest diff. peak and hole	1.320 and -0.442 e.≈$^{-3}$	

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

	x	y	z	U(eq)
C(1)	5734(6)	1586(5)	2868(4)	52(2)
C(2)	5008(5)	2059(5)	3654(4)	50(2)
C(3)	4758(5)	2650(5)	4627(4)	55(3)
C(4)	4651(5)	2195(5)	5106(4)	57(3)
C(5)	4920(6)	1429(5)	5118(4)	61(3)
C(6)	5662(6)	1302(5)	5566(5)	76(3)
C(7)	4232(6)	945(6)	5245(5)	78(3)
C(8)	4316(6)	2481(6)	5594(5)	70(3)
C(9)	4077(6)	3165(6)	5591(5)	66(3)
C(10)	4143(6)	3589(6)	5109(5)	76(3)
C(11)	4494(6)	3328(6)	4610(5)	63(3)
C(12)	4570(6)	3815(6)	4072(5)	75(3)
C(13)	4948(7)	4524(5)	4231(5)	79(3)
C(14)	3737(7)	3893(6)	3692(5)	98(4)
C(15)	6077(5)	2566(5)	4236(5)	61(3)
C(16)	6360(6)	2293(5)	3746(5)	63(3)
C(17)	6412(5)	1470(6)	2566(5)	68(3)
C(18)	6295(6)	1036(6)	2067(5)	62(3)
C(19)	5572(6)	741(5)	1881(4)	65(3)
C(20)	4932(6)	894(5)	2207(5)	54(3)
C(21)	3546(6)	888(5)	2416(4)	57(3)
C(22)	3060(6)	111(5)	1690(4)	52(2)
C(23)	3849(6)	179(5)	1632(4)	59(3)
C(24)	2060(5)	706(5)	2279(4)	49(2)
C(25)	1762(5)	386(5)	2768(4)	52(2)
C(26)	2263(6)	-89(5)	3233(4)	63(3)
C(27)	1868(6)	-825(5)	3244(5)	77(3)
C(28)	2344(6)	233(5)	3862(4)	65(3)
C(29)	958(6)	505(5)	2842(5)	70(3)
C(30)	500(6)	926(5)	2440(5)	67(3)

C(31)	797(6)	1245(5)	1967(5)	69(3)
C(32)	1604(6)	1124(5)	1877(4)	54(2)
C(33)	1924(5)	1471(5)	1329(4)	56(3)
C(34)	1576(7)	1134(6)	739(5)	92(4)
C(35)	1819(6)	2248(5)	1331(5)	81(3)
C(36)	10199(6)	3638(5)	2567(4)	53(2)
C(37)	8802(6)	3677(5)	2646(4)	52(2)
C(38)	8423(6)	4545(5)	1964(4)	59(3)
C(39)	9207(7)	4462(5)	1979(4)	59(3)
C(40)	7333(5)	3885(5)	2421(4)	56(3)
C(41)	6944(5)	4144(5)	2895(4)	51(2)
C(42)	7338(5)	4616(4)	3382(4)	51(2)
C(43)	7324(6)	4269(5)	4012(4)	70(3)
C(44)	6895(6)	5332(5)	3372(5)	75(3)
C(45)	6117(6)	3940(6)	2885(5)	63(3)
C(46)	5761(6)	3507(5)	2453(5)	61(3)
C(47)	6157(6)	3251(5)	2011(5)	62(3)
C(48)	6966(6)	3430(5)	1979(5)	63(3)
C(49)	7415(6)	3147(5)	1452(4)	62(3)
C(50)	7189(6)	3561(5)	876(4)	72(3)
C(51)	7257(6)	2367(5)	1342(5)	72(3)
C(52)	10918(6)	3807(5)	2329(4)	57(3)
C(53)	11589(6)	3451(5)	2555(4)	60(3)
C(54)	11584(5)	2923(5)	2990(4)	61(3)
C(55)	10832(6)	2812(5)	3189(4)	55(3)
C(56)	9903(6)	2294(5)	3810(5)	61(3)
C(57)	10774(6)	1587(5)	4404(4)	57(3)
C(58)	11213(6)	1910(5)	4030(5)	63(3)
C(59)	9319(6)	1565(6)	4528(4)	60(3)
C(60)	9009(6)	926(6)	4327(5)	64(3)
C(61)	9373(6)	489(6)	3861(5)	70(3)
C(62)	9797(6)	-170(6)	4138(5)	84(4)
C(63)	8758(7)	279(6)	3327(5)	80(3)
C(64)	8311(7)	666(6)	4565(5)	80(3)
C(65)	7960(7)	1063(6)	4989(5)	74(3)

C(66)	8267(7)	1699(7)	5182(5)	80(3)
C(67)	8936(6)	1969(6)	4960(4)	64(3)
C(68)	9295(7)	2660(6)	5183(5)	74(3)
C(69)	8640(7)	3207(6)	5277(6)	100(4)
C(70)	9859(7)	2530(6)	5774(5)	93(4)
Cl(1)	3792(1)	2519(1)	2458(1)	51(1)
Cl(2)	4383(1)	508(1)	3693(1)	46(1)
Cl(3)	8826(1)	2064(1)	2547(1)	53(1)
Cl(4)	9455(1)	3941(1)	3947(1)	55(1)
N(1)	5007(4)	1314(4)	2675(3)	48(2)
N(2)	5716(4)	1988(4)	3400(4)	52(2)
N(3)	5245(4)	2415(4)	4163(4)	53(2)
N(4)	4138(5)	659(4)	2088(3)	52(2)
N(5)	2869(5)	551(4)	2157(3)	55(2)
N(6)	10175(5)	3150(4)	2979(3)	50(2)
N(7)	9440(4)	3945(4)	2399(3)	53(2)
N(8)	8177(5)	4048(4)	2381(3)	51(2)
N(9)	10691(4)	2345(4)	3661(3)	53(2)
N(10)	9981(4)	1824(4)	4275(3)	55(2)
O(1)	3196(3)	1772(3)	3539(3)	58(2)
O(2)	8182(3)	2760(3)	3639(3)	64(2)
V(1)	3937(1)	1579(1)	3177(1)	51(1)
V(2)	8990(1)	2913(1)	3340(1)	56(1)

Table 3. Bond lengths [≈] and angles [∞] for **6**.

C(1)-N(1)	1.342(11)
C(1)-C(17)	1.402(12)
C(1)-N(2)	1.414(11)
C(2)-N(3)	1.337(11)
C(2)-N(2)	1.378(10)
C(2)-V(1)	2.169(10)
C(3)-C(11)	1.369(13)
C(3)-C(4)	1.404(12)
C(3)-N(3)	1.459(12)
C(4)-C(8)	1.392(13)
C(4)-C(5)	1.532(13)
C(5)-C(6)	1.511(13)
C(5)-C(7)	1.528(12)
C(5)-H(5)	1.0000
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-C(9)	1.368(13)
C(8)-H(8)	0.9500
C(9)-C(10)	1.360(13)
C(9)-H(9)	0.9500
C(10)-C(11)	1.407(13)
C(10)-H(10)	0.9500
C(11)-C(12)	1.533(14)
C(12)-C(13)	1.519(14)
C(12)-C(14)	1.543(14)
C(12)-H(12)	1.0000
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800

C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-C(16)	1.345(13)
C(15)-N(3)	1.409(11)
C(15)-H(15)	0.9500
C(16)-N(2)	1.374(12)
C(16)-H(16)	0.9500
C(17)-C(18)	1.381(13)
C(17)-H(17)	0.9500
C(18)-C(19)	1.351(12)
C(18)-H(18)	0.9500
C(19)-C(20)	1.393(12)
C(19)-H(19)	0.9500
C(20)-N(1)	1.307(11)
C(20)-N(4)	1.395(11)
C(21)-N(4)	1.371(10)
C(21)-N(5)	1.366(11)
C(21)-V(1)	2.182(11)
C(22)-C(23)	1.346(12)
C(22)-N(5)	1.403(11)
C(22)-H(22)	0.9500
C(23)-N(4)	1.407(11)
C(23)-H(23)	0.9500
C(24)-C(32)	1.361(12)
C(24)-C(25)	1.393(12)
C(24)-N(5)	1.441(10)
C(25)-C(29)	1.390(12)
C(25)-C(26)	1.543(13)
C(26)-C(28)	1.520(12)
C(26)-C(27)	1.555(13)
C(26)-H(26)	1.0000
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)	1.365(13)
C(29)-H(29)	0.9500
C(30)-C(31)	1.360(13)
C(30)-H(30)	0.9500
C(31)-C(32)	1.405(12)
C(31)-H(31)	0.9500
C(32)-C(33)	1.539(12)
C(33)-C(35)	1.497(13)
C(33)-C(34)	1.512(13)
C(33)-H(33)	1.0000
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(36)-N(6)	1.312(11)
C(36)-N(7)	1.406(11)
C(36)-C(52)	1.407(12)
C(37)-N(8)	1.338(11)
C(37)-N(7)	1.357(10)
C(37)-V(2)	2.120(10)
C(38)-C(39)	1.316(12)
C(38)-N(8)	1.423(11)
C(38)-H(38)	0.9500
C(39)-N(7)	1.382(11)
C(39)-H(39)	0.9500
C(40)-C(41)	1.395(12)
C(40)-C(48)	1.397(13)
C(40)-N(8)	1.456(11)
C(41)-C(45)	1.433(12)
C(41)-C(42)	1.498(12)

C(42)-C(43)	1.553(12)
C(42)-C(44)	1.554(12)
C(42)-H(42)	1.0000
C(43)-H(43A)	0.9800
C(43)-H(43B)	0.9800
C(43)-H(43C)	0.9800
C(44)-H(44A)	0.9800
C(44)-H(44B)	0.9800
C(44)-H(44C)	0.9800
C(45)-C(46)	1.350(13)
C(45)-H(45)	0.9500
C(46)-C(47)	1.343(12)
C(46)-H(46)	0.9500
C(47)-C(48)	1.402(12)
C(47)-H(47)	0.9500
C(48)-C(49)	1.564(13)
C(49)-C(50)	1.513(13)
C(49)-C(51)	1.528(13)
C(49)-H(49)	1.0000
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)-C(53)	1.355(12)
C(52)-H(52)	0.9500
C(53)-C(54)	1.399(13)
C(53)-H(53)	0.9500
C(54)-C(55)	1.397(12)
C(54)-H(54)	0.9500
C(55)-N(6)	1.309(11)
C(55)-N(9)	1.419(11)
C(56)-N(10)	1.365(11)
C(56)-N(9)	1.398(10)

C(56)-V(2)	2.104(11)
C(57)-C(58)	1.326(12)
C(57)-N(10)	1.395(11)
C(57)-H(57)	0.9500
C(58)-N(9)	1.396(11)
C(58)-H(58)	0.9500
C(59)-C(60)	1.380(13)
C(59)-N(10)	1.392(12)
C(59)-C(67)	1.441(13)
C(60)-C(64)	1.426(13)
C(60)-C(61)	1.515(14)
C(61)-C(63)	1.525(13)
C(61)-C(62)	1.538(14)
C(61)-H(61)	1.0000
C(62)-H(62A)	0.9800
C(62)-H(62B)	0.9800
C(62)-H(62C)	0.9800
C(63)-H(63A)	0.9800
C(63)-H(63B)	0.9800
C(63)-H(63C)	0.9800
C(64)-C(65)	1.394(14)
C(64)-H(64)	0.9500
C(65)-C(66)	1.369(14)
C(65)-H(65)	0.9500
C(66)-C(67)	1.374(13)
C(66)-H(66)	0.9500
C(67)-C(68)	1.510(14)
C(68)-C(70)	1.540(14)
C(68)-C(69)	1.546(13)
C(68)-H(68)	1.0000
C(69)-H(69A)	0.9800
C(69)-H(69B)	0.9800
C(69)-H(69C)	0.9800
C(70)-H(70A)	0.9800
C(70)-H(70B)	0.9800

C(70)-H(70C)	0.9800
Cl(1)-V(1)	2.398(3)
Cl(2)-V(1)	2.421(3)
Cl(3)-V(2)	2.388(3)
Cl(4)-V(2)	2.456(3)
N(1)-V(1)	2.275(7)
N(6)-V(2)	2.270(7)
O(1)-V(1)	1.600(5)
O(2)-V(2)	1.602(6)

N(1)-C(1)-C(17)	122.6(10)
N(1)-C(1)-N(2)	111.5(8)
C(17)-C(1)-N(2)	125.9(10)
N(3)-C(2)-N(2)	102.6(8)
N(3)-C(2)-V(1)	140.4(6)
N(2)-C(2)-V(1)	117.0(7)
C(11)-C(3)-C(4)	122.5(9)
C(11)-C(3)-N(3)	118.6(8)
C(4)-C(3)-N(3)	118.5(9)
C(8)-C(4)-C(3)	116.7(10)
C(8)-C(4)-C(5)	120.4(9)
C(3)-C(4)-C(5)	122.8(9)
C(6)-C(5)-C(7)	110.8(8)
C(6)-C(5)-C(4)	112.4(8)
C(7)-C(5)-C(4)	110.9(8)
C(6)-C(5)-H(5)	107.5
C(7)-C(5)-H(5)	107.5
C(4)-C(5)-H(5)	107.5
C(5)-C(6)-H(6A)	109.5
C(5)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(5)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(5)-C(7)-H(7A)	109.5

C(5)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(5)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(9)-C(8)-C(4)	121.1(10)
C(9)-C(8)-H(8)	119.5
C(4)-C(8)-H(8)	119.5
C(10)-C(9)-C(8)	121.6(10)
C(10)-C(9)-H(9)	119.2
C(8)-C(9)-H(9)	119.2
C(9)-C(10)-C(11)	119.4(10)
C(9)-C(10)-H(10)	120.3
C(11)-C(10)-H(10)	120.3
C(3)-C(11)-C(10)	118.6(9)
C(3)-C(11)-C(12)	122.7(9)
C(10)-C(11)-C(12)	118.7(10)
C(13)-C(12)-C(11)	115.6(9)
C(13)-C(12)-C(14)	111.3(9)
C(11)-C(12)-C(14)	109.3(9)
C(13)-C(12)-H(12)	106.7
C(11)-C(12)-H(12)	106.7
C(14)-C(12)-H(12)	106.7
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(12)-C(14)-H(14A)	109.5
C(12)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(12)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5

C(16)-C(15)-N(3)	105.5(9)
C(16)-C(15)-H(15)	127.3
N(3)-C(15)-H(15)	127.3
C(15)-C(16)-N(2)	106.8(8)
C(15)-C(16)-H(16)	126.6
N(2)-C(16)-H(16)	126.6
C(18)-C(17)-C(1)	115.8(9)
C(18)-C(17)-H(17)	122.1
C(1)-C(17)-H(17)	122.1
C(19)-C(18)-C(17)	122.0(9)
C(19)-C(18)-H(18)	119.0
C(17)-C(18)-H(18)	119.0
C(18)-C(19)-C(20)	117.9(10)
C(18)-C(19)-H(19)	121.1
C(20)-C(19)-H(19)	121.1
N(1)-C(20)-N(4)	110.3(8)
N(1)-C(20)-C(19)	122.5(9)
N(4)-C(20)-C(19)	127.2(10)
N(4)-C(21)-N(5)	103.7(8)
N(4)-C(21)-V(1)	116.0(7)
N(5)-C(21)-V(1)	140.1(7)
C(23)-C(22)-N(5)	109.0(9)
C(23)-C(22)-H(22)	125.5
N(5)-C(22)-H(22)	125.5
C(22)-C(23)-N(4)	104.4(8)
C(22)-C(23)-H(23)	127.8
N(4)-C(23)-H(23)	127.8
C(32)-C(24)-C(25)	123.2(8)
C(32)-C(24)-N(5)	117.4(8)
C(25)-C(24)-N(5)	119.3(8)
C(29)-C(25)-C(24)	117.5(9)
C(29)-C(25)-C(26)	118.0(8)
C(24)-C(25)-C(26)	124.5(8)
C(28)-C(26)-C(25)	110.9(8)
C(28)-C(26)-C(27)	110.1(8)

C(25)-C(26)-C(27)	110.3(8)
C(28)-C(26)-H(26)	108.5
C(25)-C(26)-H(26)	108.5
C(27)-C(26)-H(26)	108.5
C(26)-C(27)-H(27A)	109.5
C(26)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(26)-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)-C(25)	119.5(9)
C(30)-C(29)-H(29)	120.3
C(25)-C(29)-H(29)	120.3
C(31)-C(30)-C(29)	122.8(9)
C(31)-C(30)-H(30)	118.6
C(29)-C(30)-H(30)	118.6
C(30)-C(31)-C(32)	118.9(10)
C(30)-C(31)-H(31)	120.6
C(32)-C(31)-H(31)	120.6
C(24)-C(32)-C(31)	118.2(8)
C(24)-C(32)-C(33)	123.5(8)
C(31)-C(32)-C(33)	118.3(9)
C(35)-C(33)-C(34)	113.1(9)
C(35)-C(33)-C(32)	112.0(8)
C(34)-C(33)-C(32)	111.6(8)
C(35)-C(33)-H(33)	106.5
C(34)-C(33)-H(33)	106.5
C(32)-C(33)-H(33)	106.5
C(33)-C(34)-H(34A)	109.5

C(33)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(33)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(33)-C(35)-H(35A)	109.5
C(33)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(33)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
N(6)-C(36)-N(7)	112.3(8)
N(6)-C(36)-C(52)	121.7(9)
N(7)-C(36)-C(52)	126.0(9)
N(8)-C(37)-N(7)	103.3(8)
N(8)-C(37)-V(2)	136.4(7)
N(7)-C(37)-V(2)	120.1(7)
C(39)-C(38)-N(8)	105.6(9)
C(39)-C(38)-H(38)	127.2
N(8)-C(38)-H(38)	127.2
C(38)-C(39)-N(7)	107.4(9)
C(38)-C(39)-H(39)	126.3
N(7)-C(39)-H(39)	126.3
C(41)-C(40)-C(48)	123.2(9)
C(41)-C(40)-N(8)	120.9(9)
C(48)-C(40)-N(8)	115.8(8)
C(40)-C(41)-C(45)	115.3(9)
C(40)-C(41)-C(42)	123.8(8)
C(45)-C(41)-C(42)	120.9(9)
C(41)-C(42)-C(43)	109.8(7)
C(41)-C(42)-C(44)	110.7(8)
C(43)-C(42)-C(44)	109.3(8)
C(41)-C(42)-H(42)	109.0
C(43)-C(42)-H(42)	109.0
C(44)-C(42)-H(42)	109.0

C(42)-C(43)-H(43A)	109.5
C(42)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43B)	109.5
C(42)-C(43)-H(43C)	109.5
H(43A)-C(43)-H(43C)	109.5
H(43B)-C(43)-H(43C)	109.5
C(42)-C(44)-H(44A)	109.5
C(42)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
C(42)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
C(46)-C(45)-C(41)	121.2(9)
C(46)-C(45)-H(45)	119.4
C(41)-C(45)-H(45)	119.4
C(47)-C(46)-C(45)	122.1(9)
C(47)-C(46)-H(46)	119.0
C(45)-C(46)-H(46)	119.0
C(46)-C(47)-C(48)	120.7(10)
C(46)-C(47)-H(47)	119.7
C(48)-C(47)-H(47)	119.7
C(40)-C(48)-C(47)	117.4(9)
C(40)-C(48)-C(49)	122.2(9)
C(47)-C(48)-C(49)	120.4(10)
C(50)-C(49)-C(51)	110.8(8)
C(50)-C(49)-C(48)	111.1(8)
C(51)-C(49)-C(48)	111.6(8)
C(50)-C(49)-H(49)	107.7
C(51)-C(49)-H(49)	107.7
C(48)-C(49)-H(49)	107.7
C(49)-C(50)-H(50A)	109.5
C(49)-C(50)-H(50B)	109.5
H(50A)-C(50)-H(50B)	109.5
C(49)-C(50)-H(50C)	109.5
H(50A)-C(50)-H(50C)	109.5

H(50B)-C(50)-H(50C)	109.5
C(49)-C(51)-H(51A)	109.5
C(49)-C(51)-H(51B)	109.5
H(51A)-C(51)-H(51B)	109.5
C(49)-C(51)-H(51C)	109.5
H(51A)-C(51)-H(51C)	109.5
H(51B)-C(51)-H(51C)	109.5
C(53)-C(52)-C(36)	116.8(9)
C(53)-C(52)-H(52)	121.6
C(36)-C(52)-H(52)	121.6
C(52)-C(53)-C(54)	123.0(9)
C(52)-C(53)-H(53)	118.5
C(54)-C(53)-H(53)	118.5
C(55)-C(54)-C(53)	114.2(10)
C(55)-C(54)-H(54)	122.9
C(53)-C(54)-H(54)	122.9
N(6)-C(55)-C(54)	123.9(9)
N(6)-C(55)-N(9)	111.6(8)
C(54)-C(55)-N(9)	124.4(10)
N(10)-C(56)-N(9)	102.7(8)
N(10)-C(56)-V(2)	137.9(6)
N(9)-C(56)-V(2)	119.4(7)
C(58)-C(57)-N(10)	107.7(9)
C(58)-C(57)-H(57)	126.2
N(10)-C(57)-H(57)	126.2
C(57)-C(58)-N(9)	107.0(8)
C(57)-C(58)-H(58)	126.5
N(9)-C(58)-H(58)	126.5
C(60)-C(59)-N(10)	118.0(9)
C(60)-C(59)-C(67)	120.7(9)
N(10)-C(59)-C(67)	121.2(10)
C(59)-C(60)-C(64)	118.7(10)
C(59)-C(60)-C(61)	123.0(8)
C(64)-C(60)-C(61)	118.4(10)
C(60)-C(61)-C(63)	113.0(9)

C(60)-C(61)-C(62)	112.4(8)
C(63)-C(61)-C(62)	109.3(9)
C(60)-C(61)-H(61)	107.3
C(63)-C(61)-H(61)	107.3
C(62)-C(61)-H(61)	107.3
C(61)-C(62)-H(62A)	109.5
C(61)-C(62)-H(62B)	109.5
H(62A)-C(62)-H(62B)	109.5
C(61)-C(62)-H(62C)	109.5
H(62A)-C(62)-H(62C)	109.5
H(62B)-C(62)-H(62C)	109.5
C(61)-C(63)-H(63A)	109.5
C(61)-C(63)-H(63B)	109.5
H(63A)-C(63)-H(63B)	109.5
C(61)-C(63)-H(63C)	109.5
H(63A)-C(63)-H(63C)	109.5
H(63B)-C(63)-H(63C)	109.5
C(65)-C(64)-C(60)	119.4(11)
C(65)-C(64)-H(64)	120.3
C(60)-C(64)-H(64)	120.3
C(66)-C(65)-C(64)	121.5(10)
C(66)-C(65)-H(65)	119.3
C(64)-C(65)-H(65)	119.3
C(65)-C(66)-C(67)	120.8(10)
C(65)-C(66)-H(66)	119.6
C(67)-C(66)-H(66)	119.6
C(66)-C(67)-C(59)	118.9(11)
C(66)-C(67)-C(68)	121.3(10)
C(59)-C(67)-C(68)	119.8(9)
C(67)-C(68)-C(70)	108.4(9)
C(67)-C(68)-C(69)	112.1(9)
C(70)-C(68)-C(69)	111.3(9)
C(67)-C(68)-H(68)	108.3
C(70)-C(68)-H(68)	108.3
C(69)-C(68)-H(68)	108.3

C(68)-C(69)-H(69A)	109.5
C(68)-C(69)-H(69B)	109.5
H(69A)-C(69)-H(69B)	109.5
C(68)-C(69)-H(69C)	109.5
H(69A)-C(69)-H(69C)	109.5
H(69B)-C(69)-H(69C)	109.5
C(68)-C(70)-H(70A)	109.5
C(68)-C(70)-H(70B)	109.5
H(70A)-C(70)-H(70B)	109.5
C(68)-C(70)-H(70C)	109.5
H(70A)-C(70)-H(70C)	109.5
H(70B)-C(70)-H(70C)	109.5
C(20)-N(1)-C(1)	119.1(8)
C(20)-N(1)-V(1)	121.4(6)
C(1)-N(1)-V(1)	119.4(6)
C(16)-N(2)-C(2)	112.3(8)
C(16)-N(2)-C(1)	127.2(8)
C(2)-N(2)-C(1)	120.3(8)
C(2)-N(3)-C(15)	112.8(8)
C(2)-N(3)-C(3)	128.4(8)
C(15)-N(3)-C(3)	118.8(8)
C(21)-N(4)-C(20)	121.7(9)
C(21)-N(4)-C(23)	112.7(8)
C(20)-N(4)-C(23)	125.6(8)
C(21)-N(5)-C(22)	110.1(7)
C(21)-N(5)-C(24)	124.7(8)
C(22)-N(5)-C(24)	124.5(8)
C(55)-N(6)-C(36)	120.3(8)
C(55)-N(6)-V(2)	120.2(6)
C(36)-N(6)-V(2)	119.4(7)
C(37)-N(7)-C(39)	112.0(8)
C(37)-N(7)-C(36)	117.5(9)
C(39)-N(7)-C(36)	130.4(8)
C(37)-N(8)-C(38)	111.7(7)
C(37)-N(8)-C(40)	124.6(8)

C(38)-N(8)-C(40)	122.8(8)
C(56)-N(9)-C(58)	111.0(8)
C(56)-N(9)-C(55)	117.6(9)
C(58)-N(9)-C(55)	131.4(8)
C(56)-N(10)-C(59)	122.3(8)
C(56)-N(10)-C(57)	111.7(8)
C(59)-N(10)-C(57)	125.6(8)
O(1)-V(1)-C(2)	107.3(3)
O(1)-V(1)-C(21)	110.6(3)
C(2)-V(1)-C(21)	141.9(4)
O(1)-V(1)-N(1)	178.9(3)
C(2)-V(1)-N(1)	71.6(3)
C(21)-V(1)-N(1)	70.4(3)
O(1)-V(1)-Cl(1)	98.1(2)
C(2)-V(1)-Cl(1)	91.1(2)
C(21)-V(1)-Cl(1)	86.7(2)
N(1)-V(1)-Cl(1)	82.10(18)
O(1)-V(1)-Cl(2)	99.7(2)
C(2)-V(1)-Cl(2)	86.5(2)
C(21)-V(1)-Cl(2)	84.3(2)
N(1)-V(1)-Cl(2)	80.18(18)
Cl(1)-V(1)-Cl(2)	161.97(10)
O(2)-V(2)-C(56)	106.7(3)
O(2)-V(2)-C(37)	111.7(3)
C(56)-V(2)-C(37)	141.5(4)
O(2)-V(2)-N(6)	176.2(3)
C(56)-V(2)-N(6)	71.2(3)
C(37)-V(2)-N(6)	70.3(3)
O(2)-V(2)-Cl(3)	99.0(2)
C(56)-V(2)-Cl(3)	89.7(3)
C(37)-V(2)-Cl(3)	86.4(2)
N(6)-V(2)-Cl(3)	84.32(18)
O(2)-V(2)-Cl(4)	98.3(2)
C(56)-V(2)-Cl(4)	90.9(3)
C(37)-V(2)-Cl(4)	81.8(2)

N(6)-V(2)-Cl(4)	78.66(18)
Cl(3)-V(2)-Cl(4)	161.78(10)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\approx^2$x 10^3)for **6**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	51(7)	45(6)	62(7)	17(5)	11(6)	5(5)
C(2)	43(6)	65(7)	44(6)	16(5)	18(5)	4(5)
C(3)	40(6)	66(7)	58(7)	9(6)	4(5)	-1(5)
C(4)	53(6)	70(7)	48(6)	6(6)	9(5)	0(5)
C(5)	62(7)	71(8)	51(6)	2(5)	12(5)	-4(6)
C(6)	88(8)	60(7)	79(8)	-6(6)	4(7)	4(6)
C(7)	91(8)	83(8)	61(7)	10(6)	18(6)	-1(7)
C(8)	55(6)	91(9)	66(8)	4(6)	14(6)	-4(6)
C(9)	78(7)	66(8)	57(7)	-2(6)	14(6)	22(6)
C(10)	71(7)	81(8)	77(8)	16(7)	15(6)	28(6)
C(11)	51(6)	72(8)	69(7)	3(6)	23(6)	-4(6)
C(12)	78(8)	75(8)	74(8)	11(6)	21(7)	18(6)
C(13)	95(8)	59(7)	91(8)	16(6)	37(7)	3(6)
C(14)	95(9)	105(10)	93(9)	8(8)	14(8)	16(8)
C(15)	44(7)	55(7)	82(8)	9(6)	1(6)	-7(5)
C(16)	54(7)	77(8)	63(7)	11(6)	29(6)	7(6)
C(17)	36(6)	84(8)	90(9)	26(7)	25(6)	6(5)
C(18)	47(7)	79(8)	63(7)	-1(6)	23(6)	3(6)
C(19)	60(7)	90(8)	49(6)	18(6)	23(6)	6(6)
C(20)	45(7)	61(7)	54(7)	18(6)	4(6)	6(5)
C(21)	70(7)	58(7)	48(6)	23(5)	27(6)	21(6)
C(22)	71(7)	55(6)	31(5)	-1(5)	16(5)	4(5)
C(23)	68(7)	68(7)	46(6)	3(6)	29(6)	8(6)
C(24)	48(6)	52(6)	50(6)	5(5)	20(5)	3(5)
C(25)	50(6)	56(6)	55(6)	3(5)	24(5)	-4(5)
C(26)	70(7)	55(7)	71(7)	4(6)	41(6)	-1(6)
C(27)	76(7)	72(8)	88(8)	2(6)	26(6)	19(6)
C(28)	82(7)	68(7)	47(6)	7(5)	21(5)	-14(6)
C(29)	70(8)	72(8)	75(8)	19(6)	32(6)	-6(6)
C(30)	57(6)	73(8)	75(8)	5(6)	28(6)	11(6)

C(31)	54(7)	77(8)	79(8)	8(6)	20(6)	2(6)
C(32)	59(7)	53(6)	49(6)	13(5)	5(5)	1(5)
C(33)	40(5)	79(8)	49(6)	1(5)	5(5)	-6(5)
C(34)	87(8)	122(10)	67(8)	15(7)	8(7)	-25(8)
C(35)	83(8)	67(8)	100(9)	21(6)	33(7)	5(6)
C(36)	58(7)	62(7)	40(6)	-6(5)	10(5)	-8(6)
C(37)	46(6)	65(7)	44(6)	-9(5)	5(5)	-7(6)
C(38)	58(7)	54(7)	67(7)	-3(5)	21(6)	3(5)
C(39)	72(8)	50(7)	59(7)	-5(6)	17(6)	-3(6)
C(40)	49(6)	70(7)	51(6)	6(6)	14(5)	-3(5)
C(41)	63(7)	53(6)	40(6)	2(5)	17(5)	0(5)
C(42)	53(6)	43(6)	58(6)	-1(5)	6(5)	-2(5)
C(43)	84(8)	71(7)	59(7)	9(6)	22(6)	-4(6)
C(44)	77(7)	83(8)	71(7)	0(6)	31(6)	-3(6)
C(45)	45(6)	75(8)	76(8)	29(7)	34(6)	4(6)
C(46)	49(6)	64(7)	72(7)	-3(6)	14(6)	-7(6)
C(47)	55(7)	71(7)	59(7)	-5(5)	6(6)	-4(6)
C(48)	62(7)	64(7)	64(7)	10(6)	7(6)	-6(6)
C(49)	60(6)	73(8)	57(7)	-8(6)	19(5)	5(6)
C(50)	72(7)	79(8)	66(7)	-5(6)	8(6)	-10(6)
C(51)	78(7)	70(8)	66(7)	-11(6)	3(6)	7(6)
C(52)	44(6)	64(7)	64(7)	-5(5)	7(6)	-4(5)
C(53)	70(8)	66(7)	48(6)	7(6)	19(6)	-14(6)
C(54)	39(6)	82(8)	64(7)	-23(6)	21(5)	-14(5)
C(55)	68(7)	51(6)	48(6)	-11(5)	9(6)	-7(6)
C(56)	57(7)	59(7)	74(8)	-1(6)	36(6)	-8(5)
C(57)	53(7)	72(7)	45(6)	-6(5)	4(5)	5(6)
C(58)	49(6)	79(8)	61(7)	-8(6)	8(6)	2(6)
C(59)	67(7)	66(8)	47(6)	8(6)	8(6)	6(6)
C(60)	53(6)	73(8)	72(7)	27(6)	35(6)	6(6)
C(61)	63(7)	89(8)	60(7)	6(6)	16(6)	-6(6)
C(62)	65(7)	101(9)	94(9)	-3(7)	40(7)	-3(7)
C(63)	98(9)	78(8)	67(8)	8(6)	28(7)	-12(7)
C(64)	95(9)	69(8)	79(8)	3(6)	27(7)	3(7)
C(65)	84(8)	69(8)	79(8)	25(7)	47(7)	0(7)

C(66)	94(9)	96(10)	58(7)	27(7)	43(7)	18(8)
C(67)	68(7)	76(8)	52(6)	16(6)	24(6)	11(6)
C(68)	85(8)	81(9)	57(7)	5(6)	11(6)	9(7)
C(69)	83(8)	119(10)	103(9)	5(8)	34(7)	41(8)
C(70)	97(9)	100(10)	78(9)	0(7)	-5(7)	21(7)
Cl(1)	38(1)	50(1)	67(2)	19(1)	9(1)	0(1)
Cl(2)	54(1)	46(1)	43(1)	1(1)	19(1)	9(1)
Cl(3)	57(1)	50(2)	53(1)	-3(1)	4(1)	1(1)
Cl(4)	60(2)	63(2)	46(1)	4(1)	16(1)	4(1)
N(1)	48(5)	50(5)	45(5)	6(4)	4(4)	-10(4)
N(2)	30(4)	59(5)	67(6)	4(5)	10(5)	-7(4)
N(3)	47(5)	64(5)	52(5)	5(4)	17(4)	9(4)
N(4)	53(6)	71(6)	34(5)	7(4)	13(4)	9(4)
N(5)	41(5)	71(6)	52(5)	1(4)	4(4)	1(4)
N(6)	52(5)	56(5)	43(5)	-9(4)	12(4)	1(4)
N(7)	37(5)	70(6)	56(5)	-2(5)	17(4)	-2(5)
N(8)	55(5)	56(5)	45(5)	-2(4)	19(4)	-12(5)
N(9)	43(5)	62(6)	55(5)	-8(5)	8(4)	0(4)
N(10)	46(5)	67(6)	54(5)	3(4)	20(4)	5(4)
O(1)	45(4)	62(4)	69(4)	2(3)	22(3)	5(3)
O(2)	52(4)	75(5)	70(4)	6(4)	25(3)	8(3)
V(1)	45(1)	58(1)	53(1)	6(1)	17(1)	4(1)
V(2)	47(1)	71(1)	50(1)	-1(1)	15(1)	-1(1)

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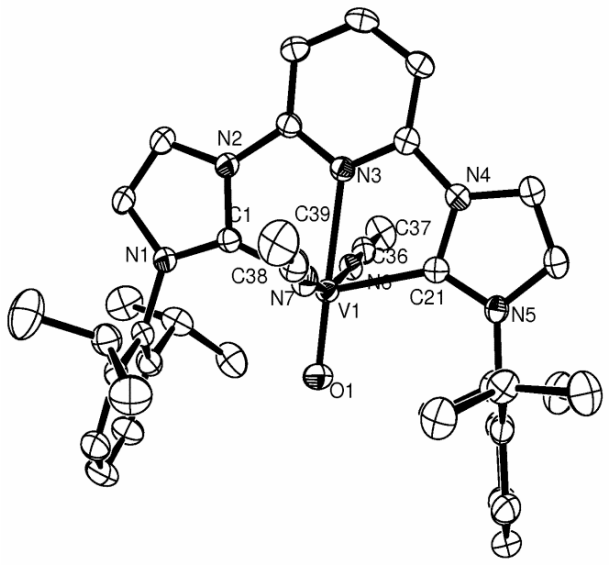
Structural Data for 7



Electronic Supplementary Information for Dalton Transactions

Table 1. Crystal data and structure refinement for **7**.

Identification code	**7**	
Empirical formula	C41 H50 B2 F8 N8 O V	
Formula weight	895.45	
Temperature	120(2) K	
Wavelength	0.71073 ≈	
Crystal system	Monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 16.851(3) ≈	α= 90∞.
	b = 12.707(4) ≈	β= 100.152(13)∞.
	c = 21.564(4) ≈	γ = 90∞.
Volume	4545.1(18) ≈^{3}	
Z	4	
Density (calculated)	1.309 Mg/m^3	
Absorption coefficient	0.292 mm^{-1}	
F(000)	1860	
Crystal size	0.50 x 0.20 x 0.02 mm^3	
Theta range for data collection	2.93 to 27.65∞.	
Index ranges	-21<=h<=21, -16<=k<=16, -28<=l<=28	
Reflections collected	66201	
Independent reflections	10463 [R(int) = 0.0687]	
Completeness to theta = 27.65∞	98.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9942 and 0.8634	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10463 / 0 / 561	
Goodness-of-fit on F^2	1.018	
Final R indices [I>2sigma(I)]	R1 = 0.0604, wR2 = 0.1382	
R indices (all data)	R1 = 0.0957, wR2 = 0.1564	
Largest diff. peak and hole	1.651 and -0.672 e.≈$^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (≈^{2}x 10^3) for **7**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
V(1)	2492(1)	212(1)	1120(1)	19(1)
F(4)	4568(2)	578(2)	3982(1)	81(1)
F(3)	5427(1)	532(1)	3301(1)	46(1)
F(8)	6623(2)	2124(2)	1380(1)	81(1)
O(1)	1588(1)	617(2)	932(1)	30(1)
F(2)	4381(1)	-598(2)	3184(1)	60(1)
F(1)	4148(1)	1119(2)	2997(1)	50(1)
N(4)	4055(1)	1385(2)	1572(1)	22(1)
N(7)	2848(1)	245(2)	239(1)	26(1)
C(36)	2557(2)	-120(2)	2608(1)	26(1)
C(38)	3132(2)	234(2)	-200(1)	30(1)
N(5)	3171(1)	2604(2)	1372(1)	22(1)
F(5)	7121(2)	907(2)	2111(1)	85(1)
N(2)	3209(1)	-1975(2)	1246(1)	23(1)
F(7)	7598(2)	2559(2)	2184(1)	94(1)
N(6)	2499(1)	6(2)	2081(1)	23(1)
C(25)	1857(2)	3244(2)	1554(1)	28(1)
F(6)	6361(2)	2209(2)	2339(1)	87(1)
C(26)	1153(2)	3803(2)	1327(2)	34(1)
C(40)	5120(2)	2247(3)	239(2)	44(1)
C(8)	-232(2)	-1938(3)	867(1)	36(1)
N(3)	3757(1)	-348(2)	1431(1)	21(1)
C(17)	4676(2)	-1776(2)	1669(1)	26(1)
C(2)	3115(2)	-3054(2)	1208(1)	29(1)
N(1)	1958(1)	-2235(2)	887(1)	23(1)
C(6)	19(2)	-1724(2)	-182(1)	34(1)
C(34)	3322(2)	4539(3)	46(2)	42(1)
C(22)	4466(2)	2325(2)	1714(1)	25(1)
C(37)	2610(2)	-243(3)	3284(1)	37(1)
C(29)	2299(2)	3577(2)	543(1)	26(1)

C(7)	-510(2)	-1752(3)	238(2)	38(1)
C(28)	1583(2)	4120(2)	341(1)	33(1)
C(21)	3249(2)	1553(2)	1360(1)	21(1)
C(27)	1020(2)	4237(2)	732(2)	36(1)
C(24)	2422(2)	3156(2)	1153(1)	24(1)
C(10)	888(2)	-2265(3)	1797(1)	35(1)
C(23)	3914(2)	3089(2)	1587(1)	26(1)
C(16)	3914(2)	-1373(2)	1459(1)	22(1)
C(5)	844(2)	-1887(2)	17(1)	27(1)
C(39)	3499(2)	213(3)	-762(1)	45(1)
C(30)	1984(2)	2766(2)	2209(1)	33(1)
C(9)	588(2)	-2088(2)	1099(1)	29(1)
C(18)	5281(2)	-1039(2)	1855(1)	28(1)
C(12)	594(2)	-1393(3)	2192(2)	43(1)
C(15)	1242(2)	-995(3)	-935(2)	48(1)
C(19)	5134(2)	34(2)	1838(1)	24(1)
C(20)	4344(2)	340(2)	1621(1)	22(1)
C(32)	1282(2)	2040(3)	2287(2)	42(1)
C(1)	2491(2)	-1460(2)	1055(1)	21(1)
N(8)	4747(2)	1500(3)	238(2)	62(1)
C(11)	650(2)	-3353(3)	2000(2)	48(1)
C(31)	2096(2)	3628(3)	2714(2)	51(1)
C(33)	2922(2)	3473(2)	116(1)	31(1)
C(13)	1412(2)	-1886(2)	-457(1)	32(1)
C(4)	1104(2)	-2069(2)	660(1)	24(1)
C(3)	2326(2)	-3220(2)	979(1)	29(1)
C(35)	2552(2)	3014(3)	-529(1)	39(1)
C(41)	5582(2)	3204(3)	247(2)	58(1)
C(14)	1381(3)	-2946(3)	-792(2)	60(1)
B(1)	4624(2)	407(3)	3372(2)	31(1)
B(2)	6950(2)	1946(3)	2009(2)	32(1)

Table 3. Bond lengths [≈] and angles [∞] for **7**.

V(1)-O(1)	1.5913(19)
V(1)-N(6)	2.087(2)
V(1)-N(7)	2.091(2)
V(1)-C(1)	2.129(3)
V(1)-C(21)	2.136(3)
V(1)-N(3)	2.236(2)
F(4)-B(1)	1.354(4)
F(3)-B(1)	1.397(4)
F(8)-B(2)	1.389(4)
F(2)-B(1)	1.380(4)
F(1)-B(1)	1.375(4)
N(4)-C(21)	1.372(3)
N(4)-C(22)	1.387(3)
N(4)-C(20)	1.413(3)
N(7)-C(38)	1.134(3)
C(36)-N(6)	1.133(3)
C(36)-C(37)	1.454(4)
C(38)-C(39)	1.455(4)
N(5)-C(21)	1.342(3)
N(5)-C(23)	1.399(3)
N(5)-C(24)	1.449(3)
F(5)-B(2)	1.362(4)
N(2)-C(1)	1.373(3)
N(2)-C(2)	1.380(3)
N(2)-C(16)	1.420(3)
F(7)-B(2)	1.341(4)
C(25)-C(26)	1.396(4)
C(25)-C(24)	1.397(4)
C(25)-C(30)	1.518(4)
F(6)-B(2)	1.360(4)
C(26)-C(27)	1.378(4)
C(26)-H(26)	0.9500
C(40)-N(8)	1.138(4)

C(40)-C(41)	1.442(5)
C(8)-C(7)	1.375(4)
C(8)-C(9)	1.396(4)
C(8)-H(8)	0.9500
N(3)-C(16)	1.328(3)
N(3)-C(20)	1.329(3)
C(17)-C(16)	1.382(4)
C(17)-C(18)	1.389(4)
C(17)-H(17)	0.9500
C(2)-C(3)	1.351(4)
C(2)-H(2)	0.9500
N(1)-C(1)	1.339(3)
N(1)-C(3)	1.395(3)
N(1)-C(4)	1.452(3)
C(6)-C(7)	1.380(4)
C(6)-C(5)	1.396(4)
C(6)-H(6)	0.9500
C(34)-C(33)	1.532(4)
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(22)-C(23)	1.339(4)
C(22)-H(22)	0.9500
C(37)-H(37A)	0.9800
C(37)-H(37B)	0.9800
C(37)-H(37C)	0.9800
C(29)-C(28)	1.391(4)
C(29)-C(24)	1.402(4)
C(29)-C(33)	1.520(4)
C(7)-H(7)	0.9500
C(28)-C(27)	1.384(4)
C(28)-H(28)	0.9500
C(27)-H(27)	0.9500
C(10)-C(9)	1.519(4)
C(10)-C(11)	1.524(5)

C(10)-C(12)	1.531(4)
C(10)-H(10)	1.0000
C(23)-H(23)	0.9500
C(5)-C(4)	1.397(4)
C(5)-C(13)	1.518(4)
C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
C(30)-C(32)	1.533(4)
C(30)-C(31)	1.533(4)
C(30)-H(30)	1.0000
C(9)-C(4)	1.395(4)
C(18)-C(19)	1.385(4)
C(18)-H(18)	0.9500
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(15)-C(13)	1.524(4)
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(19)-C(20)	1.386(4)
C(19)-H(19)	0.9500
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(33)-C(35)	1.535(4)
C(33)-H(33)	1.0000
C(13)-C(14)	1.525(4)

C(13)-H(13)	1.0000
C(3)-H(3)	0.9500
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(41)-H(41A)	0.9800
C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800

O(1)-V(1)-N(6)	97.58(9)
O(1)-V(1)-N(7)	100.15(9)
N(6)-V(1)-N(7)	162.27(9)
O(1)-V(1)-C(1)	108.46(10)
N(6)-V(1)-C(1)	86.58(9)
N(7)-V(1)-C(1)	87.51(9)
O(1)-V(1)-C(21)	107.91(10)
N(6)-V(1)-C(21)	87.82(9)
N(7)-V(1)-C(21)	87.06(9)
C(1)-V(1)-C(21)	143.63(10)
O(1)-V(1)-N(3)	177.39(9)
N(6)-V(1)-N(3)	79.87(8)
N(7)-V(1)-N(3)	82.40(8)
C(1)-V(1)-N(3)	72.04(9)
C(21)-V(1)-N(3)	71.59(9)
C(21)-N(4)-C(22)	111.5(2)
C(21)-N(4)-C(20)	118.7(2)
C(22)-N(4)-C(20)	129.9(2)
C(38)-N(7)-V(1)	171.7(2)
N(6)-C(36)-C(37)	177.6(3)
N(7)-C(38)-C(39)	179.6(4)
C(21)-N(5)-C(23)	111.1(2)
C(21)-N(5)-C(24)	123.9(2)

C(23)-N(5)-C(24)	124.9(2)
C(1)-N(2)-C(2)	111.7(2)
C(1)-N(2)-C(16)	118.9(2)
C(2)-N(2)-C(16)	129.4(2)
C(36)-N(6)-V(1)	175.3(2)
C(26)-C(25)-C(24)	116.9(3)
C(26)-C(25)-C(30)	120.1(3)
C(24)-C(25)-C(30)	123.0(2)
C(27)-C(26)-C(25)	121.3(3)
C(27)-C(26)-H(26)	119.4
C(25)-C(26)-H(26)	119.4
N(8)-C(40)-C(41)	178.9(4)
C(7)-C(8)-C(9)	121.4(3)
C(7)-C(8)-H(8)	119.3
C(9)-C(8)-H(8)	119.3
C(16)-N(3)-C(20)	120.0(2)
C(16)-N(3)-V(1)	119.82(16)
C(20)-N(3)-V(1)	120.10(17)
C(16)-C(17)-C(18)	115.9(3)
C(16)-C(17)-H(17)	122.0
C(18)-C(17)-H(17)	122.0
C(3)-C(2)-N(2)	105.8(2)
C(3)-C(2)-H(2)	127.1
N(2)-C(2)-H(2)	127.1
C(1)-N(1)-C(3)	111.2(2)
C(1)-N(1)-C(4)	124.2(2)
C(3)-N(1)-C(4)	124.5(2)
C(7)-C(6)-C(5)	121.2(3)
C(7)-C(6)-H(6)	119.4
C(5)-C(6)-H(6)	119.4
C(33)-C(34)-H(34A)	109.5
C(33)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(33)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5

H(34B)-C(34)-H(34C)	109.5
C(23)-C(22)-N(4)	106.1(2)
C(23)-C(22)-H(22)	127.0
N(4)-C(22)-H(22)	127.0
C(36)-C(37)-H(37A)	109.5
C(36)-C(37)-H(37B)	109.5
H(37A)-C(37)-H(37B)	109.5
C(36)-C(37)-H(37C)	109.5
H(37A)-C(37)-H(37C)	109.5
H(37B)-C(37)-H(37C)	109.5
C(28)-C(29)-C(24)	117.4(3)
C(28)-C(29)-C(33)	120.5(2)
C(24)-C(29)-C(33)	122.2(2)
C(8)-C(7)-C(6)	120.3(3)
C(8)-C(7)-H(7)	119.9
C(6)-C(7)-H(7)	119.9
C(27)-C(28)-C(29)	120.8(3)
C(27)-C(28)-H(28)	119.6
C(29)-C(28)-H(28)	119.6
N(5)-C(21)-N(4)	104.0(2)
N(5)-C(21)-V(1)	137.87(18)
N(4)-C(21)-V(1)	118.09(17)
C(26)-C(27)-C(28)	120.5(3)
C(26)-C(27)-H(27)	119.8
C(28)-C(27)-H(27)	119.8
C(25)-C(24)-C(29)	123.1(2)
C(25)-C(24)-N(5)	119.1(2)
C(29)-C(24)-N(5)	117.8(2)
C(9)-C(10)-C(11)	111.1(3)
C(9)-C(10)-C(12)	111.0(3)
C(11)-C(10)-C(12)	111.7(3)
C(9)-C(10)-H(10)	107.6
C(11)-C(10)-H(10)	107.6
C(12)-C(10)-H(10)	107.6
C(22)-C(23)-N(5)	107.3(2)

C(22)-C(23)-H(23)	126.4
N(5)-C(23)-H(23)	126.4
N(3)-C(16)-C(17)	122.9(2)
N(3)-C(16)-N(2)	111.4(2)
C(17)-C(16)-N(2)	125.7(2)
C(4)-C(5)-C(6)	116.8(3)
C(4)-C(5)-C(13)	122.9(2)
C(6)-C(5)-C(13)	120.3(2)
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(25)-C(30)-C(32)	111.0(3)
C(25)-C(30)-C(31)	110.8(3)
C(32)-C(30)-C(31)	110.7(3)
C(25)-C(30)-H(30)	108.1
C(32)-C(30)-H(30)	108.1
C(31)-C(30)-H(30)	108.1
C(4)-C(9)-C(8)	116.7(3)
C(4)-C(9)-C(10)	122.5(2)
C(8)-C(9)-C(10)	120.8(3)
C(19)-C(18)-C(17)	122.5(2)
C(19)-C(18)-H(18)	118.8
C(17)-C(18)-H(18)	118.8
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(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(18)-C(19)-C(20)	116.2(2)
C(18)-C(19)-H(19)	121.9
C(20)-C(19)-H(19)	121.9
N(3)-C(20)-C(19)	122.5(2)
N(3)-C(20)-N(4)	111.5(2)
C(19)-C(20)-N(4)	126.0(2)
C(30)-C(32)-H(32A)	109.5
C(30)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(30)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
N(1)-C(1)-N(2)	104.1(2)
N(1)-C(1)-V(1)	138.13(18)
N(2)-C(1)-V(1)	117.77(17)
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(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(29)-C(33)-C(34)	110.2(2)
C(29)-C(33)-C(35)	111.6(2)
C(34)-C(33)-C(35)	111.2(2)
C(29)-C(33)-H(33)	107.9
C(34)-C(33)-H(33)	107.9

C(35)-C(33)-H(33)	107.9
C(5)-C(13)-C(14)	110.2(3)
C(5)-C(13)-C(15)	113.0(3)
C(14)-C(13)-C(15)	110.4(3)
C(5)-C(13)-H(13)	107.7
C(14)-C(13)-H(13)	107.7
C(15)-C(13)-H(13)	107.7
C(9)-C(4)-C(5)	123.5(2)
C(9)-C(4)-N(1)	117.9(2)
C(5)-C(4)-N(1)	118.6(2)
C(2)-C(3)-N(1)	107.2(2)
C(2)-C(3)-H(3)	126.4
N(1)-C(3)-H(3)	126.4
C(33)-C(35)-H(35A)	109.5
C(33)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(33)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(40)-C(41)-H(41A)	109.5
C(40)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
C(40)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
C(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
F(4)-B(1)-F(1)	109.4(3)
F(4)-B(1)-F(2)	111.5(3)
F(1)-B(1)-F(2)	108.9(3)
F(4)-B(1)-F(3)	108.9(3)

F(1)-B(1)-F(3)	109.6(2)
F(2)-B(1)-F(3)	108.4(3)
F(7)-B(2)-F(6)	110.0(3)
F(7)-B(2)-F(5)	112.3(3)
F(6)-B(2)-F(5)	107.8(3)
F(7)-B(2)-F(8)	110.1(3)
F(6)-B(2)-F(8)	105.8(3)
F(5)-B(2)-F(8)	110.6(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\approx^2$x 10^3)for **7**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
V(1)	20(1)	20(1)	18(1)	1(1)	2(1)	1(1)
F(4)	92(2)	123(2)	32(1)	-4(1)	18(1)	1(2)
F(3)	32(1)	39(1)	67(1)	-9(1)	9(1)	-10(1)
F(8)	112(2)	64(2)	51(1)	-6(1)	-31(1)	14(1)
O(1)	26(1)	31(1)	32(1)	1(1)	1(1)	5(1)
F(2)	43(1)	34(1)	106(2)	-7(1)	16(1)	-11(1)
F(1)	46(1)	44(1)	55(1)	11(1)	-3(1)	-1(1)
N(4)	21(1)	25(1)	20(1)	0(1)	4(1)	-1(1)
N(7)	32(1)	26(1)	19(1)	0(1)	4(1)	-2(1)
C(36)	26(1)	26(1)	27(1)	-2(1)	5(1)	-2(1)
C(38)	37(2)	29(1)	23(1)	0(1)	2(1)	-1(1)
N(5)	24(1)	21(1)	21(1)	0(1)	5(1)	-1(1)
F(5)	115(2)	39(1)	85(2)	-6(1)	-28(2)	22(1)
N(2)	24(1)	20(1)	24(1)	-1(1)	1(1)	2(1)
F(7)	64(2)	91(2)	110(2)	36(2)	-33(2)	-36(1)
N(6)	23(1)	23(1)	23(1)	0(1)	3(1)	-2(1)
C(25)	29(1)	24(1)	32(2)	-2(1)	8(1)	-2(1)
F(6)	76(2)	118(2)	72(2)	13(2)	27(1)	35(2)
C(26)	29(2)	30(2)	43(2)	-4(1)	9(1)	0(1)
C(40)	45(2)	49(2)	38(2)	-5(2)	6(2)	-5(2)
C(8)	25(1)	45(2)	38(2)	2(1)	5(1)	0(1)
N(3)	21(1)	23(1)	19(1)	0(1)	3(1)	0(1)
C(17)	26(1)	28(1)	25(1)	3(1)	4(1)	5(1)
C(2)	31(2)	21(1)	34(2)	-1(1)	1(1)	3(1)
N(1)	24(1)	22(1)	23(1)	-2(1)	1(1)	1(1)
C(6)	35(2)	34(2)	29(2)	1(1)	-5(1)	1(1)
C(34)	48(2)	44(2)	36(2)	-2(1)	12(1)	-11(2)
C(22)	28(1)	26(1)	21(1)	1(1)	3(1)	-5(1)
C(37)	42(2)	48(2)	23(1)	1(1)	11(1)	-8(2)
C(29)	31(1)	20(1)	28(1)	-2(1)	2(1)	-3(1)

C(7)	24(1)	46(2)	41(2)	2(1)	-3(1)	0(1)
C(28)	38(2)	25(1)	33(2)	2(1)	0(1)	2(1)
C(21)	23(1)	24(1)	16(1)	1(1)	5(1)	1(1)
C(27)	29(2)	28(2)	47(2)	-2(1)	-1(1)	5(1)
C(24)	26(1)	18(1)	28(1)	-1(1)	3(1)	-1(1)
C(10)	28(2)	48(2)	28(2)	3(1)	5(1)	-1(1)
C(23)	31(1)	25(1)	23(1)	-1(1)	5(1)	-7(1)
C(16)	21(1)	25(1)	19(1)	0(1)	3(1)	0(1)
C(5)	29(1)	23(1)	27(1)	-4(1)	-1(1)	-1(1)
C(39)	59(2)	52(2)	27(2)	-3(1)	17(1)	1(2)
C(30)	38(2)	30(2)	33(2)	1(1)	15(1)	1(1)
C(9)	27(1)	30(2)	29(1)	0(1)	1(1)	-2(1)
C(18)	21(1)	41(2)	23(1)	7(1)	3(1)	5(1)
C(12)	40(2)	57(2)	34(2)	-6(2)	10(1)	-9(2)
C(15)	54(2)	53(2)	36(2)	12(2)	7(2)	4(2)
C(19)	22(1)	31(2)	20(1)	3(1)	3(1)	-1(1)
C(20)	26(1)	24(1)	16(1)	1(1)	6(1)	0(1)
C(32)	45(2)	38(2)	50(2)	6(2)	26(2)	4(1)
C(1)	22(1)	24(1)	16(1)	0(1)	2(1)	1(1)
N(8)	67(2)	64(2)	59(2)	-15(2)	17(2)	-22(2)
C(11)	56(2)	52(2)	38(2)	11(2)	14(2)	6(2)
C(31)	73(2)	46(2)	35(2)	-7(2)	11(2)	-4(2)
C(33)	38(2)	30(2)	25(1)	2(1)	7(1)	2(1)
C(13)	34(2)	36(2)	25(1)	-3(1)	3(1)	2(1)
C(4)	23(1)	22(1)	26(1)	-3(1)	-1(1)	-1(1)
C(3)	33(2)	19(1)	33(2)	-3(1)	-1(1)	2(1)
C(35)	51(2)	39(2)	28(2)	0(1)	10(1)	-2(2)
C(41)	64(2)	48(2)	58(2)	10(2)	-4(2)	-13(2)
C(14)	78(3)	48(2)	60(2)	-17(2)	31(2)	-3(2)
B(1)	33(2)	30(2)	31(2)	0(1)	8(1)	-4(1)
B(2)	30(2)	32(2)	32(2)	-5(1)	3(1)	-1(1)

Electronic Supplementary Information for Dalton Transactions

Structural Data for 9

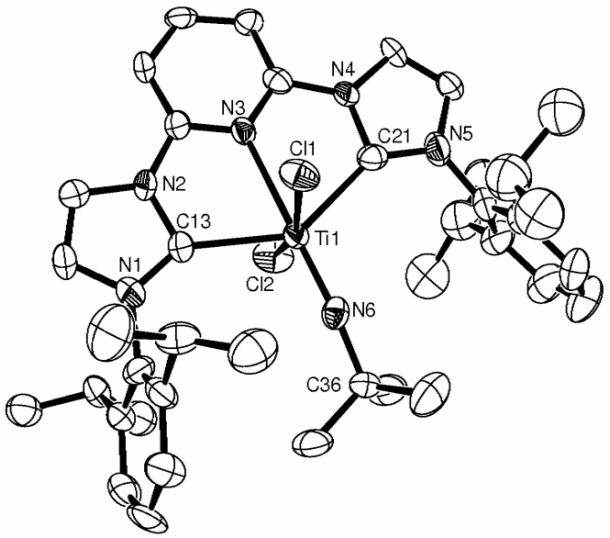


Table 1. Crystal data and structure refinement for **9**.

Identification code	05dcp024	
Empirical formula	C39 H49 Cl2 N6 O0 Ti	
Formula weight	720.64	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P212121	
Unit cell dimensions	a = 10.802(9) Å	α= 90°.
	b = 13.630(13) Å	β= 90°.
	c = 32.45(2) Å	γ = 90°.
Volume	4778(7) Å^3	
Z	4	
Density (calculated)	1.002 Mg/m^3	
Absorption coefficient	0.319 mm^{-1}	
F(000)	1524	
Crystal size	0.20 x 0.16 x 0.04 mm^3	
Theta range for data collection	2.92 to 27.49°.	

Index ranges	-13<=h<=14, -17<=k<=17, -41<=l<=41
Reflections collected	33304
Independent reflections	10871 [R(int) = 0.1118]
Completeness to theta = 27.49°	99.4 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9873 and 0.9389
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10871 / 122 / 477
Goodness-of-fit on F^2	0.973
Final R indices [I>2sigma(I)]	R1 = 0.0944, wR2 = 0.1944
R indices (all data)	R1 = 0.1728, wR2 = 0.2221
Absolute structure parameter	0.15(5)
Largest diff. peak and hole	0.414 and -0.310 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **9**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ti(1)	7673(1)	8761(1)	8237(1)	27(1)
Cl(2)	6297(2)	7430(1)	8059(1)	49(1)
Cl(1)	9266(1)	10018(1)	8186(1)	43(1)
C(7)	3174(6)	9585(5)	7781(2)	39(2)
N(4)	9676(4)	7295(3)	7885(1)	28(1)
N(3)	8391(4)	8399(3)	7576(1)	28(1)
N(5)	9828(5)	7008(4)	8530(2)	40(1)
N(2)	6983(4)	9540(4)	7364(1)	35(1)
C(3)	2894(6)	10738(5)	8377(2)	50(2)
C(19)	9629(5)	7433(4)	7125(2)	31(1)
C(2)	3657(6)	10326(4)	8077(2)	39(2)
C(22)	10564(5)	6554(4)	7926(2)	35(2)
C(9)	2657(7)	8682(5)	8005(2)	55(2)
C(6)	5349(5)	11423(5)	8324(2)	42(2)
N(1)	5692(5)	10338(3)	7729(1)	38(1)
C(5)	4550(6)	11794(5)	8615(2)	49(2)
C(36)	6377(5)	8899(4)	9099(2)	38(2)
C(8)	2196(6)	10049(5)	7499(2)	51(2)
N(6)	7102(4)	8931(3)	8712(1)	34(1)
C(14)	5507(6)	10630(5)	7321(2)	46(2)
C(1)	4878(6)	10701(5)	8062(2)	38(2)
C(12)	7353(8)	11872(6)	8678(2)	70(2)
C(17)	8233(5)	8615(5)	6852(2)	39(2)
C(4)	3321(6)	11442(5)	8650(2)	53(2)
C(20)	9239(5)	7721(4)	7515(2)	31(1)
C(23)	10665(5)	6386(5)	8326(2)	41(2)
C(24)	9533(6)	6925(5)	8962(2)	46(2)
C(10)	6620(6)	11834(5)	8280(2)	46(2)
C(16)	7897(5)	8842(5)	7254(2)	34(1)
C(13)	6580(5)	9656(4)	7767(2)	34(1)

C(25)	8820(7)	6136(5)	9097(2)	52(2)
C(21)	9182(5)	7587(4)	8266(2)	35(1)
C(33A)	10892(7)	8480(6)	9087(3)	77(2)
C(35A)	12157(13)	7895(14)	9091(6)	78(3)
C(34A)	11090(20)	9302(12)	9396(5)	85(4)
C(33B)	10892(7)	8480(6)	9087(3)	77(2)
C(35B)	12209(10)	8696(13)	9226(4)	78(3)
C(34B)	10255(16)	9468(9)	9226(5)	85(4)
C(28)	9873(8)	7416(8)	9658(2)	86(3)
C(15)	6326(6)	10153(5)	7093(2)	49(2)
C(27)	9186(9)	6624(7)	9782(2)	80(3)
C(29)	10090(6)	7616(6)	9240(2)	56(2)
C(26)	8667(8)	6018(6)	9508(2)	69(2)
C(30A)	8280(7)	5398(6)	8790(3)	71(2)
C(31A)	6868(12)	5260(40)	8807(11)	93(4)
C(32A)	8780(20)	4382(9)	8687(9)	68(3)
C(30B)	8280(7)	5398(6)	8790(3)	71(2)
C(31B)	6902(11)	5280(40)	8893(9)	93(4)
C(32B)	9031(15)	4446(10)	8881(8)	68(3)
C(11)	6562(8)	12810(6)	8051(2)	79(3)
C(18)	9083(5)	7905(5)	6796(2)	37(2)
C(37A)	5277(8)	9602(7)	9080(3)	53(2)
C(39A)	5938(9)	7828(6)	9162(3)	56(3)
C(38A)	7215(10)	9186(9)	9465(2)	67(3)
C(37B)	5029(11)	8790(20)	8950(6)	53(2)
C(39B)	7000(20)	8192(17)	9406(6)	56(3)
C(38B)	6530(30)	9865(13)	9336(7)	67(3)

Table 3. Bond lengths [Å] and angles [°] for **9**

Ti(1)-N(6)	1.677(5)	C(6)-C(5)	1.376(8)
Ti(1)-C(13)	2.281(6)	C(6)-C(1)	1.397(8)
Ti(1)-C(21)	2.286(6)	C(6)-C(10)	1.490(8)
Ti(1)-N(3)	2.332(5)	N(1)-C(13)	1.342(7)
Ti(1)-Cl(2)	2.415(2)	N(1)-C(14)	1.396(7)
Ti(1)-Cl(1)	2.433(2)	N(1)-C(1)	1.477(7)
C(7)-C(2)	1.486(9)	C(5)-C(4)	1.416(9)
C(7)-C(9)	1.535(9)	C(5)-H(5)	0.9500
C(7)-C(8)	1.536(8)	C(36)-N(6)	1.481(7)
C(7)-H(7)	1.0000	C(36)-C(37A)	1.528(7)
N(4)-C(22)	1.398(7)	C(36)-C(38B)	1.534(10)
N(4)-C(21)	1.406(7)	C(36)-C(39B)	1.540(10)
N(4)-C(20)	1.416(7)	C(36)-C(37B)	1.541(10)
N(3)-C(20)	1.316(7)	C(36)-C(38A)	1.543(8)
N(3)-C(16)	1.320(7)	C(36)-C(39A)	1.547(8)
N(5)-C(21)	1.356(7)	C(8)-H(8A)	0.9800
N(5)-C(23)	1.403(7)	C(8)-H(8B)	0.9800
N(5)-C(24)	1.444(8)	C(8)-H(8C)	0.9800
N(2)-C(13)	1.389(7)	C(14)-C(15)	1.324(9)
N(2)-C(15)	1.405(7)	C(14)-H(14)	0.9500
N(2)-C(16)	1.416(7)	C(12)-C(10)	1.516(10)
C(3)-C(4)	1.385(9)	C(12)-H(12A)	0.9800
C(3)-C(2)	1.394(9)	C(12)-H(12B)	0.9800
C(3)-H(3)	0.9500	C(12)-H(12C)	0.9800
C(19)-C(18)	1.379(8)	C(17)-C(18)	1.347(8)
C(19)-C(20)	1.390(7)	C(17)-C(16)	1.388(8)
C(19)-H(19)	0.9500	C(17)-H(17)	0.9500
C(2)-C(1)	1.416(9)	C(4)-H(4)	0.9500
C(22)-C(23)	1.323(7)	C(23)-H(23)	0.9500
C(22)-H(22)	0.9500	C(24)-C(25)	1.394(9)
C(9)-H(9A)	0.9800	C(24)-C(29)	1.435(10)
C(9)-H(9B)	0.9800	C(10)-C(11)	1.525(9)
C(9)-H(9C)	0.9800	C(10)-H(10)	1.0000

C(25)-C(26)	1.355(9)	C(32A)-H(32A)	0.9800
C(25)-C(30A)	1.530(10)	C(32A)-H(32B)	0.9800
C(33A)-C(34A)	1.520(9)	C(32A)-H(32C)	0.9800
C(33A)-C(29)	1.544(11)	C(31B)-H(31D)	0.9800
C(33A)-C(35A)	1.581(9)	C(31B)-H(31E)	0.9800
C(33A)-H(33A)	1.0000	C(31B)-H(31F)	0.9800
C(35A)-H(35A)	0.9800	C(32B)-H(32D)	0.9800
C(35A)-H(35B)	0.9800	C(32B)-H(32E)	0.9800
C(35A)-H(35C)	0.9800	C(32B)-H(32F)	0.9800
C(34A)-H(34A)	0.9800	C(11)-H(11A)	0.9800
C(34A)-H(34B)	0.9800	C(11)-H(11B)	0.9800
C(34A)-H(34C)	0.9800	C(11)-H(11C)	0.9800
C(35B)-H(35D)	0.9800	C(18)-H(18)	0.9500
C(35B)-H(35E)	0.9800	C(37A)-H(37A)	0.9800
C(35B)-H(35F)	0.9800	C(37A)-H(37B)	0.9800
C(34B)-H(34D)	0.9800	C(37A)-H(37C)	0.9800
C(34B)-H(34E)	0.9800	C(39A)-H(39A)	0.9800
C(34B)-H(34F)	0.9800	C(39A)-H(39B)	0.9800
C(28)-C(27)	1.370(12)	C(39A)-H(39C)	0.9800
C(28)-C(29)	1.404(9)	C(38A)-H(38A)	0.9800
C(28)-H(28)	0.9500	C(38A)-H(38B)	0.9800
C(15)-H(15)	0.9500	C(38A)-H(38C)	0.9800
C(27)-C(26)	1.336(11)	C(37B)-H(37D)	0.9800
C(27)-H(27)	0.9500	C(37B)-H(37E)	0.9800
C(26)-H(26)	0.9500	C(37B)-H(37F)	0.9800
C(30A)-C(32A)	1.523(9)	C(39B)-H(39D)	0.9800
C(30A)-C(31A)	1.538(10)	C(39B)-H(39E)	0.9800
C(30A)-H(30A)	1.0000	C(39B)-H(39F)	0.9800
C(31A)-H(31A)	0.9800	C(38B)-H(38D)	0.9800
C(31A)-H(31B)	0.9800	C(38B)-H(38E)	0.9800
C(31A)-H(31C)	0.9800	C(38B)-H(38F)	0.9800

N(6)-Ti(1)-C(13)	110.5(2)	N(6)-Ti(1)-N(3)	175.3(2)
N(6)-Ti(1)-C(21)	108.7(2)	C(13)-Ti(1)-N(3)	70.82(19)
C(13)-Ti(1)-C(21)	140.5(2)	C(21)-Ti(1)-N(3)	69.77(18)

N(6)-Ti(1)-Cl(2)	95.56(17)	C(1)-C(2)-C(7)	123.3(6)
C(13)-Ti(1)-Cl(2)	85.62(17)	C(23)-C(22)-N(4)	106.0(5)
C(21)-Ti(1)-Cl(2)	85.59(17)	C(23)-C(22)-H(22)	127.0
N(3)-Ti(1)-Cl(2)	79.99(12)	N(4)-C(22)-H(22)	127.0
N(6)-Ti(1)-Cl(1)	102.99(17)	C(7)-C(9)-H(9A)	109.5
C(13)-Ti(1)-Cl(1)	86.82(17)	C(7)-C(9)-H(9B)	109.5
C(21)-Ti(1)-Cl(1)	89.53(16)	H(9A)-C(9)-H(9B)	109.5
N(3)-Ti(1)-Cl(1)	81.49(12)	C(7)-C(9)-H(9C)	109.5
Cl(2)-Ti(1)-Cl(1)	161.42(7)	H(9A)-C(9)-H(9C)	109.5
C(2)-C(7)-C(9)	111.5(5)	H(9B)-C(9)-H(9C)	109.5
C(2)-C(7)-C(8)	110.3(5)	C(5)-C(6)-C(1)	116.7(6)
C(9)-C(7)-C(8)	111.2(6)	C(5)-C(6)-C(10)	120.4(6)
C(2)-C(7)-H(7)	107.9	C(1)-C(6)-C(10)	122.8(6)
C(9)-C(7)-H(7)	107.9	C(13)-N(1)-C(14)	112.8(5)
C(8)-C(7)-H(7)	107.9	C(13)-N(1)-C(1)	126.1(5)
C(22)-N(4)-C(21)	112.4(5)	C(14)-N(1)-C(1)	120.8(5)
C(22)-N(4)-C(20)	127.4(5)	C(6)-C(5)-C(4)	121.2(6)
C(21)-N(4)-C(20)	120.2(5)	C(6)-C(5)-H(5)	119.4
C(20)-N(3)-C(16)	118.9(5)	C(4)-C(5)-H(5)	119.4
C(20)-N(3)-Ti(1)	121.2(4)	N(6)-C(36)-C(37A)	110.9(5)
C(16)-N(3)-Ti(1)	119.8(4)	N(6)-C(36)-C(38B)	110.0(11)
C(21)-N(5)-C(23)	112.8(5)	C(37A)-C(36)-C(38B)	64.4(12)
C(21)-N(5)-C(24)	123.0(5)	N(6)-C(36)-C(39B)	109.6(10)
C(23)-N(5)-C(24)	123.5(5)	C(37A)-C(36)-C(39B)	139.4(11)
C(13)-N(2)-C(15)	111.3(5)	C(38B)-C(36)-C(39B)	99.5(15)
C(13)-N(2)-C(16)	122.2(5)	N(6)-C(36)-C(37B)	103.7(9)
C(15)-N(2)-C(16)	126.4(5)	C(37A)-C(36)-C(37B)	46.8(10)
C(4)-C(3)-C(2)	121.9(7)	C(38B)-C(36)-C(37B)	110.3(16)
C(4)-C(3)-H(3)	119.0	C(39B)-C(36)-C(37B)	123.6(15)
C(2)-C(3)-H(3)	119.0	N(6)-C(36)-C(38A)	109.6(6)
C(18)-C(19)-C(20)	116.2(5)	C(37A)-C(36)-C(38A)	109.2(7)
C(18)-C(19)-H(19)	121.9	C(38B)-C(36)-C(38A)	48.1(11)
C(20)-C(19)-H(19)	121.9	C(39B)-C(36)-C(38A)	53.5(11)
C(3)-C(2)-C(1)	115.5(6)	C(37B)-C(36)-C(38A)	145.1(10)
C(3)-C(2)-C(7)	121.1(6)	N(6)-C(36)-C(39A)	107.5(5)

C(37A)-C(36)-C(39A)	111.0(6)	N(5)-C(23)-H(23)	126.2
C(38B)-C(36)-C(39A)	141.0(11)	C(25)-C(24)-C(29)	122.8(6)
C(39B)-C(36)-C(39A)	57.3(11)	C(25)-C(24)-N(5)	119.2(6)
C(37B)-C(36)-C(39A)	70.0(11)	C(29)-C(24)-N(5)	117.8(6)
C(38A)-C(36)-C(39A)	108.5(7)	C(6)-C(10)-C(12)	114.4(6)
C(7)-C(8)-H(8A)	109.5	C(6)-C(10)-C(11)	109.7(6)
C(7)-C(8)-H(8B)	109.5	C(12)-C(10)-C(11)	114.0(6)
H(8A)-C(8)-H(8B)	109.5	C(6)-C(10)-H(10)	106.0
C(7)-C(8)-H(8C)	109.5	C(12)-C(10)-H(10)	106.0
H(8A)-C(8)-H(8C)	109.5	C(11)-C(10)-H(10)	106.0
H(8B)-C(8)-H(8C)	109.5	N(3)-C(16)-C(17)	122.5(5)
C(36)-N(6)-Ti(1)	166.1(4)	N(3)-C(16)-N(2)	112.9(5)
C(15)-C(14)-N(1)	107.1(6)	C(17)-C(16)-N(2)	124.6(5)
C(15)-C(14)-H(14)	126.4	N(1)-C(13)-N(2)	102.4(5)
N(1)-C(14)-H(14)	126.4	N(1)-C(13)-Ti(1)	143.4(4)
C(6)-C(1)-C(2)	124.9(6)	N(2)-C(13)-Ti(1)	114.0(4)
C(6)-C(1)-N(1)	117.7(6)	C(26)-C(25)-C(24)	117.9(7)
C(2)-C(1)-N(1)	117.3(5)	C(26)-C(25)-C(30A)	121.1(7)
C(10)-C(12)-H(12A)	109.5	C(24)-C(25)-C(30A)	120.9(6)
C(10)-C(12)-H(12B)	109.5	N(5)-C(21)-N(4)	101.2(5)
H(12A)-C(12)-H(12B)	109.5	N(5)-C(21)-Ti(1)	143.2(4)
C(10)-C(12)-H(12C)	109.5	N(4)-C(21)-Ti(1)	115.6(4)
H(12A)-C(12)-H(12C)	109.5	C(34A)-C(33A)-C(29)	115.5(10)
H(12B)-C(12)-H(12C)	109.5	C(34A)-C(33A)-C(35A)	104.2(12)
C(18)-C(17)-C(16)	117.6(5)	C(29)-C(33A)-C(35A)	95.6(9)
C(18)-C(17)-H(17)	121.2	C(34A)-C(33A)-H(33A)	113.3
C(16)-C(17)-H(17)	121.2	C(29)-C(33A)-H(33A)	113.3
C(3)-C(4)-C(5)	119.7(6)	C(35A)-C(33A)-H(33A)	113.3
C(3)-C(4)-H(4)	120.1	H(35D)-C(35B)-H(35E)	109.5
C(5)-C(4)-H(4)	120.1	H(35D)-C(35B)-H(35F)	109.5
N(3)-C(20)-C(19)	123.2(5)	H(35E)-C(35B)-H(35F)	109.5
N(3)-C(20)-N(4)	113.2(5)	H(34D)-C(34B)-H(34E)	109.5
C(19)-C(20)-N(4)	123.6(5)	H(34D)-C(34B)-H(34F)	109.5
C(22)-C(23)-N(5)	107.7(5)	H(34E)-C(34B)-H(34F)	109.5
C(22)-C(23)-H(23)	126.2	C(27)-C(28)-C(29)	121.7(9)

C(27)-C(28)-H(28)	119.1	C(36)-C(38A)-H(38A)	109.5
C(29)-C(28)-H(28)	119.1	C(36)-C(38A)-H(38B)	109.5
C(14)-C(15)-N(2)	106.3(6)	C(36)-C(38A)-H(38C)	109.5
C(14)-C(15)-H(15)	126.9	C(36)-C(37B)-H(37D)	109.5
N(2)-C(15)-H(15)	126.9	C(36)-C(37B)-H(37E)	109.5
C(26)-C(27)-C(28)	121.3(7)	C(36)-C(37B)-H(37F)	109.5
C(26)-C(27)-H(27)	119.3	C(36)-C(39B)-H(39D)	109.5
C(28)-C(27)-H(27)	119.3	C(36)-C(39B)-H(39E)	109.5
C(28)-C(29)-C(24)	114.2(8)	C(36)-C(39B)-H(39F)	109.5
C(28)-C(29)-C(33A)	123.5(8)	C(36)-C(38B)-H(38D)	109.5
C(24)-C(29)-C(33A)	122.3(6)	C(36)-C(38B)-H(38E)	109.5
C(27)-C(26)-C(25)	122.0(8)	C(36)-C(38B)-H(38F)	109.5
C(27)-C(26)-H(26)	119.0		
C(25)-C(26)-H(26)	119.0		
C(32A)-C(30A)-C(25)	127.3(13)		
C(32A)-C(30A)-C(31A)	104(3)		
C(25)-C(30A)-C(31A)	116(2)		
C(32A)-C(30A)-H(30A)	101.8		
C(25)-C(30A)-H(30A)	101.8		
C(31A)-C(30A)-H(30A)	101.8		
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(17)-C(18)-C(19)	121.6(5)		
C(17)-C(18)-H(18)	119.2		
C(19)-C(18)-H(18)	119.2		
C(36)-C(37A)-H(37A)	109.5		
C(36)-C(37A)-H(37B)	109.5		
C(36)-C(37A)-H(37C)	109.5		
C(36)-C(39A)-H(39A)	109.5		
C(36)-C(39A)-H(39B)	109.5		
C(36)-C(39A)-H(39C)	109.5		

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **9**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ti(1)	23(1)	29(1)	29(1)	1(1)	0(1)	0(1)
Cl(2)	39(1)	45(1)	64(1)	-15(1)	6(1)	-17(1)
Cl(1)	31(1)	38(1)	60(1)	-1(1)	9(1)	-6(1)
C(7)	30(4)	45(4)	43(4)	3(3)	-6(3)	6(3)
N(4)	19(3)	33(3)	31(3)	2(2)	0(2)	-1(2)
N(3)	24(3)	32(3)	27(2)	-3(2)	-5(2)	2(2)
N(5)	40(3)	41(3)	40(3)	2(3)	-8(2)	11(3)
N(2)	35(3)	41(3)	30(3)	14(2)	-1(2)	6(3)
C(3)	27(4)	71(5)	51(4)	-4(4)	-8(3)	10(3)
C(19)	34(4)	30(3)	28(3)	-8(3)	3(3)	2(3)
C(2)	39(4)	39(4)	38(3)	5(3)	5(3)	13(3)
C(22)	23(3)	37(3)	45(4)	1(3)	-5(3)	10(3)
C(9)	51(4)	58(4)	56(4)	-3(4)	1(4)	5(4)
C(6)	29(3)	51(4)	44(4)	-6(3)	-3(3)	14(3)
N(1)	34(3)	38(3)	40(3)	0(2)	0(2)	11(3)
C(5)	38(4)	55(4)	54(4)	-15(4)	0(3)	2(4)
C(36)	37(4)	43(4)	34(3)	-2(3)	8(3)	11(3)
C(8)	48(4)	54(4)	50(4)	-7(4)	3(3)	5(4)
N(6)	36(3)	33(3)	32(2)	5(2)	-3(2)	-3(2)
C(14)	41(4)	55(4)	41(4)	18(3)	-6(3)	13(4)
C(1)	50(4)	35(3)	29(3)	3(3)	11(3)	6(3)
C(12)	66(6)	79(6)	66(5)	1(4)	10(5)	-13(5)
C(17)	30(3)	54(4)	34(3)	15(3)	-5(3)	10(3)
C(4)	39(4)	54(5)	64(4)	-21(4)	3(3)	27(4)
C(20)	23(3)	26(3)	45(4)	5(3)	5(3)	-3(3)
C(23)	30(3)	47(4)	45(4)	13(3)	3(3)	14(3)
C(24)	38(4)	62(5)	39(4)	3(4)	-11(3)	18(4)
C(10)	45(4)	42(4)	52(4)	-7(3)	17(4)	-10(3)
C(16)	28(3)	45(4)	28(3)	3(3)	-3(3)	1(3)
C(13)	30(4)	41(4)	30(3)	2(3)	-5(3)	3(3)

C(25)	76(5)	35(4)	46(4)	18(3)	13(4)	19(4)
C(21)	27(3)	45(4)	33(3)	-5(3)	4(3)	-5(3)
C(33A)	77(2)	77(2)	77(2)	0(1)	0(1)	-1(1)
C(35A)	78(4)	78(4)	78(3)	0(1)	0(1)	0(1)
C(34A)	85(4)	85(4)	85(4)	0(1)	0(1)	0(1)
C(33B)	77(2)	77(2)	77(2)	0(1)	0(1)	-1(1)
C(35B)	78(4)	78(4)	78(3)	0(1)	0(1)	0(1)
C(34B)	85(4)	85(4)	85(4)	0(1)	0(1)	0(1)
C(28)	66(6)	158(10)	35(4)	4(6)	-14(4)	20(7)
C(15)	43(4)	60(5)	42(4)	16(4)	13(3)	16(4)
C(27)	107(8)	89(7)	46(5)	48(5)	10(5)	5(6)
C(29)	33(4)	95(6)	41(4)	-2(4)	-5(3)	9(4)
C(26)	104(7)	54(5)	50(5)	12(4)	12(5)	26(5)
C(30A)	71(2)	71(2)	71(2)	0(1)	1(1)	0(1)
C(31A)	93(4)	93(4)	93(4)	0(1)	0(1)	0(1)
C(32A)	68(4)	68(3)	68(4)	0(1)	0(1)	0(1)
C(30B)	71(2)	71(2)	71(2)	0(1)	1(1)	0(1)
C(31B)	93(4)	93(4)	93(4)	0(1)	0(1)	0(1)
C(32B)	68(4)	68(3)	68(4)	0(1)	0(1)	0(1)
C(11)	99(7)	64(5)	74(5)	13(5)	-2(5)	-14(5)
C(18)	27(3)	57(4)	28(3)	-11(3)	9(3)	-1(3)
C(37A)	53(4)	56(4)	49(4)	7(4)	27(4)	6(4)
C(39A)	63(5)	53(5)	53(5)	5(4)	23(4)	4(4)
C(38A)	78(7)	81(7)	40(5)	-4(5)	-2(5)	-15(5)
C(37B)	53(4)	56(4)	49(4)	7(4)	27(4)	6(4)
C(39B)	63(5)	53(5)	53(5)	5(4)	23(4)	4(4)
C(38B)	78(7)	81(7)	40(5)	-4(5)	-2(5)	-15(5)

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