Correspondence and Proofs to Dr. C. Lorber

Email: lorber@lcc-toulouse.fr, phone: (+33) 5 61 33 31 44, fax: (+33) 5 61 55 30 03

Synthesis and structure of early transition metal NHC complexes.

Christian Lorber,* and Laure Vendier

Laboratoire de Chimie de Coordination, CNRS UPR 8241, lié par convention à l'Université Paul Sabatier, 205 route de Narbonne, 31077 Toulouse Cedex 04, France

Supplementary Material

- X-ray data for all compounds: $VCl_2(NMe_2)(IMes)_2$ (**2**), $ZrCl_2(NMe_2)_2(IMes)$ (**4**), $VCl_3(IMes)_2$ (**6**), $VCl_2(IMes)(Py)_3$ (**7**), $ZrCl_4(IMes)_2$.(THF) (**8**), V(=N-2,6-^{i}Pr$_2$-C_6H_3)Cl_2(NHMe$_2$)(IMes) (**9**), Zr(=N-2,6-^{i}Pr$_2$-C_6H_3)Cl_2(NHMe$_2$)(IMes) (**10**), [V(=N-2,6-^{i}Pr$_2$-C_6H_3)Cl_3(IMes)][HIMes] (**11**), [Ti(=N-2,6-^{i}Pr$_2$-C_6H_3)Cl_3(IMes)][HIMes] (**12**), V(=O)Cl_2(NHMe$_2$)$_2$ (**13**), V(=O)Cl_2(IMes)$_2$ (**14**) (pages S2 – S79).

- X-ray data for IMes.HCl and $[VCl_2(CH_3CN)_4]_2$[HIMes] (given only as Supplementary Information) (pages S80 – S93)

- X-ray data for $[VCl_2(CH_3CN)_4]_2$[HIMes] (given only as Supplementary Information) (pages S94 – S99)

X-ray Data for Complex 2

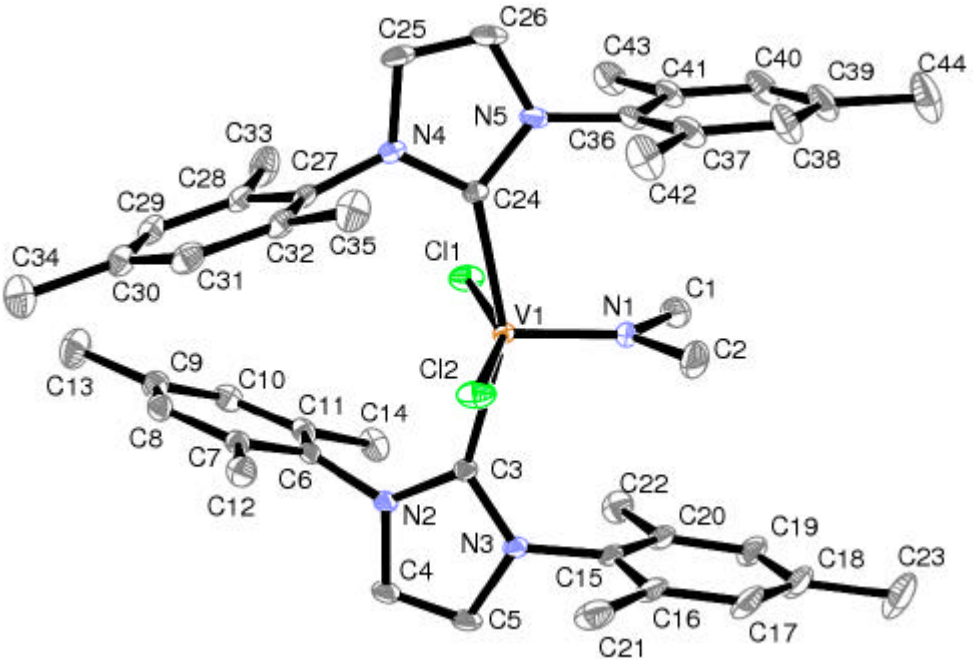

Table 1. Crystal data and structure refinement for **2**.

Empirical formula	C44 H54 Cl2 N5 V
Formula weight	774.76
Temperature	180 K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21/n
Unit cell dimensions	a = 15.1034(14) A alpha = 90 deg. b = 11.5170(11) A beta = 93.688(7) deg. c = 24.931(2) A gamma = 90 deg.
Volume	4327.7(7) A^3
Z, Calculated density	4, 1.189 Mg/m^3
Absorption coefficient	0.388 mm^-1
F(000)	1640
Crystal size	0.3078 x 0.2912 x 0.0775 mm
Theta range for data collection	3.22 to 26.31 deg.
Limiting indices	-18<=h<=18, -13<=k<=14, -31<=l<=31
Reflections collected / unique	31986 / 8847 [R(int) = 0.0646]
Completeness to theta = 26.31	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9676 and 0.8988
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8847 / 0 / 483
Goodness-of-fit on F^2	0.869
Final R indices [I>2sigma(I)]	R1 = 0.0445, wR2 = 0.0797
R indices (all data)	R1 = 0.1122, wR2 = 0.0959
Largest diff. peak and hole	0.242 and -0.226 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for cl735-2.

	x	y	z	U(eq)
C(1)	10656(2)	1527(3)	9176(1)	65(1)
C(2)	9720(2)	3143(3)	9327(1)	69(1)
C(3)	8954(2)	1828(2)	7866(1)	30(1)
C(4)	7869(2)	1042(2)	7299(1)	45(1)
C(5)	7576(2)	1002(3)	7787(1)	48(1)
C(6)	9220(2)	1579(2)	6881(1)	31(1)
C(7)	9112(2)	2521(2)	6537(1)	35(1)
C(8)	9515(2)	2463(2)	6050(1)	43(1)
C(9)	10003(2)	1510(3)	5902(1)	47(1)
C(10)	10083(2)	587(2)	6259(1)	44(1)
C(11)	9695(2)	592(2)	6747(1)	38(1)
C(12)	8572(2)	3559(2)	6676(1)	45(1)
C(13)	10430(2)	1484(3)	5368(1)	75(1)
C(14)	9783(2)	-439(2)	7113(1)	52(1)
C(15)	8158(2)	1395(2)	8706(1)	38(1)
C(16)	7640(2)	2184(3)	8967(1)	50(1)
C(17)	7543(2)	2018(3)	9514(1)	63(1)
C(18)	7922(2)	1087(3)	9791(1)	65(1)
C(19)	8412(2)	303(3)	9513(1)	57(1)
C(20)	8540(2)	428(3)	8970(1)	44(1)
C(21)	7198(2)	3202(3)	8679(1)	65(1)
C(22)	9061(2)	-450(3)	8670(1)	57(1)
C(23)	7809(2)	933(4)	10384(1)	100(2)
C(24)	11201(2)	4175(2)	8147(1)	27(1)
C(25)	12237(2)	5376(3)	7813(1)	56(1)
C(26)	12499(2)	5141(3)	8319(1)	59(1)
C(27)	10950(2)	4992(2)	7209(1)	34(1)
C(28)	11152(2)	4353(2)	6763(1)	40(1)
C(29)	10747(2)	4682(3)	6269(1)	46(1)
C(30)	10160(2)	5594(3)	6215(1)	46(1)
C(31)	9984(2)	6211(2)	6674(1)	47(1)
C(32)	10385(2)	5945(2)	7173(1)	40(1)
C(33)	11805(2)	3368(3)	6801(1)	62(1)
C(34)	9732(2)	5932(3)	5674(1)	74(1)
C(35)	10245(2)	6711(2)	7650(1)	56(1)
C(36)	11930(2)	4141(2)	9085(1)	39(1)
C(37)	11510(2)	4882(3)	9430(1)	50(1)
C(38)	11632(2)	4664(3)	9976(1)	62(1)
C(39)	12142(2)	3761(3)	10182(1)	60(1)
C(40)	12571(2)	3066(3)	9827(1)	56(1)
C(41)	12482(2)	3241(2)	9274(1)	43(1)
C(42)	10937(2)	5880(3)	9213(1)	67(1)
C(43)	12946(2)	2475(3)	8893(1)	58(1)
C(44)	12238(2)	3541(3)	10783(1)	91(1)
N(1)	10164(1)	2504(2)	8914(1)	37(1)
N(2)	8706(1)	1528(2)	7349(1)	31(1)
N(3)	8231(1)	1480(2)	8132(1)	35(1)
N(4)	11446(1)	4787(2)	7712(1)	36(1)
N(5)	11874(1)	4415(2)	8522(1)	37(1)
Cl(1)	11095(1)	1492(1)	7886(1)	47(1)
Cl(2)	9071(1)	4473(1)	8134(1)	47(1)
V(1)	10100(1)	2890(1)	8202(1)	25(1)

Table 3. Bond lengths [A] and angles [deg] for **2**.

C(1)-N(1)	1.477(3)
C(1)-H(1A)	0.98
C(1)-H(1B)	0.98
C(1)-H(1C)	0.98
C(2)-N(1)	1.464(3)
C(2)-H(2A)	0.98
C(2)-H(2B)	0.98
C(2)-H(2C)	0.98
C(3)-N(2)	1.362(3)
C(3)-N(3)	1.374(3)
C(3)-V(1)	2.238(3)
C(4)-C(5)	1.322(4)
C(4)-N(2)	1.382(3)
C(4)-H(4)	0.95
C(5)-N(3)	1.382(3)
C(5)-H(5)	0.95
C(6)-C(7)	1.386(3)
C(6)-C(11)	1.396(3)
C(6)-N(2)	1.444(3)
C(7)-C(8)	1.395(4)
C(7)-C(12)	1.501(3)
C(8)-C(9)	1.385(4)
C(8)-H(8)	0.95
C(9)-C(10)	1.387(4)
C(9)-C(13)	1.514(4)
C(10)-C(11)	1.385(4)
C(10)-H(10)	0.95
C(11)-C(14)	1.498(3)
C(12)-H(12A)	0.98
C(12)-H(12B)	0.98
C(12)-H(12C)	0.98
C(13)-H(13A)	0.98
C(13)-H(13B)	0.98
C(13)-H(13C)	0.98
C(14)-H(14A)	0.98
C(14)-H(14B)	0.98
C(14)-H(14C)	0.98
C(15)-C(16)	1.387(4)
C(15)-C(20)	1.399(4)
C(15)-N(3)	1.447(3)
C(16)-C(17)	1.396(4)
C(16)-C(21)	1.508(4)
C(17)-C(18)	1.380(4)
C(17)-H(17)	0.95
C(18)-C(19)	1.381(4)
C(18)-C(23)	1.511(4)
C(19)-C(20)	1.388(4)
C(19)-H(19)	0.95
C(20)-C(22)	1.508(4)
C(21)-H(21A)	0.98
C(21)-H(21B)	0.98
C(21)-H(21C)	0.98
C(22)-H(22A)	0.98
C(22)-H(22B)	0.98
C(22)-H(22C)	0.98
C(23)-H(23A)	0.98
C(23)-H(23B)	0.98
C(23)-H(23C)	0.98
C(24)-N(4)	1.363(3)
C(24)-N(5)	1.365(3)
C(24)-V(1)	2.237(2)
C(25)-C(26)	1.326(4)
C(25)-N(4)	1.383(3)
C(25)-H(25)	0.95

C(26)-N(5)	1.381(3)
C(26)-H(26)	0.95
C(27)-C(28)	1.384(4)
C(27)-C(32)	1.389(3)
C(27)-N(4)	1.439(3)
C(28)-C(29)	1.393(4)
C(28)-C(33)	1.502(4)
C(29)-C(30)	1.375(4)
C(29)-H(29)	0.95
C(30)-C(31)	1.386(4)
C(30)-C(34)	1.509(4)
C(31)-C(32)	1.383(4)
C(31)-H(31)	0.95
C(32)-C(35)	1.508(4)
C(33)-H(33A)	0.98
C(33)-H(33B)	0.98
C(33)-H(33C)	0.98
C(34)-H(34A)	0.98
C(34)-H(34B)	0.98
C(34)-H(34C)	0.98
C(35)-H(35A)	0.98
C(35)-H(35B)	0.98
C(35)-H(35C)	0.98
C(36)-C(41)	1.392(4)
C(36)-C(37)	1.393(4)
C(36)-N(5)	1.436(3)
C(37)-C(38)	1.384(4)
C(37)-C(42)	1.517(4)
C(38)-C(39)	1.374(4)
C(38)-H(38)	0.95
C(39)-C(40)	1.384(4)
C(39)-C(44)	1.517(4)
C(40)-C(41)	1.391(4)
C(40)-H(40)	0.95
C(41)-C(43)	1.502(4)
C(42)-H(42A)	0.98
C(42)-H(42B)	0.98
C(42)-H(42C)	0.98
C(43)-H(43A)	0.98
C(43)-H(43B)	0.98
C(43)-H(43C)	0.98
C(44)-H(44A)	0.98
C(44)-H(44B)	0.98
C(44)-H(44C)	0.98
N(1)-V(1)	1.828(2)
Cl(1)-V(1)	2.3715(8)
Cl(2)-V(1)	2.3938(8)

N(1)-C(1)-H(1A)	109.5
N(1)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
N(1)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
N(1)-C(2)-H(2A)	109.5
N(1)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
N(1)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
N(2)-C(3)-N(3)	101.7(2)
N(2)-C(3)-V(1)	130.66(18)
N(3)-C(3)-V(1)	126.79(19)
C(5)-C(4)-N(2)	106.8(3)
C(5)-C(4)-H(4)	126.6
N(2)-C(4)-H(4)	126.6
C(4)-C(5)-N(3)	106.9(3)
C(4)-C(5)-H(5)	126.6

N(3)-C(5)-H(5)	126.6
C(7)-C(6)-C(11)	122.1(2)
C(7)-C(6)-N(2)	119.0(2)
C(11)-C(6)-N(2)	118.1(2)
C(6)-C(7)-C(8)	117.4(3)
C(6)-C(7)-C(12)	121.7(2)
C(8)-C(7)-C(12)	120.9(2)
C(9)-C(8)-C(7)	122.6(3)
C(9)-C(8)-H(8)	118.7
C(7)-C(8)-H(8)	118.7
C(8)-C(9)-C(10)	117.5(3)
C(8)-C(9)-C(13)	120.9(3)
C(10)-C(9)-C(13)	121.5(3)
C(11)-C(10)-C(9)	122.4(3)
C(11)-C(10)-H(10)	118.8
C(9)-C(10)-H(10)	118.8
C(10)-C(11)-C(6)	117.8(3)
C(10)-C(11)-C(14)	120.4(3)
C(6)-C(11)-C(14)	121.8(3)
C(7)-C(12)-H(12A)	109.5
C(7)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(7)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(9)-C(13)-H(13A)	109.5
C(9)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(9)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(11)-C(14)-H(14A)	109.5
C(11)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(11)-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)-C(20)	122.0(3)
C(16)-C(15)-N(3)	120.0(2)
C(20)-C(15)-N(3)	117.6(3)
C(15)-C(16)-C(17)	117.8(3)
C(15)-C(16)-C(21)	122.2(3)
C(17)-C(16)-C(21)	120.0(3)
C(18)-C(17)-C(16)	121.9(3)
C(18)-C(17)-H(17)	119.1
C(16)-C(17)-H(17)	119.1
C(17)-C(18)-C(19)	118.4(3)
C(17)-C(18)-C(23)	120.7(3)
C(19)-C(18)-C(23)	120.9(3)
C(18)-C(19)-C(20)	122.3(3)
C(18)-C(19)-H(19)	118.8
C(20)-C(19)-H(19)	118.8
C(19)-C(20)-C(15)	117.5(3)
C(19)-C(20)-C(22)	121.6(3)
C(15)-C(20)-C(22)	121.0(3)
C(16)-C(21)-H(21A)	109.5
C(16)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(16)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(20)-C(22)-H(22A)	109.5
C(20)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(20)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(18)-C(23)-H(23A)	109.5

C(18)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(18)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
N(4)-C(24)-N(5)	102.3(2)
N(4)-C(24)-V(1)	129.17(18)
N(5)-C(24)-V(1)	127.97(19)
C(26)-C(25)-N(4)	105.9(3)
C(26)-C(25)-H(25)	127
N(4)-C(25)-H(25)	127
C(25)-C(26)-N(5)	107.7(3)
C(25)-C(26)-H(26)	126.2
N(5)-C(26)-H(26)	126.2
C(28)-C(27)-C(32)	122.3(3)
C(28)-C(27)-N(4)	118.9(2)
C(32)-C(27)-N(4)	118.0(3)
C(27)-C(28)-C(29)	117.2(3)
C(27)-C(28)-C(33)	122.0(3)
C(29)-C(28)-C(33)	120.7(3)
C(30)-C(29)-C(28)	122.6(3)
C(30)-C(29)-H(29)	118.7
C(28)-C(29)-H(29)	118.7
C(29)-C(30)-C(31)	117.9(3)
C(29)-C(30)-C(34)	121.4(3)
C(31)-C(30)-C(34)	120.7(3)
C(32)-C(31)-C(30)	122.1(3)
C(32)-C(31)-H(31)	118.9
C(30)-C(31)-H(31)	118.9
C(31)-C(32)-C(27)	117.7(3)
C(31)-C(32)-C(35)	120.3(3)
C(27)-C(32)-C(35)	121.8(3)
C(28)-C(33)-H(33A)	109.5
C(28)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(28)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(30)-C(34)-H(34A)	109.5
C(30)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(30)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(32)-C(35)-H(35A)	109.5
C(32)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(32)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(41)-C(36)-C(37)	122.3(3)
C(41)-C(36)-N(5)	119.4(3)
C(37)-C(36)-N(5)	117.9(3)
C(38)-C(37)-C(36)	117.3(3)
C(38)-C(37)-C(42)	121.6(3)
C(36)-C(37)-C(42)	121.1(3)
C(39)-C(38)-C(37)	122.7(3)
C(39)-C(38)-H(38)	118.7
C(37)-C(38)-H(38)	118.7
C(38)-C(39)-C(40)	118.2(3)
C(38)-C(39)-C(44)	120.8(3)
C(40)-C(39)-C(44)	121.0(3)
C(39)-C(40)-C(41)	122.1(3)
C(39)-C(40)-H(40)	119
C(41)-C(40)-H(40)	119
C(40)-C(41)-C(36)	117.4(3)
C(40)-C(41)-C(43)	121.5(3)
C(36)-C(41)-C(43)	121.1(3)

C(37)-C(42)-H(42A)	109.5
C(37)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(37)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(41)-C(43)-H(43A)	109.5
C(41)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43B)	109.5
C(41)-C(43)-H(43C)	109.5
H(43A)-C(43)-H(43C)	109.5
H(43B)-C(43)-H(43C)	109.5
C(39)-C(44)-H(44A)	109.5
C(39)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
C(39)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
C(2)-N(1)-C(1)	108.2(2)
C(2)-N(1)-V(1)	124.3(2)
C(1)-N(1)-V(1)	127.53(19)
C(3)-N(2)-C(4)	112.5(2)
C(3)-N(2)-C(6)	128.6(2)
C(4)-N(2)-C(6)	118.7(2)
C(3)-N(3)-C(5)	112.1(2)
C(3)-N(3)-C(15)	127.6(2)
C(5)-N(3)-C(15)	119.5(2)
C(24)-N(4)-C(25)	112.6(2)
C(24)-N(4)-C(27)	128.7(2)
C(25)-N(4)-C(27)	118.3(2)
C(24)-N(5)-C(26)	111.5(2)
C(24)-N(5)-C(36)	128.4(2)
C(26)-N(5)-C(36)	119.5(2)
N(1)-V(1)-C(24)	103.17(9)
N(1)-V(1)-C(3)	102.80(9)
C(24)-V(1)-C(3)	154.02(10)
N(1)-V(1)-Cl(1)	99.33(7)
C(24)-V(1)-Cl(1)	86.53(6)
C(3)-V(1)-Cl(1)	89.77(7)
N(1)-V(1)-Cl(2)	104.32(7)
C(24)-V(1)-Cl(2)	88.50(6)
C(3)-V(1)-Cl(2)	84.65(7)
Cl(1)-V(1)-Cl(2)	156.34(3)

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **2**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	51(2)	86(3)	55(2)	31(2)	-10(2)	-9(2)
C(2)	82(3)	88(3)	39(2)	-14(2)	20(2)	-18(2)
C(3)	26(2)	29(2)	34(2)	6(1)	1(1)	-1(1)
C(4)	38(2)	46(2)	49(2)	7(2)	-11(2)	-19(2)
C(5)	33(2)	55(2)	56(2)	14(2)	-8(2)	-22(2)
C(6)	32(2)	32(2)	28(2)	0(1)	-6(1)	-8(1)
C(7)	34(2)	29(2)	39(2)	3(1)	-6(1)	-5(1)
C(8)	52(2)	39(2)	38(2)	8(2)	-4(2)	-7(2)
C(9)	51(2)	47(2)	41(2)	-7(2)	3(2)	-6(2)
C(10)	45(2)	37(2)	48(2)	-11(2)	-3(2)	2(2)
C(11)	46(2)	28(2)	38(2)	-4(2)	-9(2)	-6(1)
C(12)	49(2)	35(2)	49(2)	7(2)	0(2)	4(2)
C(13)	100(3)	72(3)	54(2)	-6(2)	23(2)	-4(2)
C(14)	74(2)	26(2)	53(2)	0(2)	-11(2)	-2(2)
C(15)	26(2)	48(2)	41(2)	16(2)	6(1)	-7(1)
C(16)	28(2)	65(2)	59(2)	20(2)	15(2)	3(2)
C(17)	48(2)	80(3)	64(2)	18(2)	35(2)	12(2)
C(18)	49(2)	93(3)	55(2)	28(2)	25(2)	6(2)
C(19)	46(2)	71(2)	54(2)	33(2)	14(2)	1(2)
C(20)	32(2)	48(2)	51(2)	14(2)	8(2)	-4(2)
C(21)	36(2)	71(2)	89(3)	25(2)	13(2)	7(2)
C(22)	62(2)	46(2)	63(2)	17(2)	6(2)	3(2)
C(23)	101(3)	137(4)	69(3)	42(3)	50(2)	24(3)
C(24)	22(2)	26(2)	34(2)	-3(1)	5(1)	1(1)
C(25)	37(2)	64(2)	68(3)	16(2)	3(2)	-27(2)
C(26)	33(2)	69(2)	73(3)	3(2)	-4(2)	-25(2)
C(27)	33(2)	32(2)	37(2)	8(1)	10(1)	-7(1)
C(28)	37(2)	43(2)	42(2)	9(2)	15(2)	-2(1)
C(29)	53(2)	46(2)	39(2)	5(2)	17(2)	-6(2)
C(30)	51(2)	43(2)	45(2)	12(2)	7(2)	-6(2)
C(31)	50(2)	31(2)	61(2)	13(2)	13(2)	-2(2)
C(32)	47(2)	27(2)	47(2)	11(2)	14(2)	-5(1)
C(33)	69(2)	67(2)	52(2)	8(2)	26(2)	24(2)
C(34)	85(3)	81(3)	56(2)	21(2)	-5(2)	5(2)
C(35)	80(2)	32(2)	57(2)	0(2)	14(2)	3(2)
C(36)	29(2)	44(2)	41(2)	-7(2)	-7(1)	-5(1)
C(37)	38(2)	57(2)	54(2)	-10(2)	-11(2)	10(2)
C(38)	58(2)	83(3)	42(2)	-21(2)	-13(2)	21(2)
C(39)	49(2)	84(3)	44(2)	-7(2)	-20(2)	16(2)
C(40)	48(2)	64(2)	54(2)	-9(2)	-22(2)	19(2)
C(41)	33(2)	50(2)	45(2)	-10(2)	-10(1)	6(1)
C(42)	72(2)	68(2)	61(2)	-14(2)	-7(2)	29(2)
C(43)	52(2)	64(2)	58(2)	-12(2)	-4(2)	17(2)
C(44)	100(3)	126(3)	44(2)	-9(2)	-24(2)	39(3)
N(1)	35(1)	48(2)	27(1)	2(1)	2(1)	-8(1)
N(2)	32(1)	28(1)	34(1)	4(1)	-4(1)	-11(1)
N(3)	27(1)	39(1)	39(2)	11(1)	-1(1)	-10(1)
N(4)	29(1)	39(2)	40(2)	4(1)	7(1)	-9(1)
N(5)	23(1)	43(2)	45(2)	-1(1)	-2(1)	-8(1)
Cl(1)	34(1)	44(1)	66(1)	-19(1)	12(1)	2(1)
Cl(2)	29(1)	35(1)	76(1)	5(1)	3(1)	7(1)
V(1)	20(1)	27(1)	27(1)	1(1)	4(1)	-1(1)

X-ray Data for Complex 4

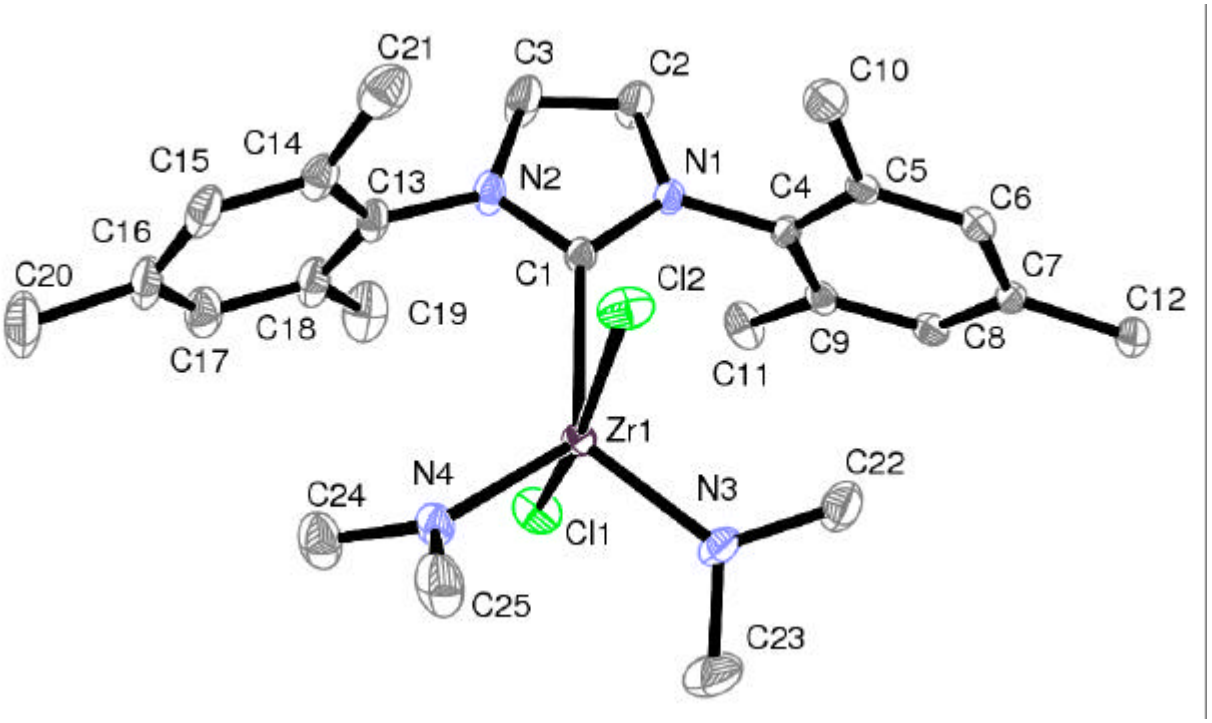

Table 5. Crystal data and structure refinement for **4**.

Empirical formula	C25 H36 Cl2 N4 Zr
Formula weight	554.7
Temperature	180 K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 1 21/c 1
Unit cell dimensions	a = 9.5739(3) A alpha = 90 deg.
	b = 16.2577(4) A beta = 101.690(3) deg.
	c = 17.9949(5) A gamma = 90 deg.
Volume	2742.80(13) A^3
Z, Calculated density	4, 1.343 Mg/m^3
Absorption coefficient	0.615 mm^-1
F(000)	1152
Crystal size	0.4 x 0.25 x 0.15 mm
Theta range for data collection	2.57 to 26.37 deg.
Limiting indices	-11<=h<=11, -20<=k<=18, -19<=l<=22
Reflections collected / unique	21290 / 5606 [R(int) = 0.0444]
Completeness to theta = 26.37	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.908 and 0.841
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5606 / 0 / 299
Goodness-of-fit on F^2	1.063
Final R indices [I>2sigma(I)]	R1 = 0.0316, wR2 = 0.081
R indices (all data)	R1 = 0.0565, wR2 = 0.1032
Largest diff. peak and hole	0.498 and -0.565 e.A^-3

Table 6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **4**.

	x	y	z	U(eq)
C(1)	1475(3)	2008(2)	9211(2)	27(1)
C(2)	106(4)	1397(2)	9934(2)	60(1)
C(3)	62(5)	2204(2)	10059(2)	68(1)
C(4)	1337(3)	482(2)	9187(2)	26(1)
C(5)	463(3)	96(2)	8567(2)	28(1)
C(6)	867(3)	-682(2)	8376(2)	30(1)
C(7)	2077(3)	-1073(2)	8787(2)	28(1)
C(8)	2855(3)	-676(2)	9409(2)	29(1)
C(9)	2513(3)	92(2)	9631(2)	28(1)
C(10)	-880(3)	490(2)	8139(2)	47(1)
C(11)	3316(4)	484(2)	10348(2)	43(1)
C(12)	2516(3)	-1909(2)	8561(2)	38(1)
C(13)	1122(4)	3438(2)	9578(2)	37(1)
C(14)	201(4)	3893(2)	9023(2)	40(1)
C(15)	488(4)	4721(2)	8971(2)	49(1)
C(16)	1601(5)	5098(2)	9435(2)	51(1)
C(17)	2409(4)	4643(2)	10011(2)	50(1)
C(18)	2191(4)	3813(2)	10099(2)	45(1)
C(19)	3066(5)	3334(2)	10755(2)	65(1)
C(20)	1923(5)	5988(2)	9319(3)	79(2)
C(21)	-1062(4)	3494(2)	8532(2)	58(1)
C(22)	3629(4)	580(2)	7703(2)	54(1)
C(23)	5580(4)	1505(3)	7777(3)	74(1)
C(24)	4143(4)	4093(2)	8464(2)	58(1)
C(25)	3752(5)	3491(2)	7238(2)	63(1)
N(1)	960(3)	1286(1)	9414(1)	32(1)
N(2)	900(3)	2572(2)	9618(2)	38(1)
N(3)	4129(3)	1407(2)	7875(2)	38(1)
N(4)	3705(3)	3364(2)	8022(1)	35(1)
Cl(1)	4883(1)	2323(1)	9545(1)	46(1)
Cl(2)	876(1)	2136(1)	7382(1)	45(1)
Zr(1)	3093(1)	2265(1)	8353(1)	24(1)

Table 7. Bond lengths [A] and angles [deg] for **4**.

C(1)-N(1)	1.353(3)
C(1)-N(2)	1.357(4)
C(1)-Zr(1)	2.435(3)
C(2)-C(3)	1.332(5)
C(2)-N(1)	1.373(4)
C(2)-H(2)	0.95
C(3)-N(2)	1.375(4)
C(3)-H(3)	0.95
C(4)-C(9)	1.394(4)
C(4)-C(5)	1.400(4)
C(4)-N(1)	1.437(3)
C(5)-C(6)	1.387(4)
C(5)-C(10)	1.501(4)
C(6)-C(7)	1.395(4)
C(6)-H(6)	0.95
C(7)-C(8)	1.373(4)
C(7)-C(12)	1.504(4)
C(8)-C(9)	1.370(4)
C(8)-H(8)	0.95
C(9)-C(11)	1.504(4)
C(10)-H(10A)	0.98
C(10)-H(10B)	0.98
C(10)-H(10C)	0.98
C(11)-H(11A)	0.98
C(11)-H(11B)	0.98
C(11)-H(11C)	0.98
C(12)-H(12A)	0.98
C(12)-H(12B)	0.98
C(12)-H(12C)	0.98
C(13)-C(18)	1.382(5)
C(13)-C(14)	1.401(4)
C(13)-N(2)	1.427(4)
C(14)-C(15)	1.381(4)
C(14)-C(21)	1.494(5)
C(15)-C(16)	1.359(5)
C(15)-H(15)	0.95
C(16)-C(17)	1.376(5)
C(16)-C(20)	1.503(5)
C(17)-C(18)	1.379(4)
C(17)-H(17)	0.95
C(18)-C(19)	1.518(5)
C(19)-H(19A)	0.98
C(19)-H(19B)	0.98
C(19)-H(19C)	0.98
C(20)-H(20A)	0.98
C(20)-H(20B)	0.98
C(20)-H(20C)	0.98
C(21)-H(21A)	0.98
C(21)-H(21B)	0.98
C(21)-H(21C)	0.98
C(22)-N(3)	1.440(4)
C(22)-H(22A)	0.98
C(22)-H(22B)	0.98
C(22)-H(22C)	0.98
C(23)-N(3)	1.444(4)
C(23)-H(23A)	0.98
C(23)-H(23B)	0.98
C(23)-H(23C)	0.98
C(24)-N(4)	1.441(4)
C(24)-H(24A)	0.98
C(24)-H(24B)	0.98
C(24)-H(24C)	0.98
C(25)-N(4)	1.437(4)
C(25)-H(25A)	0.98

C(25)-H(25B)	0.98
C(25)-H(25C)	0.98
N(3)-Zr(1)	2.003(2)
N(4)-Zr(1)	2.007(2)
Cl(1)-Zr(1)	2.4614(8)
Cl(2)-Zr(1)	2.4698(8)

N(1)-C(1)-N(2)	103.4(2)
N(1)-C(1)-Zr(1)	129.34(19)
N(2)-C(1)-Zr(1)	127.3(2)
C(3)-C(2)-N(1)	106.8(3)
C(3)-C(2)-H(2)	126.6
N(1)-C(2)-H(2)	126.6
C(2)-C(3)-N(2)	106.8(3)
C(2)-C(3)-H(3)	126.6
N(2)-C(3)-H(3)	126.6
C(9)-C(4)-C(5)	122.4(3)
C(9)-C(4)-N(1)	118.1(3)
C(5)-C(4)-N(1)	119.3(3)
C(6)-C(5)-C(4)	117.1(3)
C(6)-C(5)-C(10)	121.0(3)
C(4)-C(5)-C(10)	121.9(3)
C(5)-C(6)-C(7)	121.8(3)
C(5)-C(6)-H(6)	119.1
C(7)-C(6)-H(6)	119.1
C(8)-C(7)-C(6)	118.2(3)
C(8)-C(7)-C(12)	120.7(3)
C(6)-C(7)-C(12)	121.1(3)
C(9)-C(8)-C(7)	122.9(3)
C(9)-C(8)-H(8)	118.5
C(7)-C(8)-H(8)	118.5
C(8)-C(9)-C(4)	117.4(3)
C(8)-C(9)-C(11)	121.7(3)
C(4)-C(9)-C(11)	120.8(3)
C(5)-C(10)-H(10A)	109.5
C(5)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(5)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(9)-C(11)-H(11A)	109.5
C(9)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(9)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(7)-C(12)-H(12A)	109.5
C(7)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(7)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(18)-C(13)-C(14)	121.5(3)
C(18)-C(13)-N(2)	119.9(3)
C(14)-C(13)-N(2)	118.5(3)
C(15)-C(14)-C(13)	117.2(3)
C(15)-C(14)-C(21)	122.1(3)
C(13)-C(14)-C(21)	120.7(3)
C(16)-C(15)-C(14)	122.7(3)
C(16)-C(15)-H(15)	118.7
C(14)-C(15)-H(15)	118.7
C(15)-C(16)-C(17)	118.1(3)
C(15)-C(16)-C(20)	120.4(4)
C(17)-C(16)-C(20)	121.4(4)
C(16)-C(17)-C(18)	122.5(4)
C(16)-C(17)-H(17)	118.8
C(18)-C(17)-H(17)	118.8
C(17)-C(18)-C(13)	117.6(3)

C(17)-C(18)-C(19)	121.3(4)
C(13)-C(18)-C(19)	121.1(3)
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(16)-C(20)-H(20A)	109.5
C(16)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(16)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(14)-C(21)-H(21A)	109.5
C(14)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(14)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
N(3)-C(22)-H(22A)	109.5
N(3)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
N(3)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
N(3)-C(23)-H(23A)	109.5
N(3)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
N(3)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
N(4)-C(24)-H(24A)	109.5
N(4)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
N(4)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
N(4)-C(25)-H(25A)	109.5
N(4)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
N(4)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(1)-N(1)-C(2)	111.7(2)
C(1)-N(1)-C(4)	125.9(2)
C(2)-N(1)-C(4)	122.2(2)
C(1)-N(2)-C(3)	111.4(3)
C(1)-N(2)-C(13)	124.0(2)
C(3)-N(2)-C(13)	124.6(3)
C(22)-N(3)-C(23)	111.3(3)
C(22)-N(3)-Zr(1)	124.8(2)
C(23)-N(3)-Zr(1)	123.2(2)
C(25)-N(4)-C(24)	111.1(3)
C(25)-N(4)-Zr(1)	119.2(2)
C(24)-N(4)-Zr(1)	129.7(2)
N(3)-Zr(1)-N(4)	107.07(11)
N(3)-Zr(1)-C(1)	125.91(10)
N(4)-Zr(1)-C(1)	126.98(10)
N(3)-Zr(1)-Cl(1)	94.74(8)
N(4)-Zr(1)-Cl(1)	91.76(7)
C(1)-Zr(1)-Cl(1)	82.76(7)
N(3)-Zr(1)-Cl(2)	93.82(8)
N(4)-Zr(1)-Cl(2)	97.27(8)
C(1)-Zr(1)-Cl(2)	82.41(7)
Cl(1)-Zr(1)-Cl(2)	165.17(3)

Table 8. Anisotropic displacement parameters (A^2 x 10^3) for **4**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	34(2)	21(2)	29(2)	4(1)	11(1)	2(1)
C(2)	88(3)	31(2)	84(3)	3(2)	70(3)	0(2)
C(3)	110(3)	31(2)	90(3)	5(2)	86(3)	6(2)
C(4)	30(2)	19(1)	35(2)	2(1)	17(1)	0(1)
C(5)	22(2)	25(2)	36(2)	4(1)	8(1)	-2(1)
C(6)	29(2)	27(2)	33(2)	0(1)	6(1)	-5(1)
C(7)	30(2)	22(2)	35(2)	1(1)	14(1)	-1(1)
C(8)	23(2)	27(2)	36(2)	8(1)	3(1)	0(1)
C(9)	34(2)	25(2)	27(2)	2(1)	11(1)	-6(1)
C(10)	35(2)	37(2)	66(2)	8(2)	3(2)	4(2)
C(11)	59(2)	41(2)	26(2)	-1(1)	2(2)	-11(2)
C(12)	36(2)	27(2)	50(2)	-6(2)	8(2)	1(1)
C(13)	60(2)	24(2)	36(2)	-1(1)	31(2)	3(2)
C(14)	58(2)	33(2)	35(2)	4(1)	24(2)	10(2)
C(15)	74(3)	30(2)	52(2)	10(2)	34(2)	19(2)
C(16)	85(3)	23(2)	55(2)	-1(2)	42(2)	6(2)
C(17)	74(3)	37(2)	46(2)	-10(2)	25(2)	-2(2)
C(18)	75(3)	28(2)	40(2)	0(1)	28(2)	6(2)
C(19)	102(3)	53(2)	41(2)	0(2)	15(2)	8(2)
C(20)	129(4)	27(2)	97(4)	3(2)	60(3)	5(2)
C(21)	69(3)	60(3)	51(2)	4(2)	24(2)	14(2)
C(22)	73(3)	34(2)	66(3)	5(2)	37(2)	10(2)
C(23)	38(2)	84(3)	102(4)	-14(3)	21(2)	11(2)
C(24)	89(3)	39(2)	52(2)	4(2)	29(2)	-8(2)
C(25)	106(3)	42(2)	47(2)	10(2)	32(2)	-9(2)
N(1)	40(2)	21(1)	42(2)	-1(1)	24(1)	-2(1)
N(2)	62(2)	21(1)	40(2)	5(1)	29(1)	1(1)
N(3)	35(2)	37(2)	43(2)	1(1)	14(1)	12(1)
N(4)	43(2)	29(1)	33(1)	8(1)	11(1)	0(1)
Cl(1)	41(1)	53(1)	36(1)	11(1)	-7(1)	-3(1)
Cl(2)	33(1)	68(1)	31(1)	0(1)	2(1)	5(1)
Zr(1)	26(1)	24(1)	24(1)	4(1)	7(1)	2(1)

X-ray Data for Complex 6

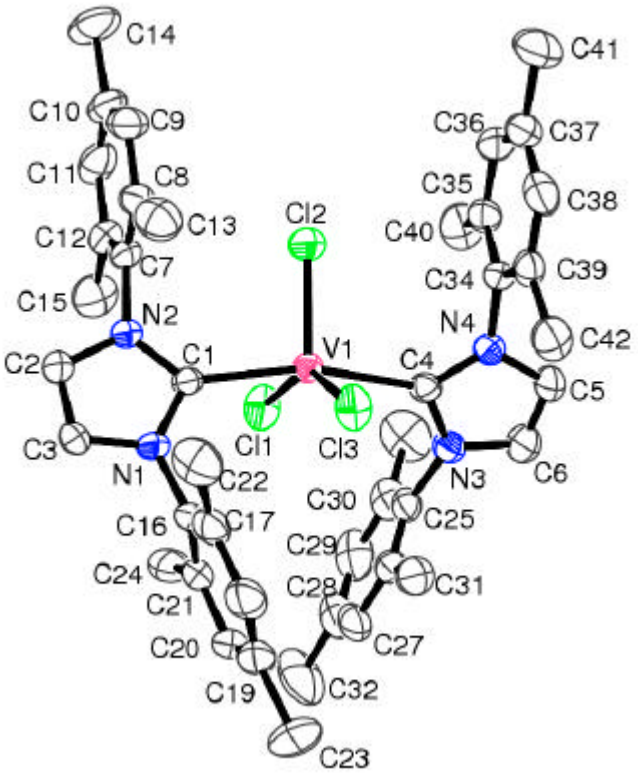

Table 9. Crystal data and structure refinement for **6**.

Empirical formula	C42 H48 Cl3 N4 V
Formula weight	766.13
Temperature	180 K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, C 2/c
Unit cell dimensions	a = 30.122(3) A alpha = 90 deg. b = 12.9535(9) A beta = 99.789(7) deg. c = 24.2742(18) A gamma = 90 deg.
Volume	9333.6(12) A^3
Z, Calculated density	8, 1.09 Mg/m^3
Absorption coefficient	0.414 mm^-1
F(000)	3216
Crystal size	0.2 x 0.12 x 0.04 mm
Theta range for data collection	1.7 to 25.46 deg.
Limiting indices	-36<=h<=36, -15<=k<=15, -29<=l<=29
Reflections collected / unique	86160 / 8635 [R(int) = 0.073]
Completeness to theta = 25.46	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.990 and 0.875
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8635 / 0 / 463
Goodness-of-fit on F^2	1.019
Final R indices [I>2sigma(I)]	R1 = 0.0504, wR2 = 0.1241
R indices (all data)	R1 = 0.086, wR2 = 0.1357
Largest diff. peak and hole	0.378 and -0.454 e.A^-3

Table 10. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **6**.

	x	y	z	U(eq)
C(1)	1257(1)	9172(2)	641(1)	30(1)
C(2)	756(1)	7970(2)	225(1)	48(1)
C(3)	540(1)	8871(2)	198(1)	50(1)
C(4)	2298(1)	11024(2)	1768(1)	32(1)
C(5)	2876(1)	12078(2)	2152(1)	49(1)
C(6)	2529(1)	12280(2)	2406(1)	55(1)
C(7)	1515(1)	7321(2)	531(1)	37(1)
C(8)	1765(1)	7226(2)	109(1)	42(1)
C(9)	2038(1)	6352(3)	111(1)	55(1)
C(10)	2054(1)	5605(2)	514(2)	57(1)
C(11)	1798(1)	5735(2)	926(2)	56(1)
C(12)	1518(1)	6592(2)	948(1)	45(1)
C(13)	1745(1)	8015(3)	-348(1)	60(1)
C(14)	2340(1)	4642(3)	494(2)	89(2)
C(15)	1240(1)	6710(3)	1404(2)	67(1)
C(16)	717(1)	10673(2)	451(1)	38(1)
C(17)	762(1)	11267(2)	-14(1)	45(1)
C(18)	621(1)	12287(2)	-17(2)	56(1)
C(19)	435(1)	12694(2)	419(2)	61(1)
C(20)	375(1)	12062(2)	859(2)	53(1)
C(21)	515(1)	11035(2)	886(1)	41(1)
C(22)	946(1)	10833(3)	-503(1)	63(1)
C(23)	285(2)	13828(2)	414(2)	96(2)
C(24)	426(1)	10358(2)	1356(1)	55(1)
C(25)	1753(1)	11683(2)	2370(1)	42(1)
C(26)	1406(1)	12289(2)	2096(1)	43(1)
C(27)	1015(1)	12356(3)	2326(2)	57(1)
C(28)	975(1)	11853(3)	2819(2)	68(1)
C(29)	1328(1)	11263(3)	3077(2)	70(1)
C(30)	1724(1)	11166(3)	2868(1)	55(1)
C(31)	1452(1)	12893(2)	1585(1)	55(1)
C(32)	542(1)	11964(4)	3071(2)	107(2)
C(33)	2102(1)	10517(4)	3163(2)	85(1)
C(34)	3048(1)	10865(2)	1444(1)	32(1)
C(35)	3271(1)	9980(2)	1655(1)	44(1)
C(36)	3585(1)	9565(2)	1360(2)	59(1)
C(37)	3687(1)	10029(3)	887(2)	59(1)
C(38)	3469(1)	10939(3)	704(1)	51(1)
C(39)	3147(1)	11372(2)	981(1)	38(1)
C(40)	3192(1)	9496(3)	2197(2)	68(1)
C(41)	4036(1)	9581(4)	572(2)	96(2)
C(42)	2926(1)	12389(2)	788(1)	55(1)
N(1)	844(1)	9592(2)	449(1)	36(1)
N(2)	1189(1)	8159(2)	492(1)	35(1)
N(3)	2176(1)	11648(2)	2173(1)	40(1)
N(4)	2732(1)	11317(2)	1761(1)	35(1)
Cl(1)	1516(1)	9381(1)	1914(1)	52(1)
Cl(2)	2357(1)	8732(1)	1119(1)	50(1)
Cl(3)	1832(1)	11200(1)	547(1)	47(1)
V(1)	1846(1)	9935(1)	1195(1)	31(1)

Table 11. Bond lengths [A] and angles [deg] for **6**.

C(1)-N(1)	1.366(3)
C(1)-N(2)	1.367(3)
C(1)-V(1)	2.262(3)
C(2)-C(3)	1.333(4)
C(2)-N(2)	1.376(3)
C(2)-H(2)	0.9500
C(3)-N(1)	1.375(3)
C(3)-H(3)	0.9500
C(4)-N(4)	1.363(3)
C(4)-N(3)	1.371(3)
C(4)-V(1)	2.266(3)
C(5)-C(6)	1.326(4)
C(5)-N(4)	1.386(3)
C(5)-H(5)	0.9500
C(6)-N(3)	1.383(4)
C(6)-H(6)	0.9500
C(7)-C(8)	1.375(4)
C(7)-C(12)	1.385(4)
C(7)-N(2)	1.456(3)
C(8)-C(9)	1.399(4)
C(8)-C(13)	1.502(4)
C(9)-C(10)	1.371(5)
C(9)-H(9)	0.9500
C(10)-C(11)	1.373(5)
C(10)-C(14)	1.522(4)
C(11)-C(12)	1.401(4)
C(11)-H(11)	0.9500
C(12)-C(15)	1.505(4)
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)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-C(21)	1.387(4)
C(16)-C(17)	1.391(4)
C(16)-N(1)	1.453(3)
C(17)-C(18)	1.388(4)
C(17)-C(22)	1.502(4)
C(18)-C(19)	1.382(5)
C(18)-H(18)	0.9500
C(19)-C(20)	1.383(5)
C(19)-C(23)	1.536(4)
C(20)-C(21)	1.394(4)
C(20)-H(20)	0.9500
C(21)-C(24)	1.498(4)
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-C(26)	1.383(4)
C(25)-C(30)	1.397(4)
C(25)-N(3)	1.437(4)
C(26)-C(27)	1.389(4)
C(26)-C(31)	1.494(4)
C(27)-C(28)	1.386(5)
C(27)-H(27)	0.9500

C(28)-C(29)	1.371(5)
C(28)-C(32)	1.542(5)
C(29)-C(30)	1.380(5)
C(29)-H(29)	0.9500
C(30)-C(33)	1.497(5)
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)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-C(39)	1.377(4)
C(34)-C(35)	1.382(4)
C(34)-N(4)	1.446(3)
C(35)-C(36)	1.387(5)
C(35)-C(40)	1.513(4)
C(36)-C(37)	1.376(5)
C(36)-H(36)	0.9500
C(37)-C(38)	1.386(5)
C(37)-C(41)	1.516(5)
C(38)-C(39)	1.391(4)
C(38)-H(38)	0.9500
C(39)-C(42)	1.513(4)
C(40)-H(40A)	0.9800
C(40)-H(40B)	0.9800
C(40)-H(40C)	0.9800
C(41)-H(41A)	0.9800
C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
Cl(1)-V(1)	2.2682(9)
Cl(2)-V(1)	2.2206(8)
Cl(3)-V(1)	2.2660(8)

N(1)-C(1)-N(2)	101.8(2)
N(1)-C(1)-V(1)	127.30(17)
N(2)-C(1)-V(1)	130.07(18)
C(3)-C(2)-N(2)	106.4(2)
C(3)-C(2)-H(2)	126.8
N(2)-C(2)-H(2)	126.8
C(2)-C(3)-N(1)	106.8(2)
C(2)-C(3)-H(3)	126.6
N(1)-C(3)-H(3)	126.6
N(4)-C(4)-N(3)	102.6(2)
N(4)-C(4)-V(1)	130.03(18)
N(3)-C(4)-V(1)	126.96(19)
C(6)-C(5)-N(4)	106.2(3)
C(6)-C(5)-H(5)	126.9
N(4)-C(5)-H(5)	126.9
C(5)-C(6)-N(3)	107.7(3)
C(5)-C(6)-H(6)	126.1
N(3)-C(6)-H(6)	126.1
C(8)-C(7)-C(12)	123.2(3)
C(8)-C(7)-N(2)	117.9(2)
C(12)-C(7)-N(2)	118.4(3)
C(7)-C(8)-C(9)	117.7(3)
C(7)-C(8)-C(13)	122.1(3)
C(9)-C(8)-C(13)	120.2(3)
C(10)-C(9)-C(8)	121.5(3)
C(10)-C(9)-H(9)	119.2
C(8)-C(9)-H(9)	119.2
C(9)-C(10)-C(11)	118.5(3)
C(9)-C(10)-C(14)	120.5(4)

C(11)-C(10)-C(14)	121.0(3)
C(10)-C(11)-C(12)	122.8(3)
C(10)-C(11)-H(11)	118.6
C(12)-C(11)-H(11)	118.6
C(7)-C(12)-C(11)	116.2(3)
C(7)-C(12)-C(15)	122.3(3)
C(11)-C(12)-C(15)	121.5(3)
C(8)-C(13)-H(13A)	109.5
C(8)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(8)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(10)-C(14)-H(14A)	109.5
C(10)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(10)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(12)-C(15)-H(15A)	109.5
C(12)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(12)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(21)-C(16)-C(17)	123.2(3)
C(21)-C(16)-N(1)	118.6(3)
C(17)-C(16)-N(1)	117.9(3)
C(18)-C(17)-C(16)	117.3(3)
C(18)-C(17)-C(22)	120.4(3)
C(16)-C(17)-C(22)	122.3(3)
C(19)-C(18)-C(17)	121.5(3)
C(19)-C(18)-H(18)	119.2
C(17)-C(18)-H(18)	119.2
C(18)-C(19)-C(20)	119.3(3)
C(18)-C(19)-C(23)	121.0(4)
C(20)-C(19)-C(23)	119.7(4)
C(19)-C(20)-C(21)	121.5(3)
C(19)-C(20)-H(20)	119.2
C(21)-C(20)-H(20)	119.2
C(16)-C(21)-C(20)	117.1(3)
C(16)-C(21)-C(24)	122.7(3)
C(20)-C(21)-C(24)	120.2(3)
C(17)-C(22)-H(22A)	109.5
C(17)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(17)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(19)-C(23)-H(23A)	109.5
C(19)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(19)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(21)-C(24)-H(24A)	109.5
C(21)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(21)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(26)-C(25)-C(30)	122.4(3)
C(26)-C(25)-N(3)	119.9(3)
C(30)-C(25)-N(3)	117.5(3)
C(25)-C(26)-C(27)	117.7(3)
C(25)-C(26)-C(31)	121.9(3)
C(27)-C(26)-C(31)	120.4(3)
C(28)-C(27)-C(26)	121.4(3)

C(28)-C(27)-H(27)	119.3
C(26)-C(27)-H(27)	119.3
C(29)-C(28)-C(27)	118.9(3)
C(29)-C(28)-C(32)	120.9(4)
C(27)-C(28)-C(32)	120.2(4)
C(28)-C(29)-C(30)	122.3(4)
C(28)-C(29)-H(29)	118.9
C(30)-C(29)-H(29)	118.9
C(29)-C(30)-C(25)	117.3(3)
C(29)-C(30)-C(33)	120.7(3)
C(25)-C(30)-C(33)	122.0(3)
C(26)-C(31)-H(31A)	109.5
C(26)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(26)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(28)-C(32)-H(32A)	109.5
C(28)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(28)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(30)-C(33)-H(33A)	109.5
C(30)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(30)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(39)-C(34)-C(35)	122.6(3)
C(39)-C(34)-N(4)	119.6(2)
C(35)-C(34)-N(4)	117.5(3)
C(34)-C(35)-C(36)	117.5(3)
C(34)-C(35)-C(40)	121.8(3)
C(36)-C(35)-C(40)	120.6(3)
C(37)-C(36)-C(35)	122.0(3)
C(37)-C(36)-H(36)	119.0
C(35)-C(36)-H(36)	119.0
C(36)-C(37)-C(38)	118.6(3)
C(36)-C(37)-C(41)	121.8(4)
C(38)-C(37)-C(41)	119.6(4)
C(37)-C(38)-C(39)	121.3(3)
C(37)-C(38)-H(38)	119.3
C(39)-C(38)-H(38)	119.3
C(34)-C(39)-C(38)	117.9(3)
C(34)-C(39)-C(42)	121.6(3)
C(38)-C(39)-C(42)	120.5(3)
C(35)-C(40)-H(40A)	109.5
C(35)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(35)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
C(37)-C(41)-H(41A)	109.5
C(37)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
C(37)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
C(39)-C(42)-H(42A)	109.5
C(39)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(39)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(1)-N(1)-C(3)	112.4(2)
C(1)-N(1)-C(16)	127.5(2)
C(3)-N(1)-C(16)	120.0(2)

C(1)-N(2)-C(2)	112.5(2)
C(1)-N(2)-C(7)	129.0(2)
C(2)-N(2)-C(7)	118.2(2)
C(4)-N(3)-C(6)	111.2(2)
C(4)-N(3)-C(25)	128.2(2)
C(6)-N(3)-C(25)	120.6(2)
C(4)-N(4)-C(5)	112.2(2)
C(4)-N(4)-C(34)	127.8(2)
C(5)-N(4)-C(34)	119.7(2)
Cl(2)-V(1)-C(1)	97.42(7)
Cl(2)-V(1)-Cl(3)	112.43(4)
C(1)-V(1)-Cl(3)	89.10(7)
Cl(2)-V(1)-C(4)	97.73(7)
C(1)-V(1)-C(4)	164.85(9)
Cl(3)-V(1)-C(4)	85.05(7)
Cl(2)-V(1)-Cl(1)	104.03(4)
C(1)-V(1)-Cl(1)	85.27(7)
Cl(3)-V(1)-Cl(1)	143.52(4)
C(4)-V(1)-Cl(1)	91.16(7)

Table 12. Anisotropic displacement parameters (A^2 x 10^3) for **6**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	30(2)	28(1)	31(2)	-3(1)	5(1)	4(1)
C(2)	33(2)	38(2)	68(2)	-16(2)	-5(2)	2(1)
C(3)	27(2)	45(2)	71(2)	-18(2)	-12(2)	6(1)
C(4)	31(2)	34(1)	31(2)	-1(1)	1(1)	4(1)
C(5)	37(2)	50(2)	58(2)	-19(2)	5(2)	-7(1)
C(6)	48(2)	60(2)	54(2)	-28(2)	2(2)	-7(2)
C(7)	35(2)	27(1)	48(2)	-6(1)	2(1)	5(1)
C(8)	35(2)	44(2)	46(2)	-10(1)	1(2)	6(1)
C(9)	41(2)	65(2)	56(2)	-23(2)	2(2)	14(2)
C(10)	53(2)	45(2)	65(2)	-22(2)	-17(2)	19(2)
C(11)	67(2)	33(2)	62(2)	3(2)	-10(2)	5(2)
C(12)	46(2)	36(2)	53(2)	-5(1)	7(2)	-1(1)
C(13)	56(2)	71(2)	52(2)	-1(2)	12(2)	4(2)
C(14)	84(3)	66(2)	101(3)	-33(2)	-29(2)	45(2)
C(15)	80(3)	57(2)	68(2)	7(2)	24(2)	-1(2)
C(16)	26(2)	34(1)	51(2)	-4(1)	1(1)	6(1)
C(17)	32(2)	47(2)	52(2)	7(2)	-4(2)	3(1)
C(18)	43(2)	47(2)	75(2)	16(2)	0(2)	4(2)
C(19)	38(2)	34(2)	105(3)	4(2)	-4(2)	7(1)
C(20)	33(2)	42(2)	81(3)	-16(2)	5(2)	7(1)
C(21)	27(2)	38(2)	55(2)	-6(1)	1(1)	3(1)
C(22)	58(2)	83(2)	44(2)	7(2)	-3(2)	7(2)
C(23)	88(3)	33(2)	165(5)	8(2)	14(3)	19(2)
C(24)	47(2)	56(2)	67(2)	-4(2)	21(2)	8(2)
C(25)	37(2)	48(2)	42(2)	-20(1)	12(2)	-9(1)
C(26)	39(2)	44(2)	48(2)	-19(1)	8(2)	-5(1)
C(27)	35(2)	69(2)	64(2)	-29(2)	3(2)	-6(2)
C(28)	53(2)	92(3)	62(3)	-36(2)	21(2)	-21(2)
C(29)	76(3)	93(3)	41(2)	-17(2)	15(2)	-28(2)
C(30)	58(2)	70(2)	36(2)	-13(2)	6(2)	-8(2)
C(31)	49(2)	52(2)	61(2)	-9(2)	0(2)	3(2)
C(32)	60(3)	166(5)	106(4)	-39(3)	46(3)	-26(3)
C(33)	84(3)	117(3)	47(2)	12(2)	-4(2)	4(3)
C(34)	28(2)	31(1)	38(2)	-2(1)	4(1)	2(1)
C(35)	34(2)	35(2)	61(2)	5(1)	-1(2)	2(1)
C(36)	40(2)	39(2)	97(3)	-9(2)	3(2)	7(2)
C(37)	35(2)	62(2)	80(3)	-32(2)	9(2)	-1(2)
C(38)	41(2)	67(2)	46(2)	-8(2)	11(2)	-14(2)
C(39)	35(2)	38(2)	41(2)	0(1)	0(1)	-5(1)
C(40)	67(2)	53(2)	80(3)	29(2)	-3(2)	4(2)
C(41)	52(2)	116(3)	128(4)	-60(3)	34(3)	-1(2)
C(42)	50(2)	48(2)	64(2)	18(2)	3(2)	-2(2)
N(1)	31(1)	29(1)	45(1)	-6(1)	0(1)	7(1)
N(2)	31(1)	31(1)	41(1)	-5(1)	4(1)	4(1)
N(3)	33(1)	46(1)	40(1)	-13(1)	4(1)	-1(1)
N(4)	32(1)	34(1)	38(1)	-1(1)	2(1)	1(1)
Cl(1)	63(1)	57(1)	38(1)	-1(1)	13(1)	-17(1)
Cl(2)	41(1)	47(1)	60(1)	-13(1)	3(1)	7(1)
Cl(3)	49(1)	48(1)	40(1)	11(1)	-2(1)	-10(1)
V(1)	30(1)	30(1)	31(1)	-1(1)	3(1)	2(1)

X-ray Data for Complex 7

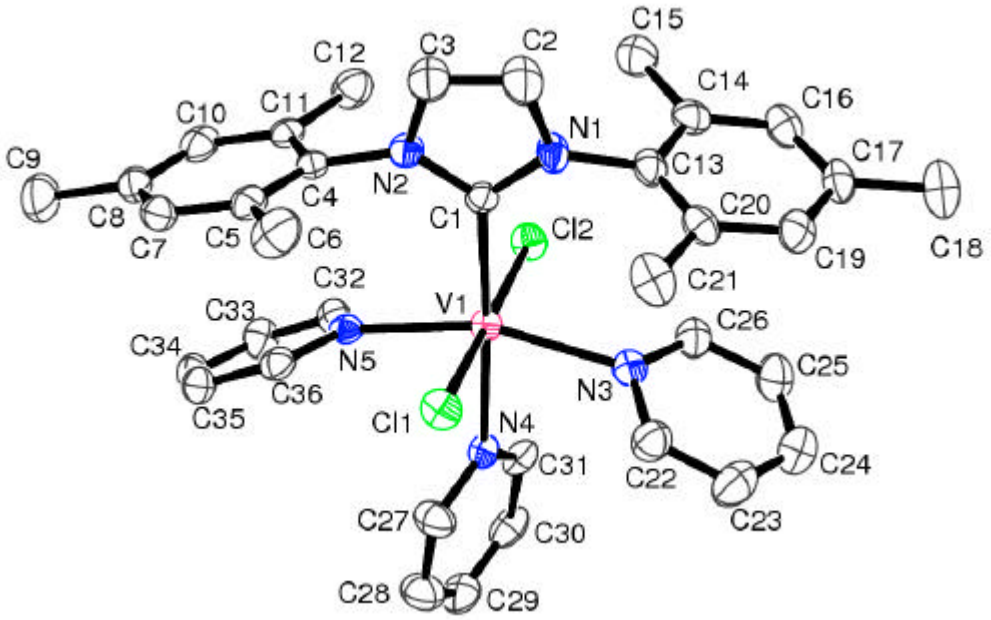

Table 13. Crystal data and structure refinement for **7**.

Empirical formula	C36 H39 Cl2 N5 V
Formula weight	663.56
Temperature	180 K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21/c
Unit cell dimensions	a = 11.5667(9) A alpha = 90 deg. b = 17.0017(10) A beta = 104.448(3) deg. c = 17.8222(12) A gamma = 90 deg.
Volume	3394.0(4) A^3
Z, Calculated density	4, 1.299 Mg/m^3
Absorption coefficient	0.482 mm^-1
F(000)	1388
Crystal size	0.17 x 0.12 x 0.03 mm
Theta range for data collection	2.4 to 24.54 deg.
Limiting indices	-13<=h<=13, -16<=k<=19, -20<=l<=20
Reflections collected / unique	29733 / 5665 [R(int) = 0.0762]
Completeness to theta = 24.54	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.990 and 0.875
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5665 / 0 / 403
Goodness-of-fit on F^2	1.003
Final R indices [I>2sigma(I)]	R1 = 0.039, wR2 = 0.0747
R indices (all data)	R1 = 0.0857, wR2 = 0.0893
Largest diff. peak and hole	0.263 and -0.313 e.A^-3

Table 14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **7**.

	x	y	z	U(eq)
V(1)	-2024(1)	12043(1)	-1414(1)	22(1)
Cl(2)	-3559(1)	12311(1)	-2635(1)	31(1)
Cl(1)	-567(1)	11787(1)	-146(1)	31(1)
N(1)	-3953(2)	12516(1)	-411(1)	29(1)
N(3)	-1621(2)	13339(1)	-1297(1)	27(1)
N(2)	-3825(2)	11272(1)	-437(1)	26(1)
N(4)	-525(2)	12098(1)	-2015(1)	23(1)
N(5)	-1900(2)	10779(1)	-1764(1)	23(1)
C(9)	-3018(3)	8058(2)	-1080(2)	60(1)
C(23)	-152(3)	14334(2)	-832(2)	55(1)
C(24)	-777(3)	14869(2)	-1348(2)	54(1)
C(18)	-4113(3)	15846(2)	-845(2)	52(1)
C(2)	-4617(3)	12222(2)	74(2)	49(1)
C(6)	-2260(3)	10364(2)	744(2)	47(1)
C(28)	1414(3)	11662(2)	-2072(2)	47(1)
C(25)	-1821(3)	14636(2)	-1826(2)	46(1)
C(3)	-4532(3)	11445(2)	53(2)	45(1)
C(15)	-5769(3)	13143(2)	-1650(2)	43(1)
C(21)	-2180(3)	13452(2)	599(2)	43(1)
C(29)	1271(3)	11975(2)	-2793(2)	42(1)
C(12)	-5105(3)	10629(2)	-1884(2)	39(1)
C(30)	235(3)	12357(2)	-3120(2)	37(1)
C(22)	-590(3)	13584(2)	-829(2)	39(1)
C(27)	504(3)	11730(2)	-1709(2)	38(1)
C(7)	-2676(3)	9242(2)	-206(2)	38(1)
C(34)	-1269(3)	9359(2)	-2329(2)	37(1)
C(8)	-3245(3)	8906(2)	-903(2)	36(1)
C(33)	-1956(3)	9896(2)	-2815(2)	35(1)
C(26)	-2226(3)	13882(2)	-1789(2)	34(1)
C(16)	-4874(3)	14474(2)	-1230(2)	35(1)
C(35)	-919(3)	9528(2)	-1556(2)	34(1)
C(17)	-4059(3)	14963(2)	-753(2)	34(1)
C(10)	-4031(3)	9362(2)	-1436(2)	34(1)
C(19)	-3182(3)	14618(2)	-171(2)	32(1)
C(14)	-4846(3)	13664(2)	-1142(2)	32(1)
C(5)	-2851(3)	10019(2)	-31(2)	30(1)
C(20)	-3104(3)	13815(2)	-54(2)	30(1)
C(31)	-645(3)	12414(2)	-2717(2)	30(1)
C(13)	-3941(3)	13349(2)	-556(2)	28(1)
C(32)	-2261(3)	10588(2)	-2517(2)	29(1)
C(36)	-1236(3)	10242(2)	-1297(2)	29(1)
C(11)	-4226(2)	10144(2)	-1301(2)	26(1)
C(1)	-3428(2)	11935(2)	-739(2)	23(1)
C(4)	-3601(2)	10465(2)	-601(2)	23(1)

Table 15. Bond lengths [A] and angles [deg] for **7**.

V(1)-N(5)	2.252(2)
V(1)-N(3)	2.252(2)
V(1)-N(4)	2.255(2)
V(1)-C(1)	2.257(3)
V(1)-Cl(2)	2.4826(9)
V(1)-Cl(1)	2.4980(9)
N(1)-C(1)	1.365(3)
N(1)-C(2)	1.384(3)
N(1)-C(13)	1.442(3)
N(3)-C(22)	1.340(4)
N(3)-C(26)	1.343(4)
N(2)-C(3)	1.369(3)
N(2)-C(1)	1.376(3)
N(2)-C(4)	1.440(3)
N(4)-C(27)	1.335(4)
N(4)-C(31)	1.336(3)
N(5)-C(36)	1.341(3)
N(5)-C(32)	1.341(3)
C(9)-C(8)	1.513(4)
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(23)-C(24)	1.366(5)
C(23)-C(22)	1.373(4)
C(23)-H(23)	0.9500
C(24)-C(25)	1.351(5)
C(24)-H(24)	0.9500
C(18)-C(17)	1.509(4)
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(2)-C(3)	1.326(4)
C(2)-H(2)	0.9500
C(6)-C(5)	1.500(4)
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800
C(28)-C(29)	1.363(4)
C(28)-C(27)	1.371(4)
C(28)-H(28)	0.9500
C(25)-C(26)	1.372(4)
C(25)-H(25)	0.9500
C(3)-H(3)	0.9500
C(15)-C(14)	1.504(4)
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(21)-C(20)	1.501(4)
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(29)-C(30)	1.360(4)
C(29)-H(29)	0.9500
C(12)-C(11)	1.505(4)
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(30)-C(31)	1.387(4)
C(30)-H(30)	0.9500
C(22)-H(22)	0.9500
C(27)-H(27)	0.9500
C(7)-C(8)	1.376(4)
C(7)-C(5)	1.384(4)
C(7)-H(7)	0.9500
C(34)-C(35)	1.366(4)
C(34)-C(33)	1.367(4)

C(34)-H(34)	0.9500
C(8)-C(10)	1.378(4)
C(33)-C(32)	1.373(4)
C(33)-H(33)	0.9500
C(26)-H(26)	0.9500
C(16)-C(17)	1.379(4)
C(16)-C(14)	1.386(4)
C(16)-H(16)	0.9500
C(35)-C(36)	1.380(4)
C(35)-H(35)	0.9500
C(17)-C(19)	1.387(4)
C(10)-C(11)	1.380(4)
C(10)-H(10)	0.9500
C(19)-C(20)	1.381(4)
C(19)-H(19)	0.9500
C(14)-C(13)	1.388(4)
C(5)-C(4)	1.385(4)
C(20)-C(13)	1.391(4)
C(31)-H(31)	0.9500
C(32)-H(32)	0.9500
C(36)-H(36)	0.9500
C(11)-C(4)	1.389(4)

N(5)-V(1)-N(3)	159.01(8)
N(5)-V(1)-N(4)	78.40(8)
N(3)-V(1)-N(4)	80.63(8)
N(5)-V(1)-C(1)	100.05(9)
N(3)-V(1)-C(1)	100.93(9)
N(4)-V(1)-C(1)	175.59(9)
N(5)-V(1)-Cl(2)	90.79(6)
N(3)-V(1)-Cl(2)	89.29(6)
N(4)-V(1)-Cl(2)	92.46(6)
C(1)-V(1)-Cl(2)	91.69(7)
N(5)-V(1)-Cl(1)	90.53(6)
N(3)-V(1)-Cl(1)	90.52(6)
N(4)-V(1)-Cl(1)	90.69(6)
C(1)-V(1)-Cl(1)	85.19(7)
Cl(2)-V(1)-Cl(1)	176.78(3)
C(1)-N(1)-C(2)	112.5(2)
C(1)-N(1)-C(13)	127.5(2)
C(2)-N(1)-C(13)	119.9(2)
C(22)-N(3)-C(26)	115.6(3)
C(22)-N(3)-V(1)	119.51(19)
C(26)-N(3)-V(1)	123.3(2)
C(3)-N(2)-C(1)	112.6(2)
C(3)-N(2)-C(4)	120.0(2)
C(1)-N(2)-C(4)	127.4(2)
C(27)-N(4)-C(31)	116.4(2)
C(27)-N(4)-V(1)	119.91(18)
C(31)-N(4)-V(1)	123.29(19)
C(36)-N(5)-C(32)	116.3(2)
C(36)-N(5)-V(1)	122.96(19)
C(32)-N(5)-V(1)	118.89(18)
C(8)-C(9)-H(9A)	109.5
C(8)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(8)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(24)-C(23)-C(22)	119.2(3)
C(24)-C(23)-H(23)	120.4
C(22)-C(23)-H(23)	120.4
C(25)-C(24)-C(23)	117.9(3)
C(25)-C(24)-H(24)	121.0
C(23)-C(24)-H(24)	121.0
C(17)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5

C(17)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(3)-C(2)-N(1)	106.5(3)
C(3)-C(2)-H(2)	126.7
N(1)-C(2)-H(2)	126.7
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(29)-C(28)-C(27)	119.0(3)
C(29)-C(28)-H(28)	120.5
C(27)-C(28)-H(28)	120.5
C(24)-C(25)-C(26)	120.4(3)
C(24)-C(25)-H(25)	119.8
C(26)-C(25)-H(25)	119.8
C(2)-C(3)-N(2)	107.0(3)
C(2)-C(3)-H(3)	126.5
N(2)-C(3)-H(3)	126.5
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(30)-C(29)-C(28)	118.4(3)
C(30)-C(29)-H(29)	120.8
C(28)-C(29)-H(29)	120.8
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(29)-C(30)-C(31)	119.6(3)
C(29)-C(30)-H(30)	120.2
C(31)-C(30)-H(30)	120.2
N(3)-C(22)-C(23)	123.9(3)
N(3)-C(22)-H(22)	118.1
C(23)-C(22)-H(22)	118.1
N(4)-C(27)-C(28)	123.9(3)
N(4)-C(27)-H(27)	118.0
C(28)-C(27)-H(27)	118.0
C(8)-C(7)-C(5)	122.4(3)
C(8)-C(7)-H(7)	118.8
C(5)-C(7)-H(7)	118.8
C(35)-C(34)-C(33)	118.6(3)
C(35)-C(34)-H(34)	120.7
C(33)-C(34)-H(34)	120.7
C(7)-C(8)-C(10)	118.3(3)
C(7)-C(8)-C(9)	121.0(3)
C(10)-C(8)-C(9)	120.7(3)
C(34)-C(33)-C(32)	119.4(3)
C(34)-C(33)-H(33)	120.3
C(32)-C(33)-H(33)	120.3
N(3)-C(26)-C(25)	123.0(3)
N(3)-C(26)-H(26)	118.5
C(25)-C(26)-H(26)	118.5
C(17)-C(16)-C(14)	122.4(3)
C(17)-C(16)-H(16)	118.8

C(14)-C(16)-H(16)	118.8
C(34)-C(35)-C(36)	119.0(3)
C(34)-C(35)-H(35)	120.5
C(36)-C(35)-H(35)	120.5
C(16)-C(17)-C(19)	117.8(3)
C(16)-C(17)-C(18)	121.9(3)
C(19)-C(17)-C(18)	120.3(3)
C(8)-C(10)-C(11)	122.0(3)
C(8)-C(10)-H(10)	119.0
C(11)-C(10)-H(10)	119.0
C(20)-C(19)-C(17)	122.6(3)
C(20)-C(19)-H(19)	118.7
C(17)-C(19)-H(19)	118.7
C(16)-C(14)-C(13)	117.4(3)
C(16)-C(14)-C(15)	121.6(3)
C(13)-C(14)-C(15)	121.0(3)
C(7)-C(5)-C(4)	117.3(3)
C(7)-C(5)-C(6)	121.5(3)
C(4)-C(5)-C(6)	121.2(3)
C(19)-C(20)-C(13)	117.2(3)
C(19)-C(20)-C(21)	122.0(3)
C(13)-C(20)-C(21)	120.8(3)
N(4)-C(31)-C(30)	122.6(3)
N(4)-C(31)-H(31)	118.7
C(30)-C(31)-H(31)	118.7
C(14)-C(13)-C(20)	122.6(3)
C(14)-C(13)-N(1)	118.3(3)
C(20)-C(13)-N(1)	118.7(3)
N(5)-C(32)-C(33)	123.3(3)
N(5)-C(32)-H(32)	118.3
C(33)-C(32)-H(32)	118.3
N(5)-C(36)-C(35)	123.4(3)
N(5)-C(36)-H(36)	118.3
C(35)-C(36)-H(36)	118.3
C(10)-C(11)-C(4)	117.7(3)
C(10)-C(11)-C(12)	121.3(3)
C(4)-C(11)-C(12)	121.1(3)
N(1)-C(1)-N(2)	101.4(2)
N(1)-C(1)-V(1)	128.79(19)
N(2)-C(1)-V(1)	128.98(19)
C(5)-C(4)-C(11)	122.2(3)
C(5)-C(4)-N(2)	119.1(3)
C(11)-C(4)-N(2)	118.5(2)

Table 16. Anisotropic displacement parameters (A^2 x 10^3) for **7**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
V(1)	23(1)	24(1)	18(1)	2(1)	6(1)	0(1)
Cl(2)	32(1)	34(1)	25(1)	3(1)	2(1)	3(1)
Cl(1)	33(1)	37(1)	20(1)	2(1)	3(1)	2(1)
N(1)	40(2)	23(1)	31(1)	0(1)	20(1)	3(1)
N(3)	30(2)	28(1)	24(1)	1(1)	9(1)	1(1)
N(2)	29(2)	26(1)	24(1)	0(1)	12(1)	-1(1)
N(4)	29(2)	23(1)	20(1)	1(1)	7(1)	-2(1)
N(5)	20(1)	28(1)	22(1)	5(1)	8(1)	-1(1)
C(9)	68(3)	32(2)	94(3)	2(2)	47(2)	6(2)
C(23)	48(3)	46(2)	68(3)	-3(2)	8(2)	-14(2)
C(24)	56(3)	34(2)	72(3)	2(2)	17(2)	-6(2)
C(18)	74(3)	30(2)	51(2)	-1(2)	15(2)	10(2)
C(2)	69(3)	36(2)	59(2)	4(2)	51(2)	8(2)
C(6)	47(2)	51(2)	38(2)	15(2)	0(2)	-7(2)
C(28)	35(2)	51(2)	59(2)	11(2)	22(2)	6(2)
C(25)	54(3)	32(2)	53(2)	9(2)	13(2)	4(2)
C(3)	58(3)	37(2)	54(2)	5(2)	42(2)	2(2)
C(15)	37(2)	41(2)	47(2)	-2(2)	7(2)	1(2)
C(21)	53(2)	43(2)	31(2)	1(2)	10(2)	11(2)
C(29)	47(2)	39(2)	49(2)	0(2)	31(2)	-6(2)
C(12)	36(2)	40(2)	38(2)	0(2)	3(2)	-7(2)
C(30)	50(2)	38(2)	27(2)	2(2)	16(2)	-16(2)
C(22)	37(2)	36(2)	39(2)	2(2)	5(2)	-3(2)
C(27)	32(2)	45(2)	37(2)	14(2)	12(2)	8(2)
C(7)	29(2)	35(2)	52(2)	22(2)	16(2)	7(2)
C(34)	42(2)	26(2)	47(2)	-2(2)	19(2)	2(2)
C(8)	38(2)	26(2)	54(2)	5(2)	27(2)	2(2)
C(33)	45(2)	32(2)	30(2)	-5(2)	14(2)	-1(2)
C(26)	38(2)	29(2)	36(2)	1(2)	11(2)	1(2)
C(16)	41(2)	32(2)	31(2)	5(2)	10(2)	11(2)
C(35)	33(2)	29(2)	40(2)	11(2)	10(2)	2(1)
C(17)	44(2)	23(2)	35(2)	-2(2)	15(2)	6(2)
C(10)	38(2)	34(2)	36(2)	-4(2)	22(2)	-7(2)
C(19)	41(2)	30(2)	28(2)	-9(1)	12(2)	-1(2)
C(14)	30(2)	36(2)	32(2)	-2(2)	14(2)	3(2)
C(5)	29(2)	31(2)	34(2)	9(2)	13(2)	-2(1)
C(20)	33(2)	33(2)	26(2)	-4(1)	13(2)	7(1)
C(31)	33(2)	29(2)	24(2)	3(1)	2(1)	-10(1)
C(13)	36(2)	24(2)	31(2)	0(1)	19(2)	4(1)
C(32)	34(2)	29(2)	26(2)	5(1)	8(2)	2(1)
C(36)	28(2)	31(2)	28(2)	5(1)	10(2)	-4(1)
C(11)	23(2)	29(2)	30(2)	5(1)	14(2)	-2(1)
C(1)	20(2)	24(2)	22(2)	1(1)	2(1)	-1(1)
C(4)	21(2)	23(2)	28(2)	3(1)	13(1)	0(1)

X-ray Data for Complex 8

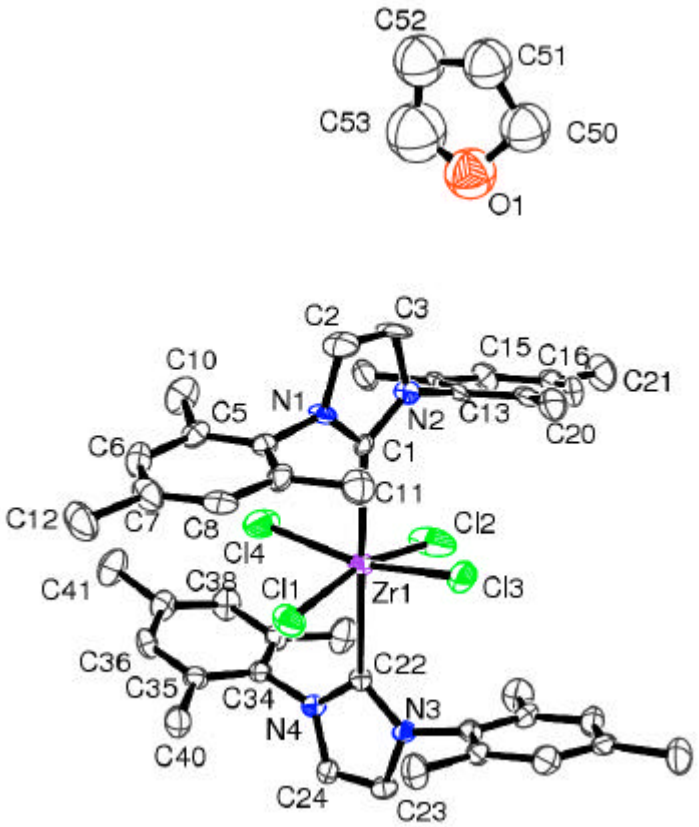

Table 17. Crystal data and structure refinement for **8**.

Empirical formula	C46 H56 Cl4 N4 O Zr
Formula weight	913.97
Temperature	180 K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 11.5961(11) A alpha = 80.854(9) deg. b = 12.8305(13) A beta = 72.645(9) deg. c = 16.8864(18) A gamma = 69.072(9) deg.
Volume	2236.0(4) A^3
Z, Calculated density	2, 1.358 Mg/m^3
Absorption coefficient	0.524 mm^-1
F(000)	952
Crystal size	0.3 x 0.2 x 0.15 mm
Theta range for data collection	2.76 to 26.37 deg.
Limiting indices	-13<=h<=14, -16<=k<=15, -20<=l<=21
Reflections collected / unique	17705 / 9136 [R(int) = 0.0725]
Completeness to theta = 26.37	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.918 and 0.8163
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9136 / 0 / 492
Goodness-of-fit on F^2	0.807
Final R indices [I>2sigma(I)]	R1 = 0.047, wR2 = 0.0777
R indices (all data)	R1 = 0.133, wR2 = 0.094
Largest diff. peak and hole	0.725 and -0.671 e.A^-3

Table 18. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **8**.

	x	y	z	U(eq)
C(1)	4645(3)	2442(3)	7170(2)	18(1)
C(2)	6552(4)	2584(4)	7099(3)	37(1)
C(3)	6530(4)	2582(4)	6316(3)	36(1)
C(4)	5209(3)	2492(3)	8498(2)	22(1)
C(5)	4762(3)	3505(3)	8867(3)	25(1)
C(6)	4665(4)	3450(4)	9711(3)	34(1)
C(7)	5013(4)	2458(4)	10170(3)	35(1)
C(8)	5472(3)	1479(4)	9767(3)	26(1)
C(9)	5586(4)	1471(3)	8924(3)	25(1)
C(10)	4450(4)	4606(3)	8378(3)	42(1)
C(11)	6106(4)	384(3)	8507(3)	38(1)
C(12)	4902(4)	2459(4)	11077(2)	48(1)
C(13)	5016(4)	2506(3)	5607(2)	21(1)
C(14)	4321(4)	3504(3)	5301(2)	21(1)
C(15)	4093(4)	3520(3)	4539(2)	30(1)
C(16)	4548(4)	2582(4)	4097(3)	29(1)
C(17)	5262(4)	1595(4)	4425(3)	33(1)
C(18)	5525(4)	1533(3)	5185(3)	26(1)
C(19)	3817(4)	4554(3)	5757(2)	37(1)
C(20)	6356(4)	471(3)	5497(3)	40(1)
C(21)	4347(4)	2632(4)	3252(2)	46(1)
C(22)	383(3)	2019(3)	8202(2)	18(1)
C(23)	-1213(3)	1280(3)	8618(2)	23(1)
C(24)	-1723(4)	2345(3)	8810(2)	25(1)
C(25)	842(3)	29(3)	7877(3)	22(1)
C(26)	1455(4)	-859(3)	8345(2)	22(1)
C(27)	2051(4)	-1875(3)	7995(3)	31(1)
C(28)	2068(4)	-2029(3)	7201(3)	27(1)
C(29)	1474(4)	-1123(3)	6746(3)	32(1)
C(30)	817(4)	-71(3)	7078(3)	26(1)
C(31)	1462(4)	-732(3)	9205(2)	36(1)
C(32)	113(4)	878(3)	6571(3)	39(1)
C(33)	2667(4)	-3170(3)	6851(3)	46(1)
C(34)	-995(3)	3977(3)	8603(2)	21(1)
C(35)	-1071(4)	4358(3)	9339(3)	24(1)
C(36)	-1292(3)	5492(3)	9356(3)	29(1)
C(37)	-1419(4)	6214(3)	8661(3)	31(1)
C(38)	-1387(4)	5791(3)	7950(3)	31(1)
C(39)	-1207(3)	4671(3)	7911(3)	24(1)
C(40)	-947(4)	3596(3)	10097(2)	35(1)
C(41)	-1573(4)	7430(3)	8674(3)	48(1)
C(42)	-1218(4)	4261(3)	7132(3)	40(1)
C(50)	10288(5)	1933(5)	4272(4)	87(2)
C(51)	11219(5)	2366(5)	4390(4)	86(2)
C(52)	10533(6)	3536(5)	4629(4)	98(2)
C(53)	9202(7)	3578(6)	4845(5)	135(3)
N(1)	5436(3)	2502(3)	7609(2)	22(1)
N(2)	5366(3)	2482(3)	6368(2)	23(1)
N(3)	70(3)	1075(3)	8249(2)	20(1)
N(4)	-747(3)	2797(3)	8554(2)	20(1)
Cl(1)	2514(1)	1702(1)	9154(1)	39(1)
Cl(2)	2037(1)	2588(1)	6399(1)	63(1)
Cl(3)	3763(1)	296(1)	7394(1)	45(1)
Cl(4)	1895(1)	4148(1)	7964(1)	50(1)
Zr(1)	2534(1)	2209(1)	7712(1)	25(1)
O(1)	9101(4)	2573(3)	4788(3)	95(1)

Table 19. Bond lengths [A] and angles [deg] for **8**.

C(1)-N(1)	1.367(4)
C(1)-N(2)	1.368(4)
C(1)-Zr(1)	2.453(4)
C(2)-C(3)	1.330(5)
C(2)-N(1)	1.354(5)
C(2)-H(2)	0.95
C(3)-N(2)	1.377(4)
C(3)-H(3)	0.95
C(4)-C(9)	1.380(5)
C(4)-C(5)	1.389(5)
C(4)-N(1)	1.444(5)
C(5)-C(6)	1.388(5)
C(5)-C(10)	1.500(5)
C(6)-C(7)	1.375(5)
C(6)-H(6)	0.95
C(7)-C(8)	1.379(5)
C(7)-C(12)	1.499(5)
C(8)-C(9)	1.392(5)
C(8)-H(8)	0.95
C(9)-C(11)	1.504(5)
C(10)-H(10A)	0.98
C(10)-H(10B)	0.98
C(10)-H(10C)	0.98
C(11)-H(11A)	0.98
C(11)-H(11B)	0.98
C(11)-H(11C)	0.98
C(12)-H(12A)	0.98
C(12)-H(12B)	0.98
C(12)-H(12C)	0.98
C(13)-C(14)	1.361(5)
C(13)-C(18)	1.385(5)
C(13)-N(2)	1.452(5)
C(14)-C(15)	1.385(5)
C(14)-C(19)	1.500(5)
C(15)-C(16)	1.370(5)
C(15)-H(15)	0.95
C(16)-C(17)	1.377(5)
C(16)-C(21)	1.502(5)
C(17)-C(18)	1.390(5)
C(17)-H(17)	0.95
C(18)-C(20)	1.483(5)
C(19)-H(19A)	0.98
C(19)-H(19B)	0.98
C(19)-H(19C)	0.98
C(20)-H(20A)	0.98
C(20)-H(20B)	0.98
C(20)-H(20C)	0.98
C(21)-H(21A)	0.98
C(21)-H(21B)	0.98
C(21)-H(21C)	0.98
C(22)-N(4)	1.363(4)
C(22)-N(3)	1.367(4)
C(22)-Zr(1)	2.471(4)
C(23)-C(24)	1.331(5)
C(23)-N(3)	1.375(4)
C(23)-H(23)	0.95
C(24)-N(4)	1.378(5)
C(24)-H(24)	0.95
C(25)-C(26)	1.379(5)
C(25)-C(30)	1.385(5)
C(25)-N(3)	1.439(4)
C(26)-C(27)	1.372(5)
C(26)-C(31)	1.489(5)
C(27)-C(28)	1.380(5)
C(27)-H(27)	0.95
C(28)-C(29)	1.369(5)

C(28)-C(33)	1.510(5)
C(29)-C(30)	1.403(5)
C(29)-H(29)	0.95
C(30)-C(32)	1.501(5)
C(31)-H(31A)	0.98
C(31)-H(31B)	0.98
C(31)-H(31C)	0.98
C(32)-H(32A)	0.98
C(32)-H(32B)	0.98
C(32)-H(32C)	0.98
C(33)-H(33A)	0.98
C(33)-H(33B)	0.98
C(33)-H(33C)	0.98
C(34)-C(35)	1.374(5)
C(34)-C(39)	1.380(5)
C(34)-N(4)	1.448(4)
C(35)-C(36)	1.388(5)
C(35)-C(40)	1.493(5)
C(36)-C(37)	1.384(5)
C(36)-H(36)	0.95
C(37)-C(38)	1.381(5)
C(37)-C(41)	1.507(5)
C(38)-C(39)	1.386(5)
C(38)-H(38)	0.95
C(39)-C(42)	1.496(5)
C(40)-H(40A)	0.98
C(40)-H(40B)	0.98
C(40)-H(40C)	0.98
C(41)-H(41A)	0.98
C(41)-H(41B)	0.98
C(41)-H(41C)	0.98
C(42)-H(42A)	0.98
C(42)-H(42B)	0.98
C(42)-H(42C)	0.98
C(50)-O(1)	1.425(6)
C(50)-C(51)	1.451(7)
C(50)-H(50A)	0.99
C(50)-H(50B)	0.99
C(51)-C(52)	1.483(6)
C(51)-H(51A)	0.99
C(51)-H(51B)	0.99
C(52)-C(53)	1.460(8)
C(52)-H(52A)	0.99
C(52)-H(52B)	0.99
C(53)-O(1)	1.357(7)
C(53)-H(53A)	0.99
C(53)-H(53B)	0.99
Cl(1)-Zr(1)	2.4136(12)
Cl(2)-Zr(1)	2.3871(13)
Cl(3)-Zr(1)	2.4102(12)
Cl(4)-Zr(1)	2.3983(12)

N(1)-C(1)-N(2)	102.0(3)
N(1)-C(1)-Zr(1)	128.1(3)
N(2)-C(1)-Zr(1)	129.8(3)
C(3)-C(2)-N(1)	108.7(4)
C(3)-C(2)-H(2)	125.6
N(1)-C(2)-H(2)	125.6
C(2)-C(3)-N(2)	105.2(4)
C(2)-C(3)-H(3)	127.4
N(2)-C(3)-H(3)	127.4
C(9)-C(4)-C(5)	123.2(4)
C(9)-C(4)-N(1)	117.7(4)
C(5)-C(4)-N(1)	118.7(4)
C(6)-C(5)-C(4)	116.5(4)
C(6)-C(5)-C(10)	121.3(4)
C(4)-C(5)-C(10)	122.2(4)
C(7)-C(6)-C(5)	123.0(4)

C(7)-C(6)-H(6)	118.5
C(5)-C(6)-H(6)	118.5
C(6)-C(7)-C(8)	117.9(4)
C(6)-C(7)-C(12)	120.2(4)
C(8)-C(7)-C(12)	121.8(4)
C(7)-C(8)-C(9)	122.2(4)
C(7)-C(8)-H(8)	118.9
C(9)-C(8)-H(8)	118.9
C(4)-C(9)-C(8)	117.2(4)
C(4)-C(9)-C(11)	122.3(4)
C(8)-C(9)-C(11)	120.5(4)
C(5)-C(10)-H(10A)	109.5
C(5)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(5)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(9)-C(11)-H(11A)	109.5
C(9)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(9)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(7)-C(12)-H(12A)	109.5
C(7)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(7)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-C(18)	123.5(4)
C(14)-C(13)-N(2)	118.5(4)
C(18)-C(13)-N(2)	117.7(4)
C(13)-C(14)-C(15)	117.2(4)
C(13)-C(14)-C(19)	122.4(4)
C(15)-C(14)-C(19)	120.4(4)
C(16)-C(15)-C(14)	122.2(4)
C(16)-C(15)-H(15)	118.9
C(14)-C(15)-H(15)	118.9
C(15)-C(16)-C(17)	118.5(4)
C(15)-C(16)-C(21)	121.3(4)
C(17)-C(16)-C(21)	120.1(4)
C(16)-C(17)-C(18)	121.7(4)
C(16)-C(17)-H(17)	119.2
C(18)-C(17)-H(17)	119.2
C(13)-C(18)-C(17)	116.9(4)
C(13)-C(18)-C(20)	123.0(4)
C(17)-C(18)-C(20)	120.1(4)
C(14)-C(19)-H(19A)	109.5
C(14)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(14)-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(16)-C(21)-H(21A)	109.5
C(16)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(16)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
N(4)-C(22)-N(3)	103.9(3)
N(4)-C(22)-Zr(1)	128.2(3)
N(3)-C(22)-Zr(1)	127.7(3)

C(24)-C(23)-N(3)	107.6(3)
C(24)-C(23)-H(23)	126.2
N(3)-C(23)-H(23)	126.2
C(23)-C(24)-N(4)	107.0(3)
C(23)-C(24)-H(24)	126.5
N(4)-C(24)-H(24)	126.5
C(26)-C(25)-C(30)	122.5(4)
C(26)-C(25)-N(3)	119.8(4)
C(30)-C(25)-N(3)	117.3(4)
C(27)-C(26)-C(25)	117.6(4)
C(27)-C(26)-C(31)	120.8(4)
C(25)-C(26)-C(31)	121.6(4)
C(26)-C(27)-C(28)	122.6(4)
C(26)-C(27)-H(27)	118.7
C(28)-C(27)-H(27)	118.7
C(29)-C(28)-C(27)	118.2(4)
C(29)-C(28)-C(33)	120.3(4)
C(27)-C(28)-C(33)	121.4(4)
C(28)-C(29)-C(30)	121.8(4)
C(28)-C(29)-H(29)	119.1
C(30)-C(29)-H(29)	119.1
C(25)-C(30)-C(29)	117.1(4)
C(25)-C(30)-C(32)	123.2(4)
C(29)-C(30)-C(32)	119.7(4)
C(26)-C(31)-H(31A)	109.5
C(26)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(26)-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(28)-C(33)-H(33A)	109.5
C(28)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(28)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(35)-C(34)-C(39)	123.3(4)
C(35)-C(34)-N(4)	119.1(4)
C(39)-C(34)-N(4)	117.5(4)
C(34)-C(35)-C(36)	117.2(4)
C(34)-C(35)-C(40)	121.9(4)
C(36)-C(35)-C(40)	120.9(4)
C(37)-C(36)-C(35)	121.9(4)
C(37)-C(36)-H(36)	119.1
C(35)-C(36)-H(36)	119.1
C(38)-C(37)-C(36)	118.2(4)
C(38)-C(37)-C(41)	120.6(4)
C(36)-C(37)-C(41)	121.2(4)
C(37)-C(38)-C(39)	122.0(4)
C(37)-C(38)-H(38)	119
C(39)-C(38)-H(38)	119
C(34)-C(39)-C(38)	117.1(4)
C(34)-C(39)-C(42)	123.1(4)
C(38)-C(39)-C(42)	119.8(4)
C(35)-C(40)-H(40A)	109.5
C(35)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(35)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
C(37)-C(41)-H(41A)	109.5
C(37)-C(41)-H(41B)	109.5

H(41A)-C(41)-H(41B)	109.5
C(37)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
C(39)-C(42)-H(42A)	109.5
C(39)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(39)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
O(1)-C(50)-C(51)	104.3(5)
O(1)-C(50)-H(50A)	110.9
C(51)-C(50)-H(50A)	110.9
O(1)-C(50)-H(50B)	110.9
C(51)-C(50)-H(50B)	110.9
H(50A)-C(50)-H(50B)	108.9
C(50)-C(51)-C(52)	107.4(5)
C(50)-C(51)-H(51A)	110.2
C(52)-C(51)-H(51A)	110.2
C(50)-C(51)-H(51B)	110.2
C(52)-C(51)-H(51B)	110.2
H(51A)-C(51)-H(51B)	108.5
C(53)-C(52)-C(51)	101.5(5)
C(53)-C(52)-H(52A)	111.5
C(51)-C(52)-H(52A)	111.5
C(53)-C(52)-H(52B)	111.5
C(51)-C(52)-H(52B)	111.5
H(52A)-C(52)-H(52B)	109.3
O(1)-C(53)-C(52)	112.0(6)
O(1)-C(53)-H(53A)	109.2
C(52)-C(53)-H(53A)	109.2
O(1)-C(53)-H(53B)	109.2
C(52)-C(53)-H(53B)	109.2
H(53A)-C(53)-H(53B)	107.9
C(2)-N(1)-C(1)	111.5(3)
C(2)-N(1)-C(4)	120.0(3)
C(1)-N(1)-C(4)	128.5(3)
C(1)-N(2)-C(3)	112.5(3)
C(1)-N(2)-C(13)	128.4(3)
C(3)-N(2)-C(13)	119.0(3)
C(22)-N(3)-C(23)	110.6(3)
C(22)-N(3)-C(25)	128.7(3)
C(23)-N(3)-C(25)	120.1(3)
C(22)-N(4)-C(24)	111.0(3)
C(22)-N(4)-C(34)	127.4(3)
C(24)-N(4)-C(34)	121.3(3)
Cl(2)-Zr(1)-Cl(4)	93.75(5)
Cl(2)-Zr(1)-Cl(3)	90.99(5)
Cl(4)-Zr(1)-Cl(3)	163.95(4)
Cl(2)-Zr(1)-Cl(1)	164.60(4)
Cl(4)-Zr(1)-Cl(1)	90.34(5)
Cl(3)-Zr(1)-Cl(1)	89.11(4)
Cl(2)-Zr(1)-C(1)	95.02(10)
Cl(4)-Zr(1)-C(1)	82.09(9)
Cl(3)-Zr(1)-C(1)	82.22(9)
Cl(1)-Zr(1)-C(1)	100.25(9)
Cl(2)-Zr(1)-C(22)	82.60(9)
Cl(4)-Zr(1)-C(22)	97.26(9)
Cl(3)-Zr(1)-C(22)	98.56(9)
Cl(1)-Zr(1)-C(22)	82.15(9)
C(1)-Zr(1)-C(22)	177.50(13)
C(53)-O(1)-C(50)	107.0(5)

Table 20. Anisotropic displacement parameters (A^2 x 10^3) for **8**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	23(2)	11(2)	20(2)	-2(2)	-6(2)	-7(2)
C(2)	28(3)	59(3)	34(3)	3(3)	-15(2)	-23(2)
C(3)	20(3)	66(3)	27(3)	0(3)	3(2)	-31(2)
C(4)	19(2)	25(3)	22(3)	-3(2)	-5(2)	-10(2)
C(5)	20(2)	25(3)	36(3)	-2(2)	-14(2)	-7(2)
C(6)	18(2)	38(3)	47(3)	-22(3)	-11(2)	0(2)
C(7)	28(3)	53(3)	23(3)	-5(3)	-10(2)	-10(2)
C(8)	8(2)	37(3)	32(3)	6(2)	-9(2)	-7(2)
C(9)	22(2)	29(3)	29(3)	-6(2)	-10(2)	-10(2)
C(10)	45(3)	25(3)	56(3)	0(3)	-25(3)	-4(2)
C(11)	31(3)	40(3)	40(3)	-6(2)	-10(2)	-8(2)
C(12)	41(3)	80(4)	27(3)	-14(3)	-8(2)	-21(3)
C(13)	17(2)	33(3)	14(2)	-4(2)	4(2)	-13(2)
C(14)	23(2)	25(3)	13(2)	-1(2)	5(2)	-12(2)
C(15)	24(3)	30(3)	29(3)	-3(2)	-4(2)	-1(2)
C(16)	22(3)	42(3)	25(3)	-9(2)	-1(2)	-14(2)
C(17)	34(3)	30(3)	32(3)	-16(2)	2(2)	-9(2)
C(18)	18(2)	29(3)	26(3)	-2(2)	6(2)	-10(2)
C(19)	38(3)	34(3)	30(3)	-9(2)	2(2)	-9(2)
C(20)	37(3)	30(3)	45(3)	-11(2)	3(2)	-8(2)
C(21)	45(3)	66(4)	31(3)	-11(3)	-16(3)	-14(3)
C(22)	13(2)	19(3)	21(2)	-3(2)	-8(2)	-1(2)
C(23)	17(2)	27(3)	28(3)	0(2)	-8(2)	-9(2)
C(24)	23(2)	27(3)	27(3)	-8(2)	-3(2)	-10(2)
C(25)	14(2)	26(3)	25(3)	-7(2)	0(2)	-7(2)
C(26)	25(2)	15(2)	23(2)	1(2)	-3(2)	-6(2)
C(27)	33(3)	19(3)	35(3)	2(2)	-7(2)	-5(2)
C(28)	23(2)	17(3)	35(3)	-3(2)	3(2)	-9(2)
C(29)	42(3)	28(3)	27(3)	-7(2)	-7(2)	-15(2)
C(30)	27(2)	22(3)	31(3)	-1(2)	-8(2)	-12(2)
C(31)	45(3)	26(3)	31(3)	-6(2)	-10(2)	-3(2)
C(32)	46(3)	37(3)	35(3)	2(2)	-21(3)	-8(2)
C(33)	57(3)	32(3)	43(3)	-15(3)	-1(3)	-11(2)
C(34)	19(2)	20(3)	23(3)	-3(2)	-2(2)	-8(2)
C(35)	22(2)	19(3)	26(3)	-2(2)	-1(2)	-5(2)
C(36)	25(3)	27(3)	25(3)	-10(2)	-2(2)	1(2)
C(37)	25(3)	19(3)	43(3)	-6(2)	-11(2)	2(2)
C(38)	39(3)	18(3)	33(3)	7(2)	-21(2)	2(2)
C(39)	15(2)	26(3)	28(3)	-11(2)	-2(2)	-2(2)
C(40)	38(3)	39(3)	31(3)	-9(2)	-8(2)	-13(2)
C(41)	63(3)	22(3)	61(4)	-3(3)	-27(3)	-9(2)
C(42)	59(3)	23(3)	41(3)	2(2)	-25(3)	-9(2)
N(1)	14(2)	35(2)	17(2)	1(2)	-2(2)	-12(2)
N(2)	22(2)	26(2)	22(2)	1(2)	-4(2)	-10(2)
N(3)	15(2)	22(2)	25(2)	-4(2)	-4(2)	-8(2)
N(4)	19(2)	20(2)	22(2)	1(2)	-6(2)	-6(2)
Cl(1)	35(1)	61(1)	26(1)	-4(1)	-9(1)	-20(1)
Cl(2)	51(1)	123(1)	33(1)	16(1)	-17(1)	-54(1)
Cl(3)	40(1)	36(1)	58(1)	-19(1)	2(1)	-17(1)
Cl(4)	30(1)	31(1)	78(1)	-13(1)	6(1)	-11(1)
Zr(1)	20(1)	31(1)	26(1)	-5(1)	-2(1)	-12(1)

X-ray Data for Complex 9

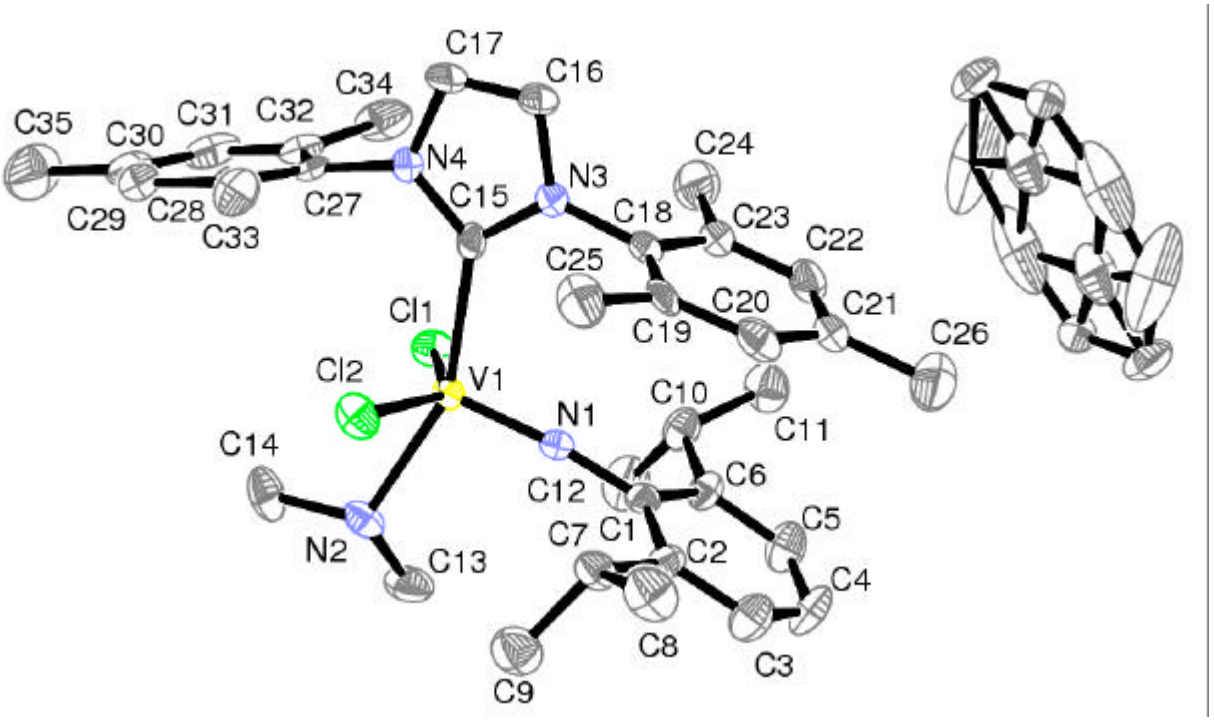

Table 21. Crystal data and structure refinement for **9**.

Identification code	cl737
Empirical formula	C35 H48 Cl2 N4 V, 0.5(C7 H8)
Formula weight	692.68
Temperature	180 K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P b c a
Unit cell dimensions	a = 13.2301(12) A alpha = 90 deg. b = 13.2393(11) A beta = 90 deg. c = 42.922(3) A gamma = 90 deg.
Volume	7518.1(11) A^3
Z, Calculated density	8, 1.224 Mg/m^3
Absorption coefficient	0.437 mm^-1
F(000)	2912
Crystal size	0.25 x 0.175 x 0.075 mm
Theta range for data collection	2.88 to 26.31 deg.
Limiting indices	-16<=h<=16, -16<=k<=11, -53<=l<=53
Reflections collected / unique	55113 / 7683 [R(int) = 0.1283]
Completeness to theta = 26.31	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9711 and 0.9454
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7683 / 4 / 411
Goodness-of-fit on F^2	0.917
Final R indices [I>2sigma(I)]	R1 = 0.0534, wR2 = 0.075
R indices (all data)	R1 = 0.1665, wR2 = 0.1008
Largest diff. peak and hole	0.522 and -0.291 e.A^-3

Table 22. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **9**.

	x	y	z	U(eq)
C(1)	681(3)	9329(3)	5927(1)	24(1)
C(2)	138(3)	10063(3)	5753(1)	26(1)
C(3)	387(3)	10213(3)	5447(1)	39(1)
C(4)	1137(4)	9670(3)	5303(1)	43(1)
C(5)	1653(3)	8935(3)	5471(1)	40(1)
C(6)	1445(3)	8742(3)	5779(1)	28(1)
C(7)	-672(3)	10681(3)	5910(1)	29(1)
C(8)	-1537(3)	10981(3)	5690(1)	45(1)
C(9)	-222(3)	11622(3)	6056(1)	45(1)
C(10)	2043(3)	7960(3)	5958(1)	34(1)
C(11)	2349(3)	7044(3)	5759(1)	46(1)
C(12)	2986(3)	8446(3)	6101(1)	49(1)
C(13)	2142(3)	10686(3)	6596(1)	42(1)
C(14)	1318(3)	10575(3)	7101(1)	42(1)
C(15)	-686(3)	7861(3)	6699(1)	24(1)
C(16)	-1866(3)	6628(3)	6618(1)	41(1)
C(17)	-1709(3)	6677(3)	6924(1)	40(1)
C(18)	-1190(3)	7457(3)	6150(1)	28(1)
C(19)	-1825(3)	8151(3)	6004(1)	30(1)
C(20)	-1787(3)	8214(3)	5684(1)	38(1)
C(21)	-1151(4)	7610(3)	5508(1)	37(1)
C(22)	-543(3)	6912(3)	5664(1)	37(1)
C(23)	-562(3)	6818(3)	5985(1)	31(1)
C(24)	90(3)	6043(3)	6149(1)	49(1)
C(25)	-2570(3)	8792(3)	6188(1)	44(1)
C(26)	-1119(4)	7705(3)	5160(1)	63(2)
C(27)	-662(3)	7705(3)	7279(1)	23(1)
C(28)	-1232(3)	8396(3)	7450(1)	24(1)
C(31)	445(3)	7469(3)	7711(1)	42(1)
C(32)	154(3)	7202(3)	7411(1)	32(1)
C(33)	-2198(3)	8850(3)	7326(1)	37(1)
C(34)	675(3)	6340(3)	7247(1)	53(2)
N(1)	470(2)	9191(2)	6243(1)	21(1)
N(2)	1179(2)	10492(2)	6760(1)	29(1)
N(3)	-1245(2)	7343(2)	6483(1)	29(1)
N(4)	-994(2)	7431(2)	6973(1)	26(1)
Cl(1)	1672(1)	8241(1)	6828(1)	30(1)
Cl(2)	-1028(1)	10185(1)	6767(1)	33(1)
V(1)	331(1)	9142(1)	6625(1)	21(1)
C(30)	-71(4)	8193(4)	7882(1)	38(1)
C(29)	-918(3)	8627(3)	7748(1)	33(1)
C(35)	266(4)	8486(4)	8208(1)	69(2)
C(51)	829(4)	5104(4)	5111(1)	77(2)
C(53)	-418(6)	4060(5)	5393(2)	112(2)
C(52)	-171(8)	4634(7)	5154(2)	56(3)
C(50)	1105(8)	5713(8)	4881(3)	68(3)
C(54)	584(8)	4554(8)	5341(3)	73(4)

Table 23. Bond lengths [A] and angles [deg] for **9**.

C(1)-N(1)	1.398(4)
C(1)-C(2)	1.419(5)
C(1)-C(6)	1.424(5)
C(2)-C(3)	1.369(5)
C(2)-C(7)	1.508(5)
C(3)-C(4)	1.372(5)
C(3)-H(3)	0.93
C(4)-C(5)	1.390(5)
C(4)-H(4)	0.93
C(5)-C(6)	1.376(5)
C(5)-H(5)	0.93
C(6)-C(10)	1.511(5)
C(7)-C(9)	1.516(5)
C(7)-C(8)	1.535(5)
C(7)-H(7)	0.98
C(8)-H(8A)	0.96
C(8)-H(8B)	0.96
C(8)-H(8C)	0.96
C(9)-H(9A)	0.96
C(9)-H(9B)	0.96
C(9)-H(9C)	0.96
C(10)-C(12)	1.533(5)
C(10)-C(11)	1.538(5)
C(10)-H(10)	0.98
C(11)-H(11A)	0.96
C(11)-H(11B)	0.96
C(11)-H(11C)	0.96
C(12)-H(12A)	0.96
C(12)-H(12B)	0.96
C(12)-H(12C)	0.96
C(13)-N(2)	1.480(4)
C(13)-H(13A)	0.96
C(13)-H(13B)	0.96
C(13)-H(13C)	0.96
C(14)-N(2)	1.476(4)
C(14)-H(14A)	0.96
C(14)-H(14B)	0.96
C(14)-H(14C)	0.96
C(15)-N(3)	1.368(4)
C(15)-N(4)	1.370(4)
C(15)-V(1)	2.188(4)
C(16)-C(17)	1.333(5)
C(16)-N(3)	1.379(4)
C(16)-H(16)	0.93
C(17)-N(4)	1.390(4)
C(17)-H(17)	0.93
C(18)-C(23)	1.382(5)
C(18)-C(19)	1.393(5)
C(18)-N(3)	1.440(5)
C(19)-C(20)	1.377(5)
C(19)-C(25)	1.522(5)
C(20)-C(21)	1.383(5)
C(20)-H(20)	0.93
C(21)-C(22)	1.395(5)
C(21)-C(26)	1.499(5)
C(22)-C(23)	1.384(5)
C(22)-H(22)	0.93
C(23)-C(24)	1.513(5)
C(24)-H(24A)	0.96
C(24)-H(24B)	0.96

C(24)-H(24C)	0.96
C(25)-H(25A)	0.96
C(25)-H(25B)	0.96
C(25)-H(25C)	0.96
C(26)-H(26A)	0.96
C(26)-H(26B)	0.96
C(26)-H(26C)	0.96
C(27)-C(32)	1.390(5)
C(27)-C(28)	1.395(5)
C(27)-N(4)	1.430(4)
C(28)-C(29)	1.378(5)
C(28)-C(33)	1.509(5)
C(31)-C(30)	1.386(6)
C(31)-C(32)	1.389(5)
C(31)-H(31)	0.93
C(32)-C(34)	1.509(5)
C(33)-H(33A)	0.96
C(33)-H(33B)	0.96
C(33)-H(33C)	0.96
C(34)-H(34A)	0.96
C(34)-H(34B)	0.96
C(34)-H(34C)	0.96
N(1)-V(1)	1.653(3)
N(2)-V(1)	2.189(3)
N(2)-H(2)	0.91
Cl(1)-V(1)	2.3076(12)
Cl(2)-V(1)	2.3474(12)
C(30)-C(29)	1.384(5)
C(30)-C(35)	1.521(6)
C(29)-H(29)	0.93
C(35)-H(35A)	0.96
C(35)-H(35B)	0.96
C(35)-H(35C)	0.96
C(51)-C(54)	1.269(10)
C(51)-C(50)	1.325(10)
C(51)-C(52)#1	1.472(11)
C(51)-C(52)	1.473(10)
C(53)-C(52)	1.320(10)
C(53)-C(54)	1.494(10)
C(53)-C(50)#1	1.517(12)
C(52)-C(54)	1.287(13)
C(52)-C(50)#1	1.327(13)
C(52)-C(51)#1	1.472(11)
C(52)-C(52)#1	1.696(19)
C(50)-C(52)#1	1.327(13)
C(50)-C(53)#1	1.517(12)

N(1)-C(1)-C(2)	119.9(4)
N(1)-C(1)-C(6)	120.1(4)
C(2)-C(1)-C(6)	120.0(4)
C(3)-C(2)-C(1)	118.7(4)
C(3)-C(2)-C(7)	121.4(4)
C(1)-C(2)-C(7)	119.8(4)
C(2)-C(3)-C(4)	122.1(4)
C(2)-C(3)-H(3)	119
C(4)-C(3)-H(3)	119
C(3)-C(4)-C(5)	119.2(4)
C(3)-C(4)-H(4)	120.4
C(5)-C(4)-H(4)	120.4
C(6)-C(5)-C(4)	122.1(4)
C(6)-C(5)-H(5)	119
C(4)-C(5)-H(5)	119

C(5)-C(6)-C(1)	117.8(4)
C(5)-C(6)-C(10)	120.7(4)
C(1)-C(6)-C(10)	121.4(4)
C(2)-C(7)-C(9)	110.6(3)
C(2)-C(7)-C(8)	113.3(3)
C(9)-C(7)-C(8)	109.5(3)
C(2)-C(7)-H(7)	107.8
C(9)-C(7)-H(7)	107.8
C(8)-C(7)-H(7)	107.8
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(6)-C(10)-C(12)	110.0(3)
C(6)-C(10)-C(11)	113.3(3)
C(12)-C(10)-C(11)	109.9(3)
C(6)-C(10)-H(10)	107.8
C(12)-C(10)-H(10)	107.8
C(11)-C(10)-H(10)	107.8
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(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
N(2)-C(13)-H(13A)	109.5
N(2)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
N(2)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
N(2)-C(14)-H(14A)	109.5
N(2)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
N(2)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
N(3)-C(15)-N(4)	102.2(3)
N(3)-C(15)-V(1)	128.6(3)
N(4)-C(15)-V(1)	129.0(3)
C(17)-C(16)-N(3)	106.7(4)
C(17)-C(16)-H(16)	126.7
N(3)-C(16)-H(16)	126.7
C(16)-C(17)-N(4)	106.8(4)
C(16)-C(17)-H(17)	126.6
N(4)-C(17)-H(17)	126.6
C(23)-C(18)-C(19)	122.4(4)
C(23)-C(18)-N(3)	118.4(4)

C(19)-C(18)-N(3)	119.1(4)
C(20)-C(19)-C(18)	117.8(4)
C(20)-C(19)-C(25)	120.5(4)
C(18)-C(19)-C(25)	121.6(4)
C(19)-C(20)-C(21)	122.1(4)
C(19)-C(20)-H(20)	119
C(21)-C(20)-H(20)	119
C(20)-C(21)-C(22)	118.2(4)
C(20)-C(21)-C(26)	120.8(4)
C(22)-C(21)-C(26)	121.0(4)
C(23)-C(22)-C(21)	121.7(4)
C(23)-C(22)-H(22)	119.1
C(21)-C(22)-H(22)	119.1
C(18)-C(23)-C(22)	117.8(4)
C(18)-C(23)-C(24)	121.3(4)
C(22)-C(23)-C(24)	120.9(4)
C(23)-C(24)-H(24A)	109.5
C(23)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(23)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(19)-C(25)-H(25A)	109.5
C(19)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(19)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(21)-C(26)-H(26A)	109.5
C(21)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(21)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(32)-C(27)-C(28)	121.2(4)
C(32)-C(27)-N(4)	119.6(4)
C(28)-C(27)-N(4)	118.9(4)
C(29)-C(28)-C(27)	118.2(4)
C(29)-C(28)-C(33)	119.5(4)
C(27)-C(28)-C(33)	122.3(4)
C(30)-C(31)-C(32)	121.8(4)
C(30)-C(31)-H(31)	119.1
C(32)-C(31)-H(31)	119.1
C(31)-C(32)-C(27)	118.3(4)
C(31)-C(32)-C(34)	119.9(4)
C(27)-C(32)-C(34)	121.7(4)
C(28)-C(33)-H(33A)	109.5
C(28)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(28)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(32)-C(34)-H(34A)	109.5
C(32)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(32)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(1)-N(1)-V(1)	172.6(3)
C(14)-N(2)-C(13)	110.7(3)
C(14)-N(2)-V(1)	112.8(2)
C(13)-N(2)-V(1)	117.1(2)

C(14)-N(2)-H(2)	105
C(13)-N(2)-H(2)	105
V(1)-N(2)-H(2)	105
C(15)-N(3)-C(16)	112.5(3)
C(15)-N(3)-C(18)	126.2(3)
C(16)-N(3)-C(18)	121.2(3)
C(15)-N(4)-C(17)	111.8(3)
C(15)-N(4)-C(27)	126.2(3)
C(17)-N(4)-C(27)	122.0(3)
N(1)-V(1)-C(15)	104.02(15)
N(1)-V(1)-N(2)	100.01(14)
C(15)-V(1)-N(2)	155.53(13)
N(1)-V(1)-Cl(1)	108.04(11)
C(15)-V(1)-Cl(1)	91.03(10)
N(2)-V(1)-Cl(1)	85.87(9)
N(1)-V(1)-Cl(2)	108.54(11)
C(15)-V(1)-Cl(2)	87.02(10)
N(2)-V(1)-Cl(2)	80.99(9)
Cl(1)-V(1)-Cl(2)	142.71(5)
C(29)-C(30)-C(31)	117.9(4)
C(29)-C(30)-C(35)	120.9(5)
C(31)-C(30)-C(35)	121.2(5)
C(28)-C(29)-C(30)	122.4(4)
C(28)-C(29)-H(29)	118.8
C(30)-C(29)-H(29)	118.8
C(30)-C(35)-H(35A)	109.5
C(30)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(30)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(54)-C(51)-C(50)	176.9(9)
C(54)-C(51)-C(52)#1	125.7(9)
C(50)-C(51)-C(52)#1	56.4(6)
C(54)-C(51)-C(52)	55.4(6)
C(50)-C(51)-C(52)	126.6(8)
C(52)#1-C(51)-C(52)	70.4(8)
C(52)-C(53)-C(54)	54.0(6)
C(52)-C(53)-C(50)#1	55.2(6)
C(54)-C(53)-C(50)#1	109.2(7)
C(54)-C(52)-C(53)	70.0(7)
C(54)-C(52)-C(50)#1	139.8(10)
C(53)-C(52)-C(50)#1	70.0(7)
C(54)-C(52)-C(51)#1	163.9(10)
C(53)-C(52)-C(51)#1	126.1(9)
C(50)#1-C(52)-C(51)#1	56.2(6)
C(54)-C(52)-C(51)	54.3(6)
C(53)-C(52)-C(51)	124.2(9)
C(50)#1-C(52)-C(51)	165.6(10)
C(51)#1-C(52)-C(51)	109.6(8)
C(54)-C(52)-C(52)#1	109.1(11)
C(53)-C(52)-C(52)#1	178.9(12)
C(50)#1-C(52)-C(52)#1	111.0(10)
C(51)#1-C(52)-C(52)#1	54.8(6)
C(51)-C(52)-C(52)#1	54.8(6)
C(51)-C(50)-C(52)#1	67.4(7)
C(51)-C(50)-C(53)#1	122.2(9)
C(52)#1-C(50)-C(53)#1	54.8(6)
C(51)-C(54)-C(52)	70.3(7)
C(51)-C(54)-C(53)	126.4(9)
C(52)-C(54)-C(53)	56.1(6)

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

Table 24. Anisotropic displacement parameters (A^2 x 10^3) for **9**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	21(3)	24(2)	26(3)	1(2)	0(2)	-5(2)
C(2)	27(3)	27(2)	25(3)	3(2)	-2(2)	-2(2)
C(3)	39(3)	46(3)	31(3)	10(2)	-7(2)	5(3)
C(4)	49(3)	60(3)	21(3)	12(2)	6(2)	3(3)
C(5)	36(3)	52(3)	31(3)	-2(3)	10(2)	8(3)
C(6)	23(3)	36(3)	24(3)	2(2)	1(2)	-1(2)
C(7)	31(3)	24(2)	31(3)	2(2)	-7(2)	3(2)
C(8)	40(3)	39(3)	57(3)	-1(3)	-7(2)	12(3)
C(9)	53(3)	38(3)	46(3)	0(2)	-9(3)	6(3)
C(10)	31(3)	42(3)	28(3)	2(2)	5(2)	9(2)
C(11)	49(3)	42(3)	48(3)	-4(3)	1(3)	14(3)
C(12)	34(3)	65(4)	49(3)	-1(3)	0(2)	14(3)
C(13)	40(3)	31(3)	55(3)	1(3)	4(3)	-13(2)
C(14)	44(3)	45(3)	38(3)	-15(2)	-20(2)	12(2)
C(15)	24(3)	24(2)	23(3)	-5(2)	6(2)	3(2)
C(16)	44(3)	41(3)	37(3)	-7(3)	12(2)	-30(2)
C(17)	47(3)	32(3)	41(3)	-8(3)	14(3)	-23(3)
C(18)	33(3)	24(2)	28(3)	-6(2)	-1(2)	-14(2)
C(19)	30(3)	29(3)	31(3)	-12(2)	3(2)	-16(2)
C(20)	35(3)	34(3)	43(3)	-6(3)	-8(2)	-9(3)
C(21)	53(4)	29(3)	29(3)	-6(2)	1(2)	-15(3)
C(22)	44(3)	32(3)	34(3)	-12(2)	8(2)	-3(2)
C(23)	37(3)	26(2)	29(3)	-4(2)	0(2)	-9(2)
C(24)	61(4)	38(3)	48(3)	-4(3)	12(3)	7(3)
C(25)	33(3)	51(3)	47(3)	-10(2)	7(2)	-3(3)
C(26)	97(5)	55(4)	37(3)	-2(3)	9(3)	-1(3)
C(27)	27(3)	22(2)	21(3)	5(2)	7(2)	-8(2)
C(28)	26(3)	26(2)	21(3)	4(2)	3(2)	-6(2)
C(31)	29(3)	48(3)	48(3)	27(3)	-5(2)	-5(3)
C(32)	30(3)	30(3)	35(3)	16(2)	6(2)	-3(2)
C(33)	28(3)	46(3)	36(3)	-1(2)	5(2)	5(2)
C(34)	57(4)	31(3)	69(4)	18(3)	21(3)	17(3)
N(1)	18(2)	19(2)	26(2)	3(2)	-1(2)	-2(2)
N(2)	29(2)	20(2)	37(2)	-3(2)	-10(2)	3(2)
N(3)	35(2)	29(2)	22(2)	-4(2)	2(2)	-9(2)
N(4)	32(2)	22(2)	24(2)	-3(2)	4(2)	-4(2)
Cl(1)	28(1)	25(1)	36(1)	5(1)	-3(1)	5(1)
Cl(2)	27(1)	30(1)	41(1)	-6(1)	0(1)	6(1)
V(1)	21(1)	20(1)	22(1)	0(1)	0(1)	0(1)
C(30)	42(3)	44(3)	29(3)	13(3)	-5(2)	-16(3)
C(29)	36(3)	32(3)	29(3)	2(2)	5(2)	-5(2)
C(35)	76(4)	91(4)	41(3)	8(3)	-15(3)	-26(3)

X-ray Data for Complex 10

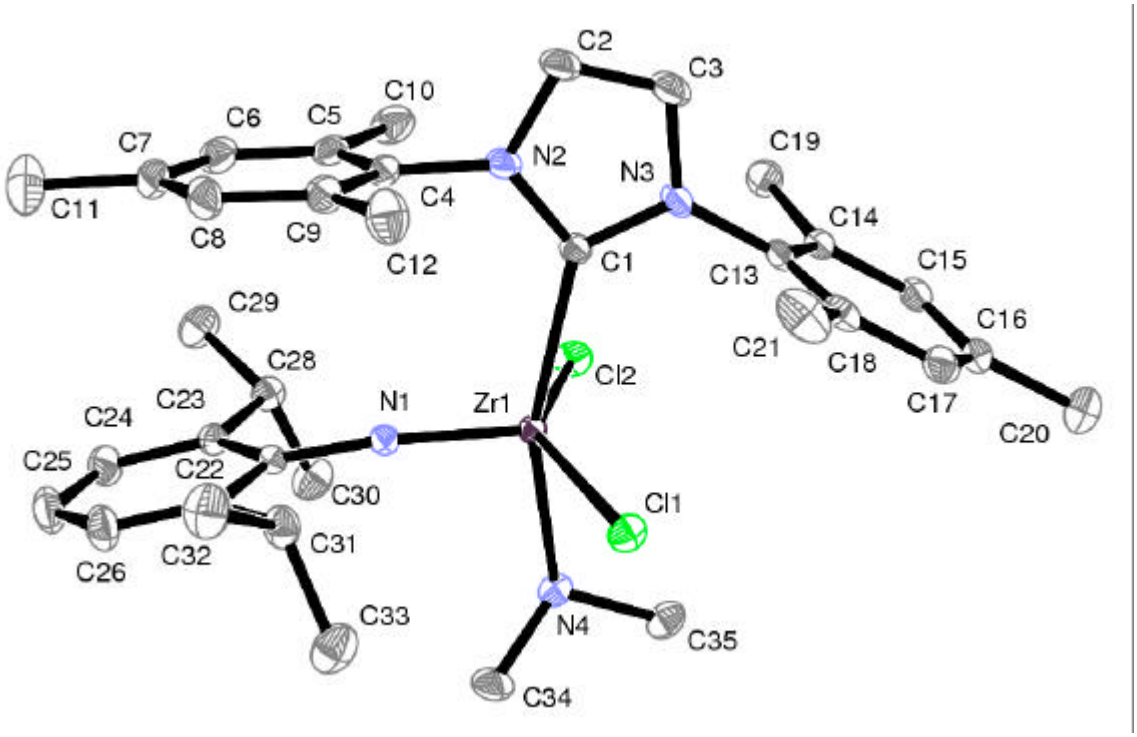

Table 25. Crystal data and structure refinement for **10**.

Empirical formula	C35 H48 Cl2 N4 Zr
Formula weight	686.89
Temperature	180 K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P b c a
Unit cell dimensions	a = 13.4366(8) A alpha = 90 deg. b = 13.3487(13) A beta = 90 deg. c = 43.139(2) A gamma = 90 deg.
Volume	7737.5(10) A^3
Z, Calculated density	8, 1.179 Mg/m^3
Absorption coefficient	0.448 mm^-1
F(000)	2880
Crystal size	0.3 x 0.2 x 0.07 mm
Theta range for data collection	0.94 to 28.9 deg.
Limiting indices	-18<=h<=17, -18<=k<=18, -57<=l<=55
Reflections collected / unique	101403 / 10083 [R(int) = 0.0544]
Completeness to theta = 28.9	98.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.967 and 0.935
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10083 / 0 / 391
Goodness-of-fit on F^2	1.062
Final R indices [I>2sigma(I)]	R1 = 0.0486, wR2 = 0.1385
R indices (all data)	R1 = 0.0681, wR2 = 0.1465
Largest diff. peak and hole	0.43 and -0.457 e.A^-3

Table 26. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **10**.

	x	y	z	U(eq)
C(1)	5756(2)	2294(2)	1708(1)	25(1)
C(2)	6929(3)	3496(3)	1624(1)	45(1)
C(3)	6784(3)	3430(3)	1930(1)	44(1)
C(4)	6235(2)	2666(2)	1161(1)	31(1)
C(5)	6845(2)	1944(2)	1023(1)	35(1)
C(6)	6789(2)	1838(3)	704(1)	39(1)
C(7)	6156(3)	2434(3)	527(1)	40(1)
C(8)	5580(3)	3146(3)	669(1)	40(1)
C(9)	5604(2)	3281(2)	991(1)	35(1)
C(10)	7542(3)	1304(3)	1209(1)	47(1)
C(11)	6107(4)	2286(3)	175(1)	65(1)
C(12)	4970(3)	4067(3)	1145(1)	51(1)
C(13)	5739(2)	2402(2)	2283(1)	26(1)
C(14)	6286(2)	1676(2)	2443(1)	26(1)
C(15)	5954(2)	1407(2)	2736(1)	31(1)
C(16)	5118(2)	1838(3)	2869(1)	39(1)
C(17)	4621(2)	2575(3)	2707(1)	39(1)
C(18)	4919(2)	2888(2)	2414(1)	34(1)
C(19)	7226(2)	1232(3)	2315(1)	38(1)
C(20)	4780(3)	1518(4)	3190(1)	63(1)
C(21)	4409(3)	3743(3)	2255(1)	54(1)
C(22)	4270(2)	719(2)	898(1)	26(1)
C(23)	4804(2)	-22(2)	733(1)	30(1)
C(24)	4559(2)	-193(3)	423(1)	40(1)
C(25)	3829(3)	351(3)	277(1)	48(1)
C(26)	3339(3)	1099(3)	437(1)	42(1)
C(27)	3544(2)	1298(2)	746(1)	32(1)
C(28)	5611(2)	-625(2)	891(1)	32(1)
C(29)	6463(3)	-940(3)	675(1)	46(1)
C(30)	5166(3)	-1557(3)	1044(1)	47(1)
C(31)	2973(2)	2104(3)	920(1)	36(1)
C(32)	2679(3)	2997(3)	716(1)	51(1)
C(33)	2054(3)	1661(3)	1075(1)	50(1)
C(34)	2726(2)	-664(3)	1573(1)	41(1)
C(35)	3471(2)	-705(2)	2086(1)	38(1)
N(1)	4458(2)	856(2)	1214(1)	24(1)
N(2)	6293(2)	2807(2)	1490(1)	34(1)
N(3)	6073(2)	2706(2)	1978(1)	30(1)
N(4)	3659(2)	-548(2)	1753(1)	29(1)
Cl(1)	3194(1)	1826(1)	1863(1)	32(1)
Cl(2)	5958(1)	-242(1)	1798(1)	34(1)
Zr(1)	4605(1)	915(1)	1635(1)	20(1)

Table 27. Bond lengths [A] and angles [deg] for **10**.

C(1)-N(3)	1.359(3)
C(1)-N(2)	1.369(4)
C(1)-Zr(1)	2.425(3)
C(2)-C(3)	1.335(5)
C(2)-N(2)	1.383(4)
C(2)-H(2)	0.95
C(3)-N(3)	1.375(4)
C(3)-H(3)	0.95
C(4)-C(9)	1.389(4)
C(4)-C(5)	1.398(5)
C(4)-N(2)	1.432(4)
C(5)-C(6)	1.385(4)
C(5)-C(10)	1.503(4)
C(6)-C(7)	1.393(5)
C(6)-H(6)	0.95
C(7)-C(8)	1.371(5)
C(7)-C(11)	1.530(5)
C(8)-C(9)	1.401(4)
C(8)-H(8)	0.95
C(9)-C(12)	1.504(5)
C(10)-H(10A)	0.98
C(10)-H(10B)	0.98
C(10)-H(10C)	0.98
C(11)-H(11A)	0.98
C(11)-H(11B)	0.98
C(11)-H(11C)	0.98
C(12)-H(12A)	0.98
C(12)-H(12B)	0.98
C(12)-H(12C)	0.98
C(13)-C(14)	1.399(4)
C(13)-C(18)	1.399(4)
C(13)-N(3)	1.446(4)
C(14)-C(15)	1.388(4)
C(14)-C(19)	1.499(4)
C(15)-C(16)	1.385(5)
C(15)-H(15)	0.95
C(16)-C(17)	1.378(5)
C(16)-C(20)	1.521(5)
C(17)-C(18)	1.388(5)
C(17)-H(17)	0.95
C(18)-C(21)	1.499(5)
C(19)-H(19A)	0.98
C(19)-H(19B)	0.98
C(19)-H(19C)	0.98
C(20)-H(20A)	0.98
C(20)-H(20B)	0.98
C(20)-H(20C)	0.98
C(21)-H(21A)	0.98
C(21)-H(21B)	0.98
C(21)-H(21C)	0.98
C(22)-N(1)	1.396(3)
C(22)-C(27)	1.408(4)
C(22)-C(23)	1.415(4)
C(23)-C(24)	1.395(4)
C(23)-C(28)	1.514(4)
C(24)-C(25)	1.372(5)
C(24)-H(24)	0.95
C(25)-C(26)	1.380(5)
C(25)-H(25)	0.95
C(26)-C(27)	1.387(4)
C(26)-H(26)	0.95
C(27)-C(31)	1.520(4)
C(28)-C(30)	1.531(5)
C(28)-C(29)	1.534(4)
C(28)-H(28)	1

C(29)-H(29A)	0.98
C(29)-H(29B)	0.98
C(29)-H(29C)	0.98
C(30)-H(30A)	0.98
C(30)-H(30B)	0.98
C(30)-H(30C)	0.98
C(31)-C(33)	1.525(5)
C(31)-C(32)	1.532(5)
C(31)-H(31)	1
C(32)-H(32A)	0.98
C(32)-H(32B)	0.98
C(32)-H(32C)	0.98
C(33)-H(33A)	0.98
C(33)-H(33B)	0.98
C(33)-H(33C)	0.98
C(34)-N(4)	1.482(4)
C(34)-H(34A)	0.98
C(34)-H(34B)	0.98
C(34)-H(34C)	0.98
C(35)-N(4)	1.470(4)
C(35)-H(35A)	0.98
C(35)-H(35B)	0.98
C(35)-H(35C)	0.98
N(1)-Zr(1)	1.830(2)
N(4)-Zr(1)	2.385(2)
N(4)-H(4)	0.93
Cl(1)-Zr(1)	2.4576(7)
Cl(2)-Zr(1)	2.4866(7)

N(3)-C(1)-N(2)	102.8(2)
N(3)-C(1)-Zr(1)	128.21(19)
N(2)-C(1)-Zr(1)	128.83(19)
C(3)-C(2)-N(2)	106.3(3)
C(3)-C(2)-H(2)	126.8
N(2)-C(2)-H(2)	126.8
C(2)-C(3)-N(3)	107.3(3)
C(2)-C(3)-H(3)	126.4
N(3)-C(3)-H(3)	126.4
C(9)-C(4)-C(5)	122.7(3)
C(9)-C(4)-N(2)	118.5(3)
C(5)-C(4)-N(2)	118.8(3)
C(6)-C(5)-C(4)	117.6(3)
C(6)-C(5)-C(10)	120.5(3)
C(4)-C(5)-C(10)	121.9(3)
C(5)-C(6)-C(7)	121.3(3)
C(5)-C(6)-H(6)	119.4
C(7)-C(6)-H(6)	119.4
C(8)-C(7)-C(6)	119.6(3)
C(8)-C(7)-C(11)	120.7(3)
C(6)-C(7)-C(11)	119.7(3)
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(4)-C(9)-C(8)	117.4(3)
C(4)-C(9)-C(12)	121.7(3)
C(8)-C(9)-C(12)	120.8(3)
C(5)-C(10)-H(10A)	109.5
C(5)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(5)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(7)-C(11)-H(11A)	109.5
C(7)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(7)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5

C(9)-C(12)-H(12A)	109.5
C(9)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(9)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-C(18)	122.3(3)
C(14)-C(13)-N(3)	118.6(2)
C(18)-C(13)-N(3)	118.9(3)
C(15)-C(14)-C(13)	117.4(3)
C(15)-C(14)-C(19)	120.2(3)
C(13)-C(14)-C(19)	122.4(3)
C(16)-C(15)-C(14)	122.0(3)
C(16)-C(15)-H(15)	119
C(14)-C(15)-H(15)	119
C(17)-C(16)-C(15)	118.7(3)
C(17)-C(16)-C(20)	121.1(3)
C(15)-C(16)-C(20)	120.2(3)
C(16)-C(17)-C(18)	122.3(3)
C(16)-C(17)-H(17)	118.8
C(18)-C(17)-H(17)	118.8
C(17)-C(18)-C(13)	117.2(3)
C(17)-C(18)-C(21)	121.0(3)
C(13)-C(18)-C(21)	121.8(3)
C(14)-C(19)-H(19A)	109.5
C(14)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(14)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(16)-C(20)-H(20A)	109.5
C(16)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(16)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(18)-C(21)-H(21A)	109.5
C(18)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(18)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
N(1)-C(22)-C(27)	120.7(2)
N(1)-C(22)-C(23)	119.4(2)
C(27)-C(22)-C(23)	119.9(2)
C(24)-C(23)-C(22)	118.5(3)
C(24)-C(23)-C(28)	120.9(3)
C(22)-C(23)-C(28)	120.5(2)
C(25)-C(24)-C(23)	121.4(3)
C(25)-C(24)-H(24)	119.3
C(23)-C(24)-H(24)	119.3
C(24)-C(25)-C(26)	119.8(3)
C(24)-C(25)-H(25)	120.1
C(26)-C(25)-H(25)	120.1
C(25)-C(26)-C(27)	121.4(3)
C(25)-C(26)-H(26)	119.3
C(27)-C(26)-H(26)	119.3
C(26)-C(27)-C(22)	118.9(3)
C(26)-C(27)-C(31)	120.6(3)
C(22)-C(27)-C(31)	120.5(2)
C(23)-C(28)-C(30)	110.3(3)
C(23)-C(28)-C(29)	114.0(3)
C(30)-C(28)-C(29)	109.4(3)
C(23)-C(28)-H(28)	107.7
C(30)-C(28)-H(28)	107.7
C(29)-C(28)-H(28)	107.7
C(28)-C(29)-H(29A)	109.5
C(28)-C(29)-H(29B)	109.5

H(29A)-C(29)-H(29B)	109.5
C(28)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(28)-C(30)-H(30A)	109.5
C(28)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(28)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(27)-C(31)-C(33)	110.6(3)
C(27)-C(31)-C(32)	113.5(3)
C(33)-C(31)-C(32)	110.2(3)
C(27)-C(31)-H(31)	107.4
C(33)-C(31)-H(31)	107.4
C(32)-C(31)-H(31)	107.4
C(31)-C(32)-H(32A)	109.5
C(31)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(31)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(31)-C(33)-H(33A)	109.5
C(31)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(31)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
N(4)-C(34)-H(34A)	109.5
N(4)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
N(4)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
N(4)-C(35)-H(35A)	109.5
N(4)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
N(4)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(22)-N(1)-Zr(1)	173.36(19)
C(1)-N(2)-C(2)	111.7(3)
C(1)-N(2)-C(4)	125.9(2)
C(2)-N(2)-C(4)	122.4(2)
C(1)-N(3)-C(3)	111.9(2)
C(1)-N(3)-C(13)	124.7(2)
C(3)-N(3)-C(13)	123.4(2)
C(35)-N(4)-C(34)	110.6(2)
C(35)-N(4)-Zr(1)	114.63(19)
C(34)-N(4)-Zr(1)	115.09(18)
C(35)-N(4)-H(4)	105.1
C(34)-N(4)-H(4)	105.1
Zr(1)-N(4)-H(4)	105.1
N(1)-Zr(1)-N(4)	96.88(9)
N(1)-Zr(1)-C(1)	103.30(9)
N(4)-Zr(1)-C(1)	159.04(9)
N(1)-Zr(1)-Cl(1)	109.56(7)
N(4)-Zr(1)-Cl(1)	84.74(6)
C(1)-Zr(1)-Cl(1)	93.68(7)
N(1)-Zr(1)-Cl(2)	109.45(7)
N(4)-Zr(1)-Cl(2)	79.69(6)
C(1)-Zr(1)-Cl(2)	88.22(7)
Cl(1)-Zr(1)-Cl(2)	139.34(3)

Table 28. Anisotropic displacement parameters (A^2 x 10^3) for **10**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	28(1)	23(1)	25(1)	4(1)	-4(1)	-4(1)
C(2)	49(2)	46(2)	41(2)	10(2)	-12(2)	-28(2)
C(3)	52(2)	41(2)	38(2)	5(1)	-13(1)	-24(2)
C(4)	35(1)	32(2)	27(1)	8(1)	-2(1)	-12(1)
C(5)	30(1)	37(2)	38(2)	12(1)	0(1)	-10(1)
C(6)	43(2)	36(2)	39(2)	4(1)	6(1)	-7(1)
C(7)	50(2)	40(2)	30(2)	7(1)	-1(1)	-11(2)
C(8)	49(2)	39(2)	32(2)	9(1)	-10(1)	-4(2)
C(9)	39(2)	33(2)	34(2)	7(1)	-3(1)	-5(1)
C(10)	34(2)	56(2)	52(2)	15(2)	1(2)	1(2)
C(11)	96(3)	64(3)	35(2)	0(2)	-2(2)	4(2)
C(12)	65(2)	48(2)	41(2)	3(2)	-7(2)	8(2)
C(13)	29(1)	27(1)	24(1)	-4(1)	-5(1)	-7(1)
C(14)	27(1)	26(1)	26(1)	-1(1)	-5(1)	-3(1)
C(15)	36(2)	31(2)	27(1)	0(1)	-7(1)	-5(1)
C(16)	39(2)	48(2)	30(2)	-11(1)	4(1)	-14(2)
C(17)	33(2)	44(2)	41(2)	-18(2)	4(1)	-2(1)
C(18)	31(1)	28(1)	41(2)	-12(1)	-11(1)	1(1)
C(19)	30(1)	47(2)	35(2)	3(1)	-4(1)	4(1)
C(20)	67(3)	87(3)	35(2)	-5(2)	13(2)	-18(2)
C(21)	59(2)	34(2)	70(3)	-13(2)	-20(2)	13(2)
C(22)	25(1)	30(1)	23(1)	-2(1)	0(1)	-6(1)
C(23)	29(1)	33(2)	27(1)	-5(1)	3(1)	-4(1)
C(24)	42(2)	49(2)	31(2)	-14(1)	5(1)	2(2)
C(25)	48(2)	69(2)	26(2)	-7(2)	-5(1)	4(2)
C(26)	43(2)	56(2)	27(2)	1(1)	-7(1)	9(2)
C(27)	30(1)	39(2)	27(1)	0(1)	-3(1)	1(1)
C(28)	34(1)	29(1)	34(2)	-4(1)	4(1)	2(1)
C(29)	45(2)	45(2)	47(2)	0(2)	12(2)	10(2)
C(30)	59(2)	35(2)	48(2)	4(2)	10(2)	0(2)
C(31)	35(2)	42(2)	30(2)	1(1)	-4(1)	10(1)
C(32)	58(2)	48(2)	45(2)	6(2)	-1(2)	13(2)
C(33)	44(2)	60(2)	47(2)	10(2)	9(2)	17(2)
C(34)	39(2)	36(2)	49(2)	-1(2)	-4(1)	-16(1)
C(35)	40(2)	36(2)	38(2)	13(1)	6(1)	1(1)
N(1)	25(1)	24(1)	23(1)	0(1)	-1(1)	-1(1)
N(2)	35(1)	37(1)	30(1)	8(1)	-7(1)	-15(1)
N(3)	35(1)	28(1)	26(1)	3(1)	-10(1)	-8(1)
N(4)	30(1)	24(1)	31(1)	2(1)	4(1)	1(1)
Cl(1)	31(1)	27(1)	37(1)	-3(1)	6(1)	5(1)
Cl(2)	28(1)	34(1)	41(1)	7(1)	-2(1)	7(1)
Zr(1)	20(1)	19(1)	20(1)	1(1)	0(1)	0(1)

X-ray Data for Complex 11

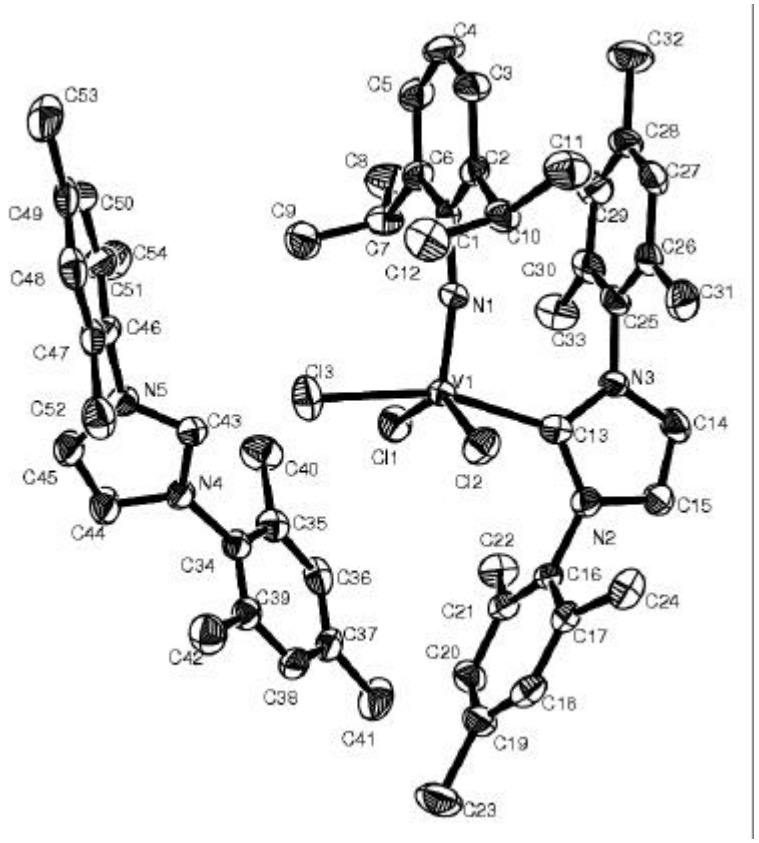

Table 29. Crystal data and structure refinement for **11**.

Empirical formula	C33 H41 Cl3 N3 V, C21 H25 N2
Formula weight	942.41
Temperature	180 K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 1 21/c 1
Unit cell dimensions	a = 16.7897(15) A alpha = 90 deg. b = 11.8681(7) A beta = 93.173(11) deg. c = 27.640(3) A gamma = 90 deg.
Volume	5499.1(8) A^3
Z, Calculated density	4, 1.138 Mg/m^3
Absorption coefficient	0.363 mm^-1
F(000)	1996
Crystal size	0.22 x 0.15 x 0.05 mm
Theta range for data collection	1.96 to 23.26 deg.
Limiting indices	-18<=h<=18, -12<=k<=12, -30<=l<=30
Reflections collected / unique	29659 / 7685 [R(int) = 0.1075]
Completeness to theta = 23.26	97.2 %
Absorption correction	Empirical (SHELXA)
Max. and min. transmission	0.979 and 0.928
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7685 / 0 / 584
Goodness-of-fit on F^2	0.832
Final R indices [I>2sigma(I)]	R1 = 0.0537, wR2 = 0.1146
R indices (all data)	R1 = 0.1096, wR2 = 0.1324
Largest diff. peak and hole	0.303 and -0.36 e.A^-3

Table 29. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **11**.

	x	y	z	U(eq)
V(1)	2591(1)	688(1)	7972(1)	23(1)
Cl(1)	2354(1)	-1240(1)	7816(1)	38(1)
Cl(2)	3050(1)	2372(1)	7647(1)	36(1)
Cl(3)	3954(1)	176(1)	8165(1)	42(1)
N(1)	2322(2)	956(3)	8532(1)	27(1)
N(2)	1298(2)	1071(3)	7063(1)	28(1)
N(3)	729(2)	1266(4)	7727(1)	27(1)
N(4)	4238(2)	-3369(3)	7722(1)	31(1)
N(5)	4828(2)	-2965(3)	8410(1)	29(1)
C(1)	2243(2)	1096(4)	9029(2)	26(1)
C(2)	2348(3)	2179(4)	9236(2)	29(1)
C(3)	2225(3)	2295(5)	9731(2)	37(1)
C(4)	2023(3)	1387(5)	10008(2)	42(1)
C(5)	1954(3)	322(5)	9802(2)	39(1)
C(6)	2061(3)	154(4)	9313(2)	30(1)
C(7)	2048(3)	-1016(5)	9093(2)	36(1)
C(8)	1490(4)	-1850(5)	9328(2)	56(2)
C(9)	2889(3)	-1489(5)	9101(2)	47(2)
C(10)	2617(3)	3149(4)	8934(2)	32(1)
C(11)	2342(3)	4307(5)	9096(2)	45(1)
C(12)	3527(3)	3131(5)	8913(2)	46(1)
C(13)	1459(3)	1033(4)	7556(2)	26(1)
C(14)	154(3)	1433(5)	7364(2)	38(1)
C(15)	504(3)	1313(5)	6947(2)	37(1)
C(16)	1853(2)	867(4)	6686(2)	23(1)
C(17)	2201(3)	1787(4)	6470(2)	27(1)
C(18)	2727(3)	1566(5)	6108(2)	32(1)
C(19)	2876(3)	477(5)	5956(2)	36(1)
C(20)	2484(3)	-400(5)	6169(2)	35(1)
C(21)	1955(3)	-228(4)	6533(2)	29(1)
C(22)	1464(3)	-1208(5)	6703(2)	39(1)
C(23)	3449(3)	236(6)	5564(2)	55(2)
C(24)	2001(3)	2985(5)	6587(2)	39(1)
C(25)	543(3)	1366(5)	8233(2)	30(1)
C(26)	573(3)	2416(5)	8441(2)	33(1)
C(27)	342(3)	2500(5)	8920(2)	38(1)
C(28)	94(3)	1580(5)	9173(2)	40(2)
C(29)	61(3)	548(5)	8944(2)	40(1)
C(30)	284(3)	400(5)	8469(2)	35(1)
C(31)	821(3)	3433(5)	8159(2)	43(1)
C(32)	-142(3)	1689(6)	9692(2)	59(2)
C(33)	235(3)	-730(5)	8221(2)	47(2)
C(34)	3683(3)	-3402(4)	7296(2)	28(1)
C(35)	2961(3)	-3968(4)	7325(2)	34(1)
C(36)	2490(3)	-4059(4)	6901(2)	36(1)
C(37)	2719(3)	-3628(5)	6462(2)	37(1)
C(38)	3432(3)	-3054(5)	6456(2)	36(1)
C(39)	3941(3)	-2908(4)	6872(2)	32(1)
C(40)	2712(3)	-4452(5)	7794(2)	52(2)
C(41)	2203(4)	-3800(6)	6001(2)	61(2)
C(42)	4697(3)	-2260(5)	6862(2)	46(2)
C(43)	4204(3)	-2700(4)	8107(2)	26(1)
C(44)	4908(3)	-4041(5)	7776(2)	45(2)
C(45)	5271(3)	-3793(5)	8202(2)	44(1)
C(46)	5052(3)	-2409(4)	8869(2)	26(1)
C(47)	5566(3)	-1502(4)	8854(2)	31(1)
C(48)	5804(3)	-999(5)	9290(2)	37(1)
C(49)	5555(3)	-1408(5)	9723(2)	41(1)
C(50)	5051(3)	-2331(5)	9722(2)	41(1)
C(51)	4792(3)	-2865(5)	9294(2)	34(1)
C(52)	5849(3)	-1066(5)	8379(2)	42(1)

C(53)	5812(3)	-840(6)	10204(2)	62(2)
C(54)	4271(3)	-3889(5)	9298(2)	50(2)

Table 30. Bond lengths [A] and angles [deg] for **11**.

V(1)-N(1)	1.668(4)
V(1)-C(13)	2.204(5)
V(1)-Cl(2)	2.3386(15)
V(1)-Cl(1)	2.3576(16)
V(1)-Cl(3)	2.3993(14)
N(1)-C(1)	1.397(6)
N(2)-C(13)	1.376(6)
N(2)-C(15)	1.383(6)
N(2)-C(16)	1.455(5)
N(3)-C(13)	1.365(5)
N(3)-C(14)	1.367(6)
N(3)-C(25)	1.456(6)
N(4)-C(43)	1.332(6)
N(4)-C(44)	1.380(6)
N(4)-C(34)	1.461(6)
N(5)-C(43)	1.342(6)
N(5)-C(45)	1.379(6)
N(5)-C(46)	1.459(6)
C(1)-C(6)	1.408(7)
C(1)-C(2)	1.414(7)
C(2)-C(3)	1.402(6)
C(2)-C(10)	1.506(7)
C(3)-C(4)	1.375(8)
C(3)-H(3)	0.95
C(4)-C(5)	1.389(8)
C(4)-H(4)	0.95
C(5)-C(6)	1.388(7)
C(5)-H(5)	0.95
C(6)-C(7)	1.515(7)
C(7)-C(9)	1.518(7)
C(7)-C(8)	1.531(7)
C(7)-H(7)	1
C(8)-H(8A)	0.98
C(8)-H(8B)	0.98
C(8)-H(8C)	0.98
C(9)-H(9A)	0.98
C(9)-H(9B)	0.98
C(9)-H(9C)	0.98
C(10)-C(11)	1.525(7)
C(10)-C(12)	1.531(7)
C(10)-H(10)	1
C(11)-H(11A)	0.98
C(11)-H(11B)	0.98
C(11)-H(11C)	0.98
C(12)-H(12A)	0.98
C(12)-H(12B)	0.98
C(12)-H(12C)	0.98
C(14)-C(15)	1.331(7)
C(14)-H(14)	0.95
C(15)-H(15)	0.95
C(16)-C(21)	1.380(7)
C(16)-C(17)	1.389(6)
C(17)-C(18)	1.394(7)
C(17)-C(24)	1.501(7)
C(18)-C(19)	1.387(7)
C(18)-H(18)	0.95
C(19)-C(20)	1.381(7)
C(19)-C(23)	1.514(7)
C(20)-C(21)	1.394(6)
C(20)-H(20)	0.95

C(21)-C(22)	1.516(7)
C(22)-H(22A)	0.98
C(22)-H(22B)	0.98
C(22)-H(22C)	0.98
C(23)-H(23A)	0.98
C(23)-H(23B)	0.98
C(23)-H(23C)	0.98
C(24)-H(24A)	0.98
C(24)-H(24B)	0.98
C(24)-H(24C)	0.98
C(25)-C(26)	1.372(7)
C(25)-C(30)	1.400(7)
C(26)-C(27)	1.403(7)
C(26)-C(31)	1.507(7)
C(27)-C(28)	1.374(8)
C(27)-H(27)	0.95
C(28)-C(29)	1.379(8)
C(28)-C(32)	1.514(7)
C(29)-C(30)	1.395(7)
C(29)-H(29)	0.95
C(30)-C(33)	1.507(8)
C(31)-H(31A)	0.98
C(31)-H(31B)	0.98
C(31)-H(31C)	0.98
C(32)-H(32A)	0.98
C(32)-H(32B)	0.98
C(32)-H(32C)	0.98
C(33)-H(33A)	0.98
C(33)-H(33B)	0.98
C(33)-H(33C)	0.98
C(34)-C(35)	1.393(7)
C(34)-C(39)	1.399(7)
C(35)-C(36)	1.380(7)
C(35)-C(40)	1.498(7)
C(36)-C(37)	1.390(7)
C(36)-H(36)	0.95
C(37)-C(38)	1.379(7)
C(37)-C(41)	1.514(7)
C(38)-C(39)	1.404(7)
C(38)-H(38)	0.95
C(39)-C(42)	1.486(7)
C(40)-H(40A)	0.98
C(40)-H(40B)	0.98
C(40)-H(40C)	0.98
C(41)-H(41A)	0.98
C(41)-H(41B)	0.98
C(41)-H(41C)	0.98
C(42)-H(42A)	0.98
C(42)-H(42B)	0.98
C(42)-H(42C)	0.98
C(43)-H(43)	0.95
C(44)-C(45)	1.326(7)
C(44)-H(44)	0.95
C(45)-H(45)	0.95
C(46)-C(47)	1.382(7)
C(46)-C(51)	1.387(7)
C(47)-C(48)	1.384(7)
C(47)-C(52)	1.512(7)
C(48)-C(49)	1.377(8)
C(48)-H(48)	0.95
C(49)-C(50)	1.383(8)
C(49)-C(53)	1.533(7)
C(50)-C(51)	1.390(7)
C(50)-H(50)	0.95
C(51)-C(54)	1.497(7)
C(52)-H(52A)	0.98
C(52)-H(52B)	0.98
C(52)-H(52C)	0.98

C(53)-H(53A)	0.98
C(53)-H(53B)	0.98
C(53)-H(53C)	0.98
C(54)-H(54A)	0.98
C(54)-H(54B)	0.98
C(54)-H(54C)	0.98

N(1)-V(1)-C(13)	100.30(17)
N(1)-V(1)-Cl(2)	107.80(15)
C(13)-V(1)-Cl(2)	86.24(13)
N(1)-V(1)-Cl(1)	107.61(15)
C(13)-V(1)-Cl(1)	87.33(13)
Cl(2)-V(1)-Cl(1)	144.59(6)
N(1)-V(1)-Cl(3)	98.35(13)
C(13)-V(1)-Cl(3)	161.35(12)
Cl(2)-V(1)-Cl(3)	88.37(5)
Cl(1)-V(1)-Cl(3)	86.77(5)
C(1)-N(1)-V(1)	168.8(3)
C(13)-N(2)-C(15)	111.7(4)
C(13)-N(2)-C(16)	127.2(4)
C(15)-N(2)-C(16)	121.1(4)
C(13)-N(3)-C(14)	112.8(4)
C(13)-N(3)-C(25)	126.4(4)
C(14)-N(3)-C(25)	120.8(4)
C(43)-N(4)-C(44)	109.2(4)
C(43)-N(4)-C(34)	127.3(4)
C(44)-N(4)-C(34)	123.5(4)
C(43)-N(5)-C(45)	109.0(4)
C(43)-N(5)-C(46)	126.3(4)
C(45)-N(5)-C(46)	124.5(4)
N(1)-C(1)-C(6)	119.2(4)
N(1)-C(1)-C(2)	119.3(4)
C(6)-C(1)-C(2)	121.5(4)
C(3)-C(2)-C(1)	117.5(5)
C(3)-C(2)-C(10)	122.1(5)
C(1)-C(2)-C(10)	120.4(4)
C(4)-C(3)-C(2)	121.4(5)
C(4)-C(3)-H(3)	119.3
C(2)-C(3)-H(3)	119.3
C(3)-C(4)-C(5)	120.1(5)
C(3)-C(4)-H(4)	119.9
C(5)-C(4)-H(4)	119.9
C(6)-C(5)-C(4)	121.2(5)
C(6)-C(5)-H(5)	119.4
C(4)-C(5)-H(5)	119.4
C(5)-C(6)-C(1)	118.1(5)
C(5)-C(6)-C(7)	121.4(5)
C(1)-C(6)-C(7)	120.3(4)
C(6)-C(7)-C(9)	109.9(4)
C(6)-C(7)-C(8)	114.8(4)
C(9)-C(7)-C(8)	110.2(5)
C(6)-C(7)-H(7)	107.2
C(9)-C(7)-H(7)	107.2
C(8)-C(7)-H(7)	107.2
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(2)-C(10)-C(11)	114.9(4)
C(2)-C(10)-C(12)	110.0(4)

C(11)-C(10)-C(12)	110.0(4)
C(2)-C(10)-H(10)	107.2
C(11)-C(10)-H(10)	107.2
C(12)-C(10)-H(10)	107.2
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
N(3)-C(13)-N(2)	101.8(4)
N(3)-C(13)-V(1)	128.5(3)
N(2)-C(13)-V(1)	129.7(3)
C(15)-C(14)-N(3)	106.9(4)
C(15)-C(14)-H(14)	126.5
N(3)-C(14)-H(14)	126.5
C(14)-C(15)-N(2)	106.7(4)
C(14)-C(15)-H(15)	126.6
N(2)-C(15)-H(15)	126.6
C(21)-C(16)-C(17)	123.1(4)
C(21)-C(16)-N(2)	118.1(4)
C(17)-C(16)-N(2)	118.6(4)
C(16)-C(17)-C(18)	117.3(5)
C(16)-C(17)-C(24)	123.1(4)
C(18)-C(17)-C(24)	119.4(4)
C(19)-C(18)-C(17)	121.7(5)
C(19)-C(18)-H(18)	119.1
C(17)-C(18)-H(18)	119.1
C(20)-C(19)-C(18)	118.3(4)
C(20)-C(19)-C(23)	119.9(5)
C(18)-C(19)-C(23)	121.8(5)
C(19)-C(20)-C(21)	122.3(5)
C(19)-C(20)-H(20)	118.8
C(21)-C(20)-H(20)	118.8
C(16)-C(21)-C(20)	117.0(5)
C(16)-C(21)-C(22)	123.3(4)
C(20)-C(21)-C(22)	119.3(5)
C(21)-C(22)-H(22A)	109.5
C(21)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(21)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(19)-C(23)-H(23A)	109.5
C(19)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(19)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(17)-C(24)-H(24A)	109.5
C(17)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(17)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(26)-C(25)-C(30)	123.7(4)
C(26)-C(25)-N(3)	118.1(5)
C(30)-C(25)-N(3)	118.0(4)
C(25)-C(26)-C(27)	117.0(5)
C(25)-C(26)-C(31)	121.1(4)
C(27)-C(26)-C(31)	122.0(5)
C(28)-C(27)-C(26)	122.1(5)

C(28)-C(27)-H(27)	118.9
C(26)-C(27)-H(27)	118.9
C(27)-C(28)-C(29)	118.5(5)
C(27)-C(28)-C(32)	121.2(5)
C(29)-C(28)-C(32)	120.3(5)
C(28)-C(29)-C(30)	122.5(5)
C(28)-C(29)-H(29)	118.7
C(30)-C(29)-H(29)	118.7
C(29)-C(30)-C(25)	116.2(5)
C(29)-C(30)-C(33)	122.0(5)
C(25)-C(30)-C(33)	121.8(4)
C(26)-C(31)-H(31A)	109.5
C(26)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(26)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(28)-C(32)-H(32A)	109.5
C(28)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(28)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(30)-C(33)-H(33A)	109.5
C(30)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(30)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(35)-C(34)-C(39)	124.1(4)
C(35)-C(34)-N(4)	119.0(4)
C(39)-C(34)-N(4)	116.8(4)
C(36)-C(35)-C(34)	116.7(5)
C(36)-C(35)-C(40)	122.0(5)
C(34)-C(35)-C(40)	121.3(5)
C(35)-C(36)-C(37)	122.6(5)
C(35)-C(36)-H(36)	118.7
C(37)-C(36)-H(36)	118.7
C(38)-C(37)-C(36)	118.3(4)
C(38)-C(37)-C(41)	120.9(5)
C(36)-C(37)-C(41)	120.8(5)
C(37)-C(38)-C(39)	122.7(5)
C(37)-C(38)-H(38)	118.7
C(39)-C(38)-H(38)	118.7
C(34)-C(39)-C(38)	115.6(4)
C(34)-C(39)-C(42)	122.5(4)
C(38)-C(39)-C(42)	122.0(5)
C(35)-C(40)-H(40A)	109.5
C(35)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(35)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
C(37)-C(41)-H(41A)	109.5
C(37)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
C(37)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
C(39)-C(42)-H(42A)	109.5
C(39)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(39)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
N(4)-C(43)-N(5)	107.0(4)
N(4)-C(43)-H(43)	126.5
N(5)-C(43)-H(43)	126.5

C(45)-C(44)-N(4)	107.4(5)
C(45)-C(44)-H(44)	126.3
N(4)-C(44)-H(44)	126.3
C(44)-C(45)-N(5)	107.3(4)
C(44)-C(45)-H(45)	126.3
N(5)-C(45)-H(45)	126.3
C(47)-C(46)-C(51)	123.7(4)
C(47)-C(46)-N(5)	117.3(4)
C(51)-C(46)-N(5)	118.8(4)
C(46)-C(47)-C(48)	117.5(5)
C(46)-C(47)-C(52)	121.2(4)
C(48)-C(47)-C(52)	121.3(5)
C(49)-C(48)-C(47)	121.1(5)
C(49)-C(48)-H(48)	119.5
C(47)-C(48)-H(48)	119.5
C(48)-C(49)-C(50)	119.6(5)
C(48)-C(49)-C(53)	120.9(6)
C(50)-C(49)-C(53)	119.5(6)
C(49)-C(50)-C(51)	121.6(5)
C(49)-C(50)-H(50)	119.2
C(51)-C(50)-H(50)	119.2
C(46)-C(51)-C(50)	116.4(5)
C(46)-C(51)-C(54)	122.2(4)
C(50)-C(51)-C(54)	121.4(5)
C(47)-C(52)-H(52A)	109.5
C(47)-C(52)-H(52B)	109.5
H(52A)-C(52)-H(52B)	109.5
C(47)-C(52)-H(52C)	109.5
H(52A)-C(52)-H(52C)	109.5
H(52B)-C(52)-H(52C)	109.5
C(49)-C(53)-H(53A)	109.5
C(49)-C(53)-H(53B)	109.5
H(53A)-C(53)-H(53B)	109.5
C(49)-C(53)-H(53C)	109.5
H(53A)-C(53)-H(53C)	109.5
H(53B)-C(53)-H(53C)	109.5
C(51)-C(54)-H(54A)	109.5
C(51)-C(54)-H(54B)	109.5
H(54A)-C(54)-H(54B)	109.5
C(51)-C(54)-H(54C)	109.5
H(54A)-C(54)-H(54C)	109.5
H(54B)-C(54)-H(54C)	109.5

Table 32. Anisotropic displacement parameters (A^2 x 10^3) for **11**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
V(1)	24(1)	25(1)	21(1)	0(1)	4(1)	1(1)
Cl(1)	46(1)	27(1)	41(1)	-7(1)	-3(1)	4(1)
Cl(2)	38(1)	34(1)	35(1)	10(1)	2(1)	-6(1)
Cl(3)	27(1)	39(1)	61(1)	9(1)	5(1)	4(1)
N(1)	26(2)	33(3)	22(2)	0(2)	5(2)	4(2)
N(2)	29(2)	28(3)	26(2)	-1(2)	0(2)	1(2)
N(3)	23(2)	35(3)	22(2)	-2(2)	3(2)	1(2)
N(4)	36(2)	28(3)	26(2)	-6(2)	-5(2)	10(2)
N(5)	34(2)	25(3)	27(2)	-5(2)	-1(2)	2(2)
C(1)	18(2)	37(4)	22(3)	-3(2)	0(2)	8(2)
C(2)	30(3)	30(4)	24(3)	-5(2)	-6(2)	5(2)
C(3)	40(3)	45(4)	27(3)	-13(3)	-1(2)	2(3)
C(4)	50(3)	55(5)	21(3)	-1(3)	4(2)	0(3)
C(5)	40(3)	48(4)	29(3)	9(3)	4(2)	2(3)
C(6)	30(3)	35(4)	25(3)	6(2)	4(2)	1(2)

C(7)	42(3)	38(4)	29(3)	0(2)	8(2)	-7(2)
C(8)	74(4)	46(4)	51(4)	5(3)	24(3)	-15(3)
C(9)	55(4)	39(4)	46(3)	7(3)	10(3)	12(3)
C(10)	38(3)	29(3)	31(3)	-6(2)	3(2)	1(2)
C(11)	60(3)	34(4)	42(3)	-10(3)	4(3)	-5(3)
C(12)	47(3)	40(4)	50(3)	-5(3)	6(3)	-7(3)
C(13)	32(3)	21(3)	26(3)	-1(2)	5(2)	-4(2)
C(14)	22(3)	53(4)	40(3)	-6(3)	4(2)	8(2)
C(15)	30(3)	51(4)	29(3)	-7(3)	-4(2)	6(2)
C(16)	23(2)	26(3)	19(2)	0(2)	1(2)	-1(2)
C(17)	27(3)	29(3)	25(3)	4(2)	-4(2)	0(2)
C(18)	31(3)	39(4)	26(3)	8(2)	-5(2)	-10(2)
C(19)	28(3)	51(4)	30(3)	-4(3)	5(2)	2(3)
C(20)	34(3)	37(4)	34(3)	-8(2)	2(2)	3(2)
C(21)	29(3)	33(4)	24(3)	3(2)	-1(2)	-3(2)
C(22)	52(3)	28(3)	38(3)	-2(2)	4(2)	-8(3)
C(23)	46(3)	78(5)	41(3)	-1(3)	21(3)	-3(3)
C(24)	41(3)	35(4)	40(3)	4(3)	-8(2)	-1(2)
C(25)	21(2)	41(4)	30(3)	-6(3)	5(2)	2(2)
C(26)	22(2)	43(4)	33(3)	-3(3)	-2(2)	7(2)
C(27)	29(3)	45(4)	38(3)	-10(3)	0(2)	14(3)
C(28)	22(3)	70(5)	29(3)	-3(3)	7(2)	6(3)
C(29)	28(3)	53(4)	39(3)	4(3)	8(2)	-5(3)
C(30)	17(2)	48(4)	40(3)	-6(3)	7(2)	-5(2)
C(31)	50(3)	33(4)	47(3)	1(3)	0(3)	11(3)
C(32)	45(3)	97(6)	35(3)	-7(3)	14(3)	1(3)
C(33)	45(3)	47(4)	49(3)	-7(3)	9(3)	-16(3)
C(34)	32(3)	23(3)	30(3)	-7(2)	-2(2)	4(2)
C(35)	43(3)	22(4)	37(3)	-4(2)	4(2)	1(2)
C(36)	28(3)	30(4)	50(4)	-19(3)	-6(2)	1(2)
C(37)	45(3)	33(4)	32(3)	-9(3)	-10(2)	14(3)
C(38)	46(3)	33(4)	30(3)	5(2)	1(2)	12(3)
C(39)	35(3)	27(3)	33(3)	-1(2)	-1(2)	5(2)
C(40)	65(4)	42(4)	52(4)	6(3)	18(3)	-4(3)
C(41)	64(4)	66(5)	49(4)	-21(3)	-25(3)	17(3)
C(42)	38(3)	47(4)	54(4)	7(3)	7(3)	-2(3)
C(43)	33(3)	20(3)	26(3)	-1(2)	2(2)	0(2)
C(44)	48(3)	45(4)	43(3)	-16(3)	-9(3)	19(3)
C(45)	48(3)	44(4)	37(3)	-12(3)	-9(3)	20(3)
C(46)	29(3)	24(3)	25(3)	-2(2)	-5(2)	3(2)
C(47)	23(3)	30(4)	39(3)	-3(2)	-5(2)	9(2)
C(48)	24(3)	31(4)	56(4)	-14(3)	-7(2)	4(2)
C(49)	27(3)	45(4)	48(4)	-19(3)	-15(2)	16(3)
C(50)	42(3)	53(4)	27(3)	-3(3)	2(2)	12(3)
C(51)	35(3)	36(4)	30(3)	1(2)	0(2)	0(2)
C(52)	31(3)	40(4)	54(4)	11(3)	7(2)	3(2)
C(53)	57(4)	62(5)	62(4)	-38(3)	-33(3)	21(3)
C(54)	55(4)	49(4)	46(3)	11(3)	2(3)	-10(3)

X-ray Data for Complex 12

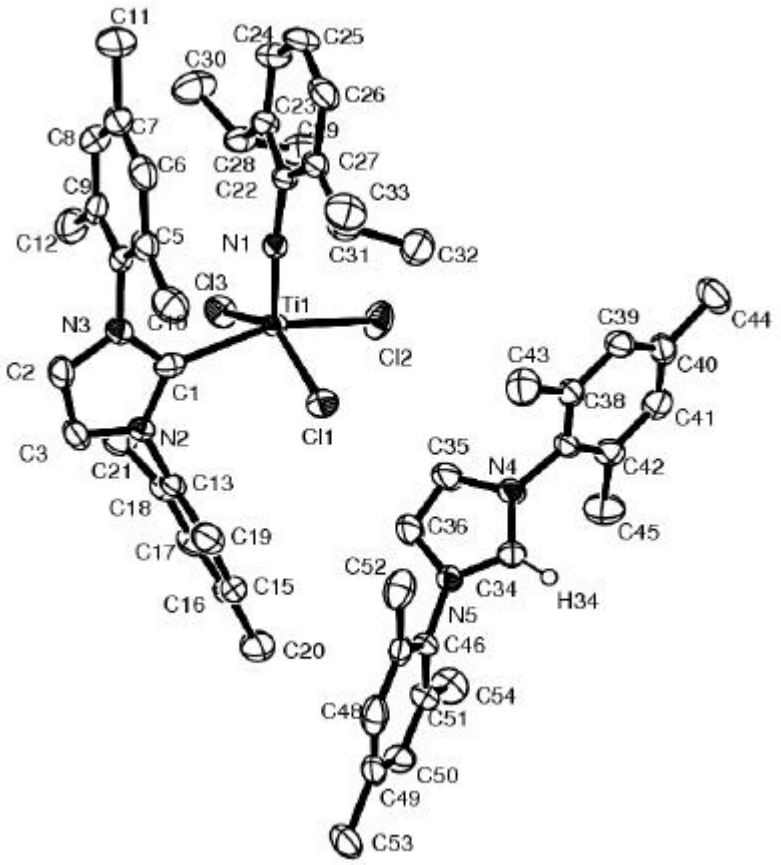

Table 33. Crystal data and structure refinement for **12**.

Empirical formula	C33 H41 Cl3 N3 Ti, C21 H25 N2
Formula weight	939.37
Temperature	180 K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 1 21/c 1
Unit cell dimensions	a = 16.8092(9) A alpha = 90 deg. b = 11.8860(6) A beta = 93.217(3) deg. c = 27.6624(11) A gamma = 90 deg.
Volume	5518.1(5) A^3
Z, Calculated density	4, 1.131 Mg/m^3
Absorption coefficient	0.337 mm^-1
F(000)	1992
Crystal size	0.15 x 0.1 x 0.02 mm
Theta range for data collection	1.21 to 22.79 deg.
Limiting indices	-18<=h<=18, -12<=k<=12, -30<=l<=30
Reflections collected / unique	35370 / 7359 [R(int) = 0.0637]
Completeness to theta = 22.79	98.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.993 and 0.858
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7359 / 0 / 584
Goodness-of-fit on F^2	1.017
Final R indices [I>2sigma(I)]	R1 = 0.0483, wR2 = 0.1187
R indices (all data)	R1 = 0.0784, wR2 = 0.1291
Largest diff. peak and hole	0.314 and -0.309 e.A^-3

Table 34. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **12**.

	x	y	z	U(eq)
C(1)	8558(2)	3974(3)	7455(1)	29(1)
C(2)	9866(2)	3557(3)	7645(1)	41(1)
C(3)	9514(2)	3690(3)	8064(1)	37(1)
C(4)	9464(2)	3637(3)	6774(1)	31(1)
C(5)	9413(2)	2571(3)	6565(1)	34(1)
C(6)	9634(2)	2492(3)	6085(1)	38(1)
C(7)	9889(2)	3404(4)	5835(1)	40(1)
C(8)	9933(2)	4446(4)	6063(1)	44(1)
C(9)	9721(2)	4586(3)	6541(1)	37(1)
C(10)	9160(2)	1558(3)	6842(1)	45(1)
C(11)	10129(3)	3285(4)	5317(1)	64(1)
C(12)	9778(3)	5721(4)	6783(1)	50(1)
C(13)	8162(2)	4149(3)	8313(1)	28(1)
C(14)	7812(2)	3222(3)	8531(1)	29(1)
C(15)	7285(2)	3457(3)	8889(1)	34(1)
C(16)	7122(2)	4541(3)	9035(1)	35(1)
C(17)	7513(2)	5410(3)	8826(1)	38(1)
C(18)	8057(2)	5245(3)	8466(1)	31(1)
C(19)	8023(2)	2045(3)	8413(1)	39(1)
C(20)	6546(3)	4762(4)	9426(1)	53(1)
C(21)	8537(2)	6213(3)	8288(1)	42(1)
C(22)	7747(2)	3892(3)	5962(1)	26(1)
C(23)	7934(2)	4830(3)	5673(1)	32(1)
C(24)	8058(2)	4642(4)	5188(1)	41(1)
C(25)	7984(2)	3598(4)	4987(1)	43(1)
C(26)	7769(2)	2685(4)	5262(1)	40(1)
C(27)	7643(2)	2813(3)	5755(1)	28(1)
C(28)	7957(2)	5986(3)	5894(1)	36(1)
C(29)	7108(3)	6464(4)	5886(1)	51(1)
C(30)	8509(3)	6811(4)	5657(2)	62(1)
C(31)	7361(2)	1844(3)	6057(1)	35(1)
C(32)	6454(2)	1874(4)	6077(1)	46(1)
C(33)	7634(3)	686(3)	5891(1)	49(1)
C(34)	4197(2)	2723(3)	8118(1)	30(1)
C(35)	4861(3)	4103(4)	7799(1)	54(1)
C(36)	5230(3)	3837(4)	8222(1)	50(1)
C(37)	3664(2)	3431(3)	7311(1)	29(1)
C(38)	3920(2)	2942(3)	6890(1)	31(1)
C(39)	3427(2)	3091(3)	6474(1)	36(1)
C(40)	2712(2)	3654(3)	6475(1)	39(1)
C(41)	2471(2)	4078(3)	6909(1)	39(1)
C(42)	2944(2)	3988(3)	7338(1)	35(1)
C(43)	4687(2)	2304(4)	6882(1)	49(1)
C(44)	2199(3)	3812(4)	6014(1)	60(1)
C(45)	2680(3)	4476(4)	7805(1)	54(1)
C(46)	5047(2)	2422(3)	8870(1)	26(1)
C(47)	5566(2)	1526(3)	8847(1)	30(1)
C(48)	5808(2)	1022(3)	9283(2)	42(1)
C(49)	5559(2)	1390(4)	9721(1)	41(1)
C(50)	5048(2)	2299(4)	9725(1)	43(1)
C(51)	4782(2)	2852(3)	9303(1)	32(1)
C(52)	5861(2)	1122(3)	8372(1)	46(1)
C(53)	5831(3)	797(4)	10190(2)	64(1)
C(54)	4243(3)	3854(4)	9311(1)	51(1)
N(1)	7638(2)	4041(2)	6453(1)	25(1)
N(2)	8725(2)	3939(2)	7947(1)	27(1)
N(3)	9279(2)	3740(2)	7280(1)	31(1)
N(4)	4208(2)	3409(2)	7735(1)	33(1)
N(5)	4813(2)	2987(2)	8422(1)	30(1)
Cl(1)	6949(1)	2602(1)	7351(1)	38(1)

Cl(2)	6004(1)	4857(1)	6856(1)	45(1)
Cl(3)	7659(1)	6257(1)	7175(1)	39(1)
Ti(1)	7369(1)	4319(1)	7024(1)	26(1)

Table 35. Bond lengths [A] and angles [deg] for **12**.

C(1)-N(3)	1.359(4)
C(1)-N(2)	1.374(4)
C(1)-Ti(1)	2.306(4)
C(2)-C(3)	1.342(5)
C(2)-N(3)	1.388(4)
C(2)-H(2)	0.9300
C(3)-N(2)	1.381(5)
C(3)-H(3)	0.9300
C(4)-C(9)	1.381(5)
C(4)-C(5)	1.393(5)
C(4)-N(3)	1.455(4)
C(5)-C(6)	1.403(5)
C(5)-C(10)	1.500(5)
C(6)-C(7)	1.368(5)
C(6)-H(6)	0.9300
C(7)-C(8)	1.390(5)
C(7)-C(11)	1.517(5)
C(8)-C(9)	1.399(5)
C(8)-H(8)	0.9300
C(9)-C(12)	1.506(5)
C(10)-H(10A)	0.9600
C(10)-H(10B)	0.9600
C(10)-H(10C)	0.9600
C(11)-H(11A)	0.9600
C(11)-H(11B)	0.9600
C(11)-H(11C)	0.9600
C(12)-H(12A)	0.9600
C(12)-H(12B)	0.9600
C(12)-H(12C)	0.9600
C(13)-C(18)	1.384(5)
C(13)-C(14)	1.402(5)
C(13)-N(2)	1.445(4)
C(14)-C(15)	1.393(5)
C(14)-C(19)	1.484(5)
C(15)-C(16)	1.382(5)
C(15)-H(15)	0.9300
C(16)-C(17)	1.369(5)
C(16)-C(20)	1.516(5)
C(17)-C(18)	1.403(5)
C(17)-H(17)	0.9300
C(18)-C(21)	1.504(5)
C(19)-H(19A)	0.9600
C(19)-H(19B)	0.9600
C(19)-H(19C)	0.9600
C(20)-H(20A)	0.9600
C(20)-H(20B)	0.9600
C(20)-H(20C)	0.9600
C(21)-H(21A)	0.9600
C(21)-H(21B)	0.9600
C(21)-H(21C)	0.9600
C(22)-N(1)	1.392(4)
C(22)-C(27)	1.411(5)
C(22)-C(23)	1.417(5)
C(23)-C(24)	1.387(5)
C(23)-C(28)	1.503(5)
C(24)-C(25)	1.363(5)
C(24)-H(24)	0.9300
C(25)-C(26)	1.385(5)

C(25)-H(25)	0.9300
C(26)-C(27)	1.402(5)
C(26)-H(26)	0.9300
C(27)-C(31)	1.514(5)
C(28)-C(30)	1.524(5)
C(28)-C(29)	1.535(5)
C(28)-H(28)	0.9800
C(29)-H(29A)	0.9600
C(29)-H(29B)	0.9600
C(29)-H(29C)	0.9600
C(30)-H(30A)	0.9600
C(30)-H(30B)	0.9600
C(30)-H(30C)	0.9600
C(31)-C(33)	1.529(5)
C(31)-C(32)	1.530(5)
C(31)-H(31)	0.9800
C(32)-H(32A)	0.9600
C(32)-H(32B)	0.9600
C(32)-H(32C)	0.9600
C(33)-H(33A)	0.9600
C(33)-H(33B)	0.9600
C(33)-H(33C)	0.9600
C(34)-N(5)	1.334(4)
C(34)-N(4)	1.337(4)
C(34)-H(34)	0.9300
C(35)-C(36)	1.330(5)
C(35)-N(4)	1.376(5)
C(35)-H(35)	0.9300
C(36)-N(5)	1.366(5)
C(36)-H(36)	0.9300
C(37)-C(42)	1.384(5)
C(37)-C(38)	1.392(5)
C(37)-N(4)	1.448(4)
C(38)-C(39)	1.391(5)
C(38)-C(43)	1.497(5)
C(39)-C(40)	1.375(5)
C(39)-H(39)	0.9300
C(40)-C(41)	1.383(5)
C(40)-C(44)	1.511(5)
C(41)-C(42)	1.394(5)
C(41)-H(41)	0.9300
C(42)-C(45)	1.506(5)
C(43)-H(43A)	0.9600
C(43)-H(43B)	0.9600
C(43)-H(43C)	0.9600
C(44)-H(44A)	0.9600
C(44)-H(44B)	0.9600
C(44)-H(44C)	0.9600
C(45)-H(45A)	0.9600
C(45)-H(45B)	0.9600
C(45)-H(45C)	0.9600
C(46)-C(47)	1.381(5)
C(46)-C(51)	1.397(5)
C(46)-N(5)	1.445(4)
C(47)-C(48)	1.389(5)
C(47)-C(52)	1.507(5)
C(48)-C(49)	1.374(5)
C(48)-H(48)	0.9300
C(49)-C(50)	1.380(6)
C(49)-C(53)	1.523(5)
C(50)-C(51)	1.393(5)
C(50)-H(50)	0.9300
C(51)-C(54)	1.497(5)
C(52)-H(52A)	0.9600
C(52)-H(52B)	0.9600
C(52)-H(52C)	0.9600
C(53)-H(53A)	0.9600
C(53)-H(53B)	0.9600

C(53)-H(53C)	0.9600
C(54)-H(54A)	0.9600
C(54)-H(54B)	0.9600
C(54)-H(54C)	0.9600
N(1)-Ti(1)	1.701(3)
Cl(1)-Ti(1)	2.3572(11)
Cl(2)-Ti(1)	2.4022(12)
Cl(3)-Ti(1)	2.3862(11)

N(3)-C(1)-N(2)	102.2(3)
N(3)-C(1)-Ti(1)	128.1(2)
N(2)-C(1)-Ti(1)	129.8(3)
C(3)-C(2)-N(3)	106.3(3)
C(3)-C(2)-H(2)	126.9
N(3)-C(2)-H(2)	126.9
C(2)-C(3)-N(2)	106.6(3)
C(2)-C(3)-H(3)	126.7
N(2)-C(3)-H(3)	126.7
C(9)-C(4)-C(5)	124.2(3)
C(9)-C(4)-N(3)	118.0(3)
C(5)-C(4)-N(3)	117.6(3)
C(4)-C(5)-C(6)	116.1(4)
C(4)-C(5)-C(10)	122.1(3)
C(6)-C(5)-C(10)	121.8(4)
C(7)-C(6)-C(5)	122.3(4)
C(7)-C(6)-H(6)	118.9
C(5)-C(6)-H(6)	118.9
C(6)-C(7)-C(8)	119.1(3)
C(6)-C(7)-C(11)	120.8(4)
C(8)-C(7)-C(11)	120.1(4)
C(7)-C(8)-C(9)	121.6(4)
C(7)-C(8)-H(8)	119.2
C(9)-C(8)-H(8)	119.2
C(4)-C(9)-C(8)	116.6(4)
C(4)-C(9)-C(12)	122.5(3)
C(8)-C(9)-C(12)	120.8(4)
C(5)-C(10)-H(10A)	109.5
C(5)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(5)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(7)-C(11)-H(11A)	109.5
C(7)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(7)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(9)-C(12)-H(12A)	109.5
C(9)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(9)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(18)-C(13)-C(14)	122.9(3)
C(18)-C(13)-N(2)	118.5(3)
C(14)-C(13)-N(2)	118.2(3)
C(15)-C(14)-C(13)	116.6(3)
C(15)-C(14)-C(19)	121.0(3)
C(13)-C(14)-C(19)	122.3(3)
C(16)-C(15)-C(14)	122.5(3)
C(16)-C(15)-H(15)	118.7
C(14)-C(15)-H(15)	118.7
C(17)-C(16)-C(15)	118.3(3)
C(17)-C(16)-C(20)	120.8(4)
C(15)-C(16)-C(20)	121.0(4)
C(16)-C(17)-C(18)	122.7(4)
C(16)-C(17)-H(17)	118.6

C(18)-C(17)-H(17)	118.6
C(13)-C(18)-C(17)	116.6(3)
C(13)-C(18)-C(21)	122.7(3)
C(17)-C(18)-C(21)	120.5(3)
C(14)-C(19)-H(19A)	109.5
C(14)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(14)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(16)-C(20)-H(20A)	109.5
C(16)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(16)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(18)-C(21)-H(21A)	109.5
C(18)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(18)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
N(1)-C(22)-C(27)	119.3(3)
N(1)-C(22)-C(23)	119.7(3)
C(27)-C(22)-C(23)	120.9(3)
C(24)-C(23)-C(22)	117.9(3)
C(24)-C(23)-C(28)	122.6(3)
C(22)-C(23)-C(28)	119.5(3)
C(25)-C(24)-C(23)	121.9(4)
C(25)-C(24)-H(24)	119.1
C(23)-C(24)-H(24)	119.1
C(24)-C(25)-C(26)	120.6(3)
C(24)-C(25)-H(25)	119.7
C(26)-C(25)-H(25)	119.7
C(25)-C(26)-C(27)	120.6(4)
C(25)-C(26)-H(26)	119.7
C(27)-C(26)-H(26)	119.7
C(26)-C(27)-C(22)	118.0(3)
C(26)-C(27)-C(31)	121.6(3)
C(22)-C(27)-C(31)	120.3(3)
C(23)-C(28)-C(30)	114.6(3)
C(23)-C(28)-C(29)	109.2(3)
C(30)-C(28)-C(29)	110.0(3)
C(23)-C(28)-H(28)	107.6
C(30)-C(28)-H(28)	107.6
C(29)-C(28)-H(28)	107.6
C(28)-C(29)-H(29A)	109.5
C(28)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(28)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(28)-C(30)-H(30A)	109.5
C(28)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(28)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(27)-C(31)-C(33)	114.2(3)
C(27)-C(31)-C(32)	110.2(3)
C(33)-C(31)-C(32)	110.4(3)
C(27)-C(31)-H(31)	107.3
C(33)-C(31)-H(31)	107.3
C(32)-C(31)-H(31)	107.3
C(31)-C(32)-H(32A)	109.5
C(31)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(31)-C(32)-H(32C)	109.5

H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(31)-C(33)-H(33A)	109.5
C(31)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(31)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
N(5)-C(34)-N(4)	108.1(3)
N(5)-C(34)-H(34)	126.0
N(4)-C(34)-H(34)	126.0
C(36)-C(35)-N(4)	107.5(3)
C(36)-C(35)-H(35)	126.3
N(4)-C(35)-H(35)	126.3
C(35)-C(36)-N(5)	107.9(4)
C(35)-C(36)-H(36)	126.1
N(5)-C(36)-H(36)	126.1
C(42)-C(37)-C(38)	123.9(3)
C(42)-C(37)-N(4)	118.7(3)
C(38)-C(37)-N(4)	117.4(3)
C(39)-C(38)-C(37)	116.1(3)
C(39)-C(38)-C(43)	121.8(3)
C(37)-C(38)-C(43)	122.1(3)
C(40)-C(39)-C(38)	122.7(3)
C(40)-C(39)-H(39)	118.6
C(38)-C(39)-H(39)	118.6
C(39)-C(40)-C(41)	118.5(3)
C(39)-C(40)-C(44)	121.1(4)
C(41)-C(40)-C(44)	120.5(4)
C(40)-C(41)-C(42)	122.0(4)
C(40)-C(41)-H(41)	119.0
C(42)-C(41)-H(41)	119.0
C(37)-C(42)-C(41)	116.7(3)
C(37)-C(42)-C(45)	122.0(3)
C(41)-C(42)-C(45)	121.2(4)
C(38)-C(43)-H(43A)	109.5
C(38)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43B)	109.5
C(38)-C(43)-H(43C)	109.5
H(43A)-C(43)-H(43C)	109.5
H(43B)-C(43)-H(43C)	109.5
C(40)-C(44)-H(44A)	109.5
C(40)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
C(40)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
C(42)-C(45)-H(45A)	109.5
C(42)-C(45)-H(45B)	109.5
H(45A)-C(45)-H(45B)	109.5
C(42)-C(45)-H(45C)	109.5
H(45A)-C(45)-H(45C)	109.5
H(45B)-C(45)-H(45C)	109.5
C(47)-C(46)-C(51)	123.8(3)
C(47)-C(46)-N(5)	117.4(3)
C(51)-C(46)-N(5)	118.7(3)
C(46)-C(47)-C(48)	116.5(3)
C(46)-C(47)-C(52)	121.8(3)
C(48)-C(47)-C(52)	121.7(4)
C(49)-C(48)-C(47)	122.7(4)
C(49)-C(48)-H(48)	118.7
C(47)-C(48)-H(48)	118.7
C(48)-C(49)-C(50)	118.5(3)
C(48)-C(49)-C(53)	120.8(4)
C(50)-C(49)-C(53)	120.7(4)
C(49)-C(50)-C(51)	122.2(4)
C(49)-C(50)-H(50)	118.9
C(51)-C(50)-H(50)	118.9

C(50)-C(51)-C(46)	116.3(3)
C(50)-C(51)-C(54)	121.9(3)
C(46)-C(51)-C(54)	121.8(3)
C(47)-C(52)-H(52A)	109.5
C(47)-C(52)-H(52B)	109.5
H(52A)-C(52)-H(52B)	109.5
C(47)-C(52)-H(52C)	109.5
H(52A)-C(52)-H(52C)	109.5
H(52B)-C(52)-H(52C)	109.5
C(49)-C(53)-H(53A)	109.5
C(49)-C(53)-H(53B)	109.5
H(53A)-C(53)-H(53B)	109.5
C(49)-C(53)-H(53C)	109.5
H(53A)-C(53)-H(53C)	109.5
H(53B)-C(53)-H(53C)	109.5
C(51)-C(54)-H(54A)	109.5
C(51)-C(54)-H(54B)	109.5
H(54A)-C(54)-H(54B)	109.5
C(51)-C(54)-H(54C)	109.5
H(54A)-C(54)-H(54C)	109.5
H(54B)-C(54)-H(54C)	109.5
C(22)-N(1)-Ti(1)	171.1(2)
C(1)-N(2)-C(3)	112.3(3)
C(1)-N(2)-C(13)	125.7(3)
C(3)-N(2)-C(13)	122.0(3)
C(1)-N(3)-C(2)	112.7(3)
C(1)-N(3)-C(4)	127.1(3)
C(2)-N(3)-C(4)	120.2(3)
C(34)-N(4)-C(35)	108.1(3)
C(34)-N(4)-C(37)	128.1(3)
C(35)-N(4)-C(37)	123.8(3)
C(34)-N(5)-C(36)	108.5(3)
C(34)-N(5)-C(46)	126.6(3)
C(36)-N(5)-C(46)	124.7(3)
N(1)-Ti(1)-C(1)	100.27(13)
N(1)-Ti(1)-Cl(1)	106.81(10)
C(1)-Ti(1)-Cl(1)	85.26(9)
N(1)-Ti(1)-Cl(3)	106.76(10)
C(1)-Ti(1)-Cl(3)	85.33(9)
Cl(1)-Ti(1)-Cl(3)	146.24(4)
N(1)-Ti(1)-Cl(2)	99.94(10)
C(1)-Ti(1)-Cl(2)	159.76(9)
Cl(1)-Ti(1)-Cl(2)	90.06(4)
Cl(3)-Ti(1)-Cl(2)	87.73(4)

Table 36. Anisotropic displacement parameters (A^2 x 10^3) for **12**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	40(3)	22(2)	26(2)	-2(2)	8(2)	-6(2)
C(2)	22(2)	66(3)	35(2)	-3(2)	0(2)	5(2)
C(3)	29(3)	52(3)	28(2)	-2(2)	-8(2)	4(2)
C(4)	19(2)	49(3)	26(2)	-4(2)	4(2)	-1(2)
C(5)	25(2)	46(3)	31(2)	-6(2)	-1(2)	7(2)
C(6)	27(2)	49(3)	37(2)	-12(2)	-3(2)	7(2)
C(7)	27(2)	65(3)	30(2)	-10(2)	5(2)	3(2)
C(8)	33(2)	64(3)	34(2)	4(2)	7(2)	-6(2)
C(9)	19(2)	55(3)	37(2)	-5(2)	3(2)	-6(2)
C(10)	48(3)	44(3)	42(2)	0(2)	-3(2)	7(2)
C(11)	54(3)	108(4)	31(2)	-9(2)	13(2)	2(3)
C(12)	45(3)	57(3)	47(2)	-10(2)	6(2)	-12(2)

C(13)	28(2)	37(2)	18(2)	-3(2)	-2(2)	2(2)
C(14)	30(2)	37(2)	18(2)	1(2)	-6(2)	0(2)
C(15)	28(2)	46(3)	27(2)	5(2)	-1(2)	-6(2)
C(16)	33(2)	49(3)	24(2)	-3(2)	3(2)	4(2)
C(17)	42(3)	41(3)	29(2)	-6(2)	0(2)	7(2)
C(18)	32(2)	38(2)	22(2)	-1(2)	-4(2)	0(2)
C(19)	45(3)	39(3)	33(2)	4(2)	-5(2)	-1(2)
C(20)	46(3)	79(3)	36(2)	-3(2)	9(2)	4(3)
C(21)	52(3)	40(2)	33(2)	-5(2)	2(2)	-7(2)
C(22)	22(2)	38(2)	18(2)	-1(2)	1(2)	5(2)
C(23)	29(2)	42(2)	24(2)	3(2)	0(2)	2(2)
C(24)	50(3)	51(3)	24(2)	4(2)	5(2)	-2(2)
C(25)	50(3)	63(3)	17(2)	-3(2)	3(2)	1(2)
C(26)	38(3)	50(3)	29(2)	-10(2)	-7(2)	2(2)
C(27)	25(2)	37(2)	23(2)	-3(2)	0(2)	3(2)
C(28)	46(3)	34(2)	29(2)	4(2)	7(2)	-5(2)
C(29)	63(3)	46(3)	46(2)	6(2)	11(2)	7(2)
C(30)	83(4)	52(3)	54(3)	5(2)	21(3)	-16(3)
C(31)	40(3)	37(2)	28(2)	-5(2)	2(2)	2(2)
C(32)	42(3)	49(3)	48(2)	-3(2)	5(2)	-4(2)
C(33)	62(3)	41(3)	42(2)	-6(2)	3(2)	2(2)
C(34)	32(2)	28(2)	29(2)	3(2)	2(2)	0(2)
C(35)	66(3)	60(3)	35(2)	18(2)	-14(2)	-33(3)
C(36)	52(3)	55(3)	40(2)	14(2)	-15(2)	-27(2)
C(37)	33(2)	29(2)	24(2)	6(2)	-6(2)	-6(2)
C(38)	32(2)	28(2)	31(2)	4(2)	-2(2)	-6(2)
C(39)	46(3)	37(2)	26(2)	-2(2)	2(2)	-9(2)
C(40)	39(3)	37(2)	40(2)	12(2)	-11(2)	-11(2)
C(41)	33(3)	35(2)	48(3)	15(2)	1(2)	2(2)
C(42)	44(3)	27(2)	32(2)	8(2)	0(2)	-3(2)
C(43)	45(3)	51(3)	51(3)	-7(2)	5(2)	1(2)
C(44)	65(3)	63(3)	47(3)	16(2)	-24(2)	-14(3)
C(45)	67(3)	54(3)	43(2)	1(2)	12(2)	12(3)
C(46)	26(2)	30(2)	23(2)	6(2)	-4(2)	-2(2)
C(47)	20(2)	30(2)	38(2)	2(2)	-2(2)	-5(2)
C(48)	26(2)	31(2)	67(3)	7(2)	-6(2)	2(2)
C(49)	34(3)	46(3)	41(2)	15(2)	-13(2)	-16(2)
C(50)	48(3)	53(3)	26(2)	-2(2)	2(2)	-13(2)
C(51)	34(2)	34(2)	28(2)	3(2)	-2(2)	2(2)
C(52)	34(3)	45(3)	60(3)	-9(2)	9(2)	0(2)
C(53)	57(3)	76(4)	55(3)	32(2)	-29(2)	-22(3)
C(54)	56(3)	48(3)	48(3)	-9(2)	6(2)	7(2)
N(1)	23(2)	30(2)	23(2)	-2(1)	1(1)	0(1)
N(2)	28(2)	32(2)	21(2)	0(1)	1(1)	0(2)
N(3)	30(2)	39(2)	24(2)	-4(1)	1(2)	-1(2)
N(4)	41(2)	30(2)	27(2)	7(1)	-4(2)	-9(2)
N(5)	30(2)	30(2)	28(2)	4(1)	-2(2)	-3(2)
Cl(1)	40(1)	40(1)	33(1)	7(1)	3(1)	-5(1)
Cl(2)	28(1)	43(1)	66(1)	8(1)	5(1)	6(1)
Cl(3)	46(1)	32(1)	39(1)	-7(1)	-2(1)	2(1)
Ti(1)	26(1)	31(1)	20(1)	-1(1)	4(1)	2(1)

X-ray Data for Complex 13

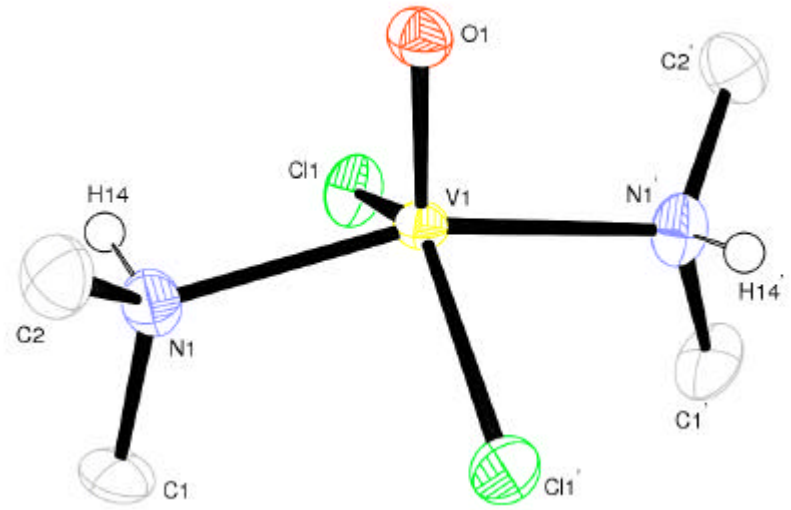

Table 37.

Formula	$C_4 H_{14} Cl_2 N_2 O V$		
Crystal Class	Monoclinic		
Space Group	C 2/c		
a (Å)	16.693(3)	alpha	90
b (Å)	9.6467(19)	beta	111.99(3)
c (Å)	6.5779(13)	gamma	90
Volume	982.2(4)		
Z	4		
Radiation type	Mo K?		
Wavelength (Å)	0.710730		
Density	1.54		
M(g.mol^{-1})	228.01		
μ(mm^{-1})	1.50		
Temperature (K)	180		
Size (mm)	0.09x 0.12x 0.60		
Colour	pale blue		
Shape	stick		
Cell from	8000 Reflections		
Theta range	2.49 to 26.02		
Diffractometer type	IPDS		
Scan type	Phi		
Absorption type	multi-scan		
Transmission range	0.52	0.88	
Reflections measured	4718		
Independent reflections	923		
Rint	0.09		
Hmin, Hmax	-20	20	
Kmin, Kmax	-11	11	
Lmin, Lmax	-8	8	
Refinement	on F		
R-factor	0.0721		
Weighted R-factor	0.0547		
Delta Rho min	-1.18		

Delta Rho max	1.41	
Reflections used	749	
sigma(I) limit		3.00
Number of parameters		48
Goodness of fit		0.904

Table 38 Atom coordinates and Uiso or Ueq:

Atom	x/a	y/b	z/c	U(equiv)
V(1)	0.5000	0.17633(11)	0.2500	0.0164
Cl(1)	0.59649(7)	0.26295(14)	0.57720(17)	0.0289
O(1)	0.5000	0.0114(5)	0.2500	0.0228
N(1)	0.4039(2)	0.2140(5)	0.3890(6)	0.0259
C(1)	0.3784(4)	0.3606(5)	0.3895(9)	0.0360
C(2)	0.3266(3)	0.1216(6)	0.2988(8)	0.0322

Atom	x/a	y/b	z/c	U(iso)
H(11)	0.4314	0.4196	0.4505	0.044(6)
H(12)	0.3436	0.3905	0.2362	0.044(6)
H(13)	0.3431	0.3709	0.4823	0.044(6)
H(14)	0.4305	0.1922	0.5246	0.044(6)
H(21)	0.3459	0.0233	0.3006	0.044(6)
H(22)	0.2913	0.1497	0.1448	0.044(6)
H(23)	0.2908	0.1301	0.3909	0.044(6)

Table 39. Thermal parameters:

Atom	u(11)	u(22)	u(33)	u(23)	u(13)	u(12)
V(1)	0.0156(5)	0.0143(6)	0.0183(6)	0.0000	0.0050(4)	0.0000
Cl(1)	0.0292(6)	0.0371(8)	0.0183(6)	-0.0052(4)	0.0065(4)	-0.0078(4)
O(1)	0.0200(19)	0.020(2)	0.028(2)	0.0000	0.0090(17)	0.0000
N(1)	0.021(2)	0.036(2)	0.0195(19)	0.0025(15)	0.0069(15)	0.0048(15)
C(1)	0.053(3)	0.021(3)	0.040(3)	0.003(2)	0.025(2)	0.018(2)
C(2)	0.023(2)	0.038(3)	0.036(3)	0.002(2)	0.011(2)	-0.004(2)

Table 40. Distances and angles:

V(1)	- Cl(1)	2.3085(11)
V(1)	- O(1)	1.591(5)
V(1)	- N(1)	2.154(4)
N(1)	- C(1)	1.477(6)
N(1)	- C(2)	1.497(6)

Cl(1)	- V(1)	- Cl(1')	137.55(8)
Cl(1)	- V(1)	- O(1)	111.22(4)
Cl(1)	- V(1)	- N(1)	85.04(11)
Cl(1)	- V(1)	- N(1')	87.95(10)
O(1)	- V(1)	- N(1)	99.71(13)
N(1)	- V(1)	- N(1')	160.6(3)
V(1)	- N(1)	- C(1)	115.1(3)
V(1)	- N(1)	- C(2)	113.6(3)
C(1)	- N(1)	- C(2)	111.3(4)

Symmetry code :
' : 1-x, y, -z+1/2

X-ray Data for Complex 14

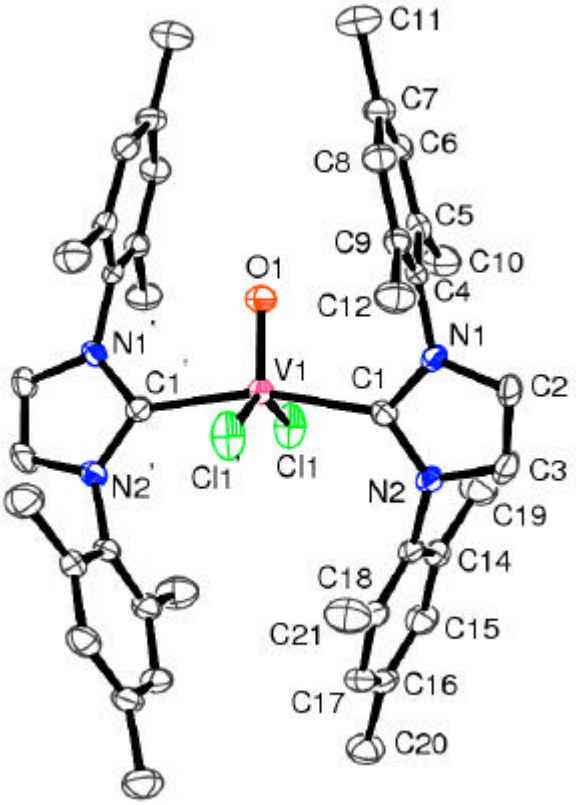

Table 41. Crystal data and structure refinement for **14**.

Empirical formula	C42 H48 Cl2 N4 O V
Formula weight	746.68
Temperature	180 K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, C 1 2/c 1
Unit cell dimensions	a = 18.693(3) A alpha = 90 deg. b = 14.468(3) A beta = 100.50(2) deg. c = 14.673(2) A gamma = 90 deg.
Volume	3901.9(12) A^3
Z, Calculated density	4, 1.271 Mg/m^3
Absorption coefficient	0.428 mm^-1
F(000)	1572
Crystal size	0.2 x 0.17 x 0.1 mm
Theta range for data collection	3.15 to 25.68 deg.
Limiting indices	-22<=h<=22, -16<=k<=17, -17<=l<=17
Reflections collected / unique	14141 / 3698 [R(int) = 0.07]
Completeness to theta = 25.68	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9578 and 0.921
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3698 / 0 / 233
Goodness-of-fit on F^2	0.918
Final R indices [I>2sigma(I)]	R1 = 0.0434, wR2 = 0.0764
R indices (all data)	R1 = 0.0945, wR2 = 0.0891
Largest diff. peak and hole	0.242 and -0.276 e.A^-3

Table 42. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **14**.

	x	y	z	U(eq)
C(1)	6100(1)	2462(2)	7247(2)	19(1)
C(2)	7155(1)	2178(2)	6730(2)	34(1)
C(3)	7160(2)	3065(2)	6972(2)	37(1)
C(4)	6332(1)	847(2)	6785(2)	20(1)
C(5)	6433(1)	297(2)	7571(2)	22(1)
C(6)	6236(1)	-625(2)	7451(2)	24(1)
C(7)	5974(1)	-999(2)	6588(2)	24(1)
C(8)	5905(1)	-426(2)	5823(2)	25(1)
C(9)	6077(1)	503(2)	5905(2)	22(1)
C(10)	6744(2)	676(2)	8510(2)	34(1)
C(11)	5780(2)	-2007(2)	6497(2)	39(1)
C(12)	5977(2)	1120(2)	5065(2)	32(1)
C(13)	6404(1)	4096(2)	7738(2)	24(1)
C(14)	6737(1)	4195(2)	8659(2)	27(1)
C(15)	6645(2)	5031(2)	9089(2)	30(1)
C(16)	6242(2)	5743(2)	8623(2)	28(1)
C(17)	5945(2)	5623(2)	7701(2)	29(1)
C(18)	6020(2)	4804(2)	7233(2)	26(1)
C(19)	7178(2)	3442(2)	9189(2)	39(1)
C(20)	6123(2)	6634(2)	9118(2)	39(1)
C(21)	5695(2)	4726(2)	6223(2)	42(1)
N(1)	6505(1)	1816(1)	6896(1)	22(1)
N(2)	6519(1)	3233(1)	7287(1)	24(1)
O(1)	5000	1150(2)	7500	40(1)
Cl(1)	5380(1)	2693(1)	9019(1)	40(1)
V(1)	5000	2233(1)	7500	22(1)

Table 43. Bond lengths [A] and angles [deg] for **14**.

C(1)-N(2)	1.358(3)
C(1)-N(1)	1.363(3)
C(1)-V(1)	2.180(2)
C(2)-C(3)	1.332(3)
C(2)-N(1)	1.384(3)
C(2)-H(2)	0.93
C(3)-N(2)	1.383(3)
C(3)-H(3)	0.93
C(4)-C(9)	1.385(3)
C(4)-C(5)	1.386(3)
C(4)-N(1)	1.440(3)
C(5)-C(6)	1.386(3)
C(5)-C(10)	1.499(3)
C(6)-C(7)	1.382(3)
C(6)-H(6)	0.93
C(7)-C(8)	1.381(3)
C(7)-C(11)	1.503(3)
C(8)-C(9)	1.382(3)
C(8)-H(8)	0.93
C(9)-C(12)	1.507(3)
C(10)-H(10A)	0.96
C(10)-H(10B)	0.96
C(10)-H(10C)	0.96
C(11)-H(11A)	0.96
C(11)-H(11B)	0.96
C(11)-H(11C)	0.96
C(12)-H(12A)	0.96
C(12)-H(12B)	0.96
C(12)-H(12C)	0.96
C(13)-C(18)	1.385(3)
C(13)-C(14)	1.388(3)
C(13)-N(2)	1.447(3)
C(14)-C(15)	1.390(3)
C(14)-C(19)	1.496(3)
C(15)-C(16)	1.381(4)
C(15)-H(15)	0.93
C(16)-C(17)	1.376(4)
C(16)-C(20)	1.516(3)
C(17)-C(18)	1.390(3)
C(17)-H(17)	0.93
C(18)-C(21)	1.501(4)
C(19)-H(19A)	0.96
C(19)-H(19B)	0.96
C(19)-H(19C)	0.96
C(20)-H(20A)	0.96
C(20)-H(20B)	0.96
C(20)-H(20C)	0.96
C(21)-H(21A)	0.96
C(21)-H(21B)	0.96
C(21)-H(21C)	0.96
O(1)-V(1)	1.567(2)
Cl(1)-V(1)	2.3099(8)
V(1)-C(1)#1	2.180(3)
V(1)-Cl(1)#1	2.3099(8)

N(2)-C(1)-N(1)	103.0(2)
N(2)-C(1)-V(1)	132.19(17)
N(1)-C(1)-V(1)	124.52(17)
C(3)-C(2)-N(1)	106.4(2)
C(3)-C(2)-H(2)	126.8
N(1)-C(2)-H(2)	126.8
C(2)-C(3)-N(2)	107.1(2)
C(2)-C(3)-H(3)	126.5
N(2)-C(3)-H(3)	126.5
C(9)-C(4)-C(5)	122.7(2)

C(9)-C(4)-N(1)	119.2(2)
C(5)-C(4)-N(1)	118.1(2)
C(6)-C(5)-C(4)	117.1(2)
C(6)-C(5)-C(10)	121.3(2)
C(4)-C(5)-C(10)	121.7(2)
C(7)-C(6)-C(5)	122.3(2)
C(7)-C(6)-H(6)	118.9
C(5)-C(6)-H(6)	118.9
C(8)-C(7)-C(6)	118.4(2)
C(8)-C(7)-C(11)	121.6(2)
C(6)-C(7)-C(11)	120.0(2)
C(7)-C(8)-C(9)	121.7(2)
C(7)-C(8)-H(8)	119.1
C(9)-C(8)-H(8)	119.1
C(8)-C(9)-C(4)	117.8(2)
C(8)-C(9)-C(12)	120.8(2)
C(4)-C(9)-C(12)	121.3(2)
C(5)-C(10)-H(10A)	109.5
C(5)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(5)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(7)-C(11)-H(11A)	109.5
C(7)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(7)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(9)-C(12)-H(12A)	109.5
C(9)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(9)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(18)-C(13)-C(14)	122.7(2)
C(18)-C(13)-N(2)	119.9(2)
C(14)-C(13)-N(2)	117.2(2)
C(13)-C(14)-C(15)	117.5(2)
C(13)-C(14)-C(19)	122.5(2)
C(15)-C(14)-C(19)	120.0(2)
C(16)-C(15)-C(14)	121.7(3)
C(16)-C(15)-H(15)	119.2
C(14)-C(15)-H(15)	119.2
C(17)-C(16)-C(15)	118.6(2)
C(17)-C(16)-C(20)	120.7(2)
C(15)-C(16)-C(20)	120.7(3)
C(16)-C(17)-C(18)	122.3(2)
C(16)-C(17)-H(17)	118.8
C(18)-C(17)-H(17)	118.8
C(13)-C(18)-C(17)	117.1(3)
C(13)-C(18)-C(21)	123.4(2)
C(17)-C(18)-C(21)	119.5(2)
C(14)-C(19)-H(19A)	109.5
C(14)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(14)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(16)-C(20)-H(20A)	109.5
C(16)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(16)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(18)-C(21)-H(21A)	109.5
C(18)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5

C(18)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(1)-N(1)-C(2)	111.9(2)
C(1)-N(1)-C(4)	125.5(2)
C(2)-N(1)-C(4)	122.3(2)
C(1)-N(2)-C(3)	111.7(2)
C(1)-N(2)-C(13)	126.6(2)
C(3)-N(2)-C(13)	120.9(2)
O(1)-V(1)-C(1)	98.74(6)
O(1)-V(1)-C(1)#1	98.74(6)
C(1)-V(1)-C(1)#1	162.52(13)
O(1)-V(1)-Cl(1)	106.72(2)
C(1)-V(1)-Cl(1)	89.27(7)
C(1)#1-V(1)-Cl(1)	85.71(7)
O(1)-V(1)-Cl(1)#1	106.72(2)
C(1)-V(1)-Cl(1)#1	85.71(7)
C(1)#1-V(1)-Cl(1)#1	89.27(7)
Cl(1)-V(1)-Cl(1)#1	146.55(5)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,y,-z+3/2

Table 44. Anisotropic displacement parameters (A^2 x 10^3) for **14**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	20(1)	19(2)	18(1)	-2(1)	1(1)	2(1)
C(2)	20(2)	32(2)	56(2)	-9(2)	19(2)	-3(1)
C(3)	23(2)	30(2)	62(2)	-8(2)	21(2)	-10(1)
C(4)	14(1)	16(2)	33(2)	-1(1)	6(1)	3(1)
C(5)	17(2)	26(2)	23(2)	0(1)	2(1)	5(1)
C(6)	23(2)	22(2)	28(2)	3(1)	6(1)	4(1)
C(7)	29(2)	18(2)	27(2)	-2(1)	6(1)	0(1)
C(8)	30(2)	24(2)	22(2)	-6(1)	5(1)	-1(1)
C(9)	20(2)	21(2)	25(2)	2(1)	7(1)	2(1)
C(10)	40(2)	30(2)	30(2)	0(1)	-3(1)	3(1)
C(11)	56(2)	24(2)	35(2)	0(1)	3(2)	-6(1)
C(12)	43(2)	25(2)	27(2)	1(1)	10(2)	1(1)
C(13)	21(2)	16(2)	36(2)	-5(1)	10(1)	-4(1)
C(14)	20(2)	22(2)	36(2)	-4(1)	-1(1)	-3(1)
C(15)	33(2)	28(2)	29(2)	-8(1)	3(1)	-6(1)
C(16)	31(2)	18(2)	37(2)	-5(1)	13(1)	-6(1)
C(17)	31(2)	17(2)	39(2)	4(1)	9(1)	1(1)
C(18)	28(2)	20(2)	32(2)	2(1)	9(1)	-4(1)
C(19)	42(2)	32(2)	39(2)	-6(2)	-4(2)	3(2)
C(20)	48(2)	27(2)	44(2)	-8(2)	16(2)	1(2)
C(21)	58(2)	33(2)	32(2)	-1(1)	4(2)	3(2)
N(1)	19(1)	19(1)	29(1)	-3(1)	8(1)	-5(1)
N(2)	22(1)	19(1)	32(1)	-5(1)	9(1)	-3(1)
O(1)	30(2)	20(2)	75(2)	0	22(2)	0
Cl(1)	30(1)	63(1)	25(1)	-1(1)	5(1)	-2(1)
V(1)	19(1)	19(1)	29(1)	0	7(1)	0

X-ray Data for Complex IMes.HCl

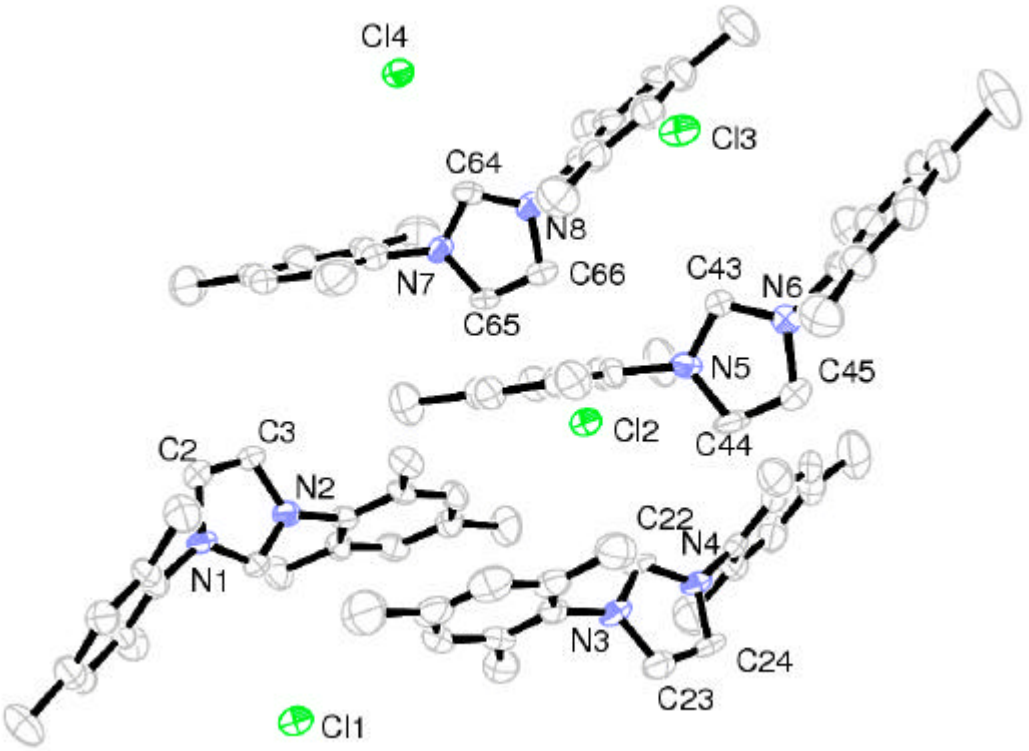

Table 45. Crystal data and structure refinement for **IMes.HCl**.

Empirical formula	C21 H25 Cl N2
Formula weight	340.88
Temperature	180 K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 16.2380(18) A alpha = 93.658(9) deg.
	b = 16.3664(16) A beta = 116.037(11) deg.
	c = 16.5630(18) A gamma = 90.853(9) deg.
Volume	3942.4(7) A^3
Z, Calculated density	8, 1.149 Mg/m^3
Absorption coefficient	0.198 mm^-1
F(000)	1456
Crystal size	0.17 x 0.11 x 0.05 mm
Theta range for data collection	2.58 to 25.68 deg.
Limiting indices	-19<=h<=19, -19<=k<=19, -15<=l<=20
Reflections collected / unique	29327 / 14914 [R(int) = 0.0956]
Completeness to theta = 25.68	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.998 and 0.95518
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	14914 / 0 / 879
Goodness-of-fit on F^2	0.738
Final R indices [I>2sigma(I)]	R1 = 0.044, wR2 = 0.0606
R indices (all data)	R1 = 0.2065, wR2 = 0.0871
Largest diff. peak and hole	0.219 and -0.249 e.A^-3

Table 46. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **IMes.HCl**.

	x	y	z	U(eq)
C(1)	6898(2)	8024(2)	-3799(2)	32(1)
C(2)	6677(2)	7736(2)	-2622(2)	39(1)
C(3)	7494(2)	8144(2)	-2315(2)	39(1)
C(4)	5449(2)	7274(2)	-4187(2)	32(1)
C(5)	5324(2)	6435(2)	-4149(2)	37(1)
C(6)	4516(3)	6060(2)	-4798(2)	42(1)
C(7)	3852(3)	6487(3)	-5448(2)	43(1)
C(8)	4012(2)	7325(2)	-5427(2)	39(1)
C(9)	4792(2)	7740(2)	-4796(2)	33(1)
C(10)	6033(2)	5943(2)	-3464(2)	50(1)
C(11)	2990(2)	6061(2)	-6176(2)	61(1)
C(12)	4927(2)	8655(2)	-4799(2)	47(1)
C(13)	8406(2)	8758(2)	-3034(2)	30(1)
C(14)	9242(2)	8379(2)	-2726(2)	32(1)
C(15)	9976(2)	8839(2)	-2697(2)	39(1)
C(16)	9900(3)	9626(2)	-2950(2)	38(1)
C(17)	9052(3)	9973(2)	-3245(2)	41(1)
C(18)	8285(2)	9544(2)	-3299(2)	34(1)
C(19)	9316(2)	7509(2)	-2475(2)	47(1)
C(20)	10725(2)	10105(2)	-2907(2)	58(1)
C(21)	7376(2)	9941(2)	-3626(2)	47(1)
C(22)	11689(3)	7725(2)	-3810(2)	43(1)
C(23)	11220(3)	7314(2)	-5243(3)	60(1)
C(24)	12062(3)	7665(3)	-4929(2)	62(1)
C(25)	10154(3)	7021(3)	-4558(2)	40(1)
C(26)	9390(3)	7488(3)	-4873(2)	47(1)
C(27)	8582(3)	7152(3)	-4918(2)	54(1)
C(28)	8553(3)	6379(3)	-4663(3)	58(1)
C(29)	9324(4)	5926(3)	-4359(3)	59(1)
C(30)	10142(3)	6239(3)	-4305(2)	46(1)
C(31)	9424(2)	8347(2)	-5129(2)	65(1)
C(32)	7650(3)	6018(3)	-4725(3)	97(2)
C(33)	10993(3)	5753(2)	-3946(2)	65(1)
C(34)	13203(3)	8354(3)	-3461(3)	40(1)
C(35)	13292(3)	9174(3)	-3592(3)	49(1)
C(36)	14128(3)	9575(3)	-3079(3)	55(1)
C(37)	14848(3)	9190(3)	-2453(3)	55(1)
C(38)	14712(3)	8381(3)	-2326(3)	53(1)
C(39)	13907(3)	7939(3)	-2836(3)	43(1)
C(40)	12503(2)	9610(2)	-4259(3)	73(1)
C(41)	15770(3)	9641(2)	-1910(3)	86(2)
C(42)	13784(2)	7046(2)	-2716(2)	62(1)
C(43)	12963(2)	3146(2)	-1269(2)	32(1)
C(44)	12476(3)	3282(2)	-2718(2)	40(1)
C(45)	13231(3)	2850(2)	-2454(2)	42(1)
C(46)	11540(2)	3896(2)	-1992(2)	34(1)
C(47)	11635(3)	4732(2)	-1820(2)	39(1)
C(48)	10861(3)	5133(2)	-1881(2)	39(1)
C(49)	10038(2)	4703(2)	-2104(2)	36(1)
C(50)	9986(2)	3865(2)	-2270(2)	38(1)
C(51)	10739(3)	3439(2)	-2211(2)	35(1)
C(52)	12528(2)	5197(2)	-1564(2)	61(1)
C(53)	9217(2)	5151(2)	-2153(2)	54(1)
C(54)	10681(2)	2518(2)	-2384(2)	48(1)
C(55)	14297(3)	2308(2)	-993(2)	34(1)
C(56)	14211(3)	1470(3)	-1161(2)	40(1)
C(57)	14948(3)	1034(2)	-602(3)	50(1)
C(58)	15726(3)	1418(3)	81(3)	47(1)
C(59)	15758(2)	2255(3)	213(2)	44(1)
C(60)	15048(3)	2728(2)	-315(3)	38(1)
C(61)	13373(2)	1037(2)	-1902(2)	56(1)

C(62)	16511(2)	935(2)	696(3)	87(2)
C(63)	15116(2)	3646(2)	-148(2)	53(1)
C(64)	11719(3)	7318(2)	1194(2)	39(1)
C(65)	11355(3)	7655(2)	-177(2)	48(1)
C(66)	12138(3)	7257(2)	99(2)	52(1)
C(67)	10297(3)	8086(3)	484(2)	41(1)
C(68)	9483(3)	7616(3)	145(2)	48(1)
C(69)	8726(3)	8019(4)	104(2)	66(2)
C(70)	8764(4)	8830(4)	379(3)	77(2)
C(71)	9592(4)	9258(3)	724(3)	70(2)
C(72)	10383(3)	8895(3)	779(2)	47(1)
C(73)	9405(3)	6723(2)	-145(2)	70(1)
C(74)	7918(3)	9254(3)	329(3)	126(2)
C(75)	11294	9356	1171	63
C(76)	13158(2)	6622(3)	1510(2)	36(1)
C(77)	13139(3)	5781(3)	1317(2)	43(1)
C(78)	13926(3)	5388(2)	1795(3)	49(1)
C(79)	14693(3)	5794(3)	2448(3)	53(1)
C(80)	14671(3)	6629(3)	2645(2)	47(1)
C(81)	13894(3)	7062(2)	2159(2)	37(1)
C(82)	12290(2)	5307(2)	620(2)	65(1)
C(83)	15568(2)	5363(2)	2966(2)	74(1)
C(84)	13892(2)	7977(2)	2340(2)	55(1)
N(1)	6313(2)	7661(2)	-3551(2)	34(1)
N(2)	7627(2)	8313(2)	-3054(2)	32(1)
N(3)	10997(2)	7349(2)	-4528(2)	43(1)
N(4)	12347(2)	7915(2)	-4041(2)	43(1)
N(5)	12317(2)	3464(2)	-1978(2)	32(1)
N(6)	13525(2)	2774(2)	-1546(2)	33(1)
N(7)	11097(2)	7689(2)	510(2)	36(1)
N(8)	12348(2)	7042(2)	959(2)	39(1)
Cl(1)	6473(1)	8272(1)	-5901(1)	47(1)
Cl(2)	11786(1)	7298(1)	-1940(1)	45(1)
Cl(3)	13500(1)	3181(1)	907(1)	51(1)
Cl(4)	11725(1)	7942(1)	3044(1)	40(1)

Table 47. Bond lengths [A] and angles [deg] for **IMes.HCl**.

C(1)-N(2)	1.332(3)
C(1)-N(1)	1.333(4)
C(1)-H(1)	0.93
C(2)-C(3)	1.343(4)
C(2)-N(1)	1.382(4)
C(2)-H(2)	0.93
C(3)-N(2)	1.376(4)
C(3)-H(3)	0.93
C(4)-C(9)	1.384(4)
C(4)-C(5)	1.395(4)
C(4)-N(1)	1.439(4)
C(5)-C(6)	1.380(4)
C(5)-C(10)	1.503(4)
C(6)-C(7)	1.382(4)
C(6)-H(6)	0.93
C(7)-C(8)	1.388(4)
C(7)-C(11)	1.510(4)
C(8)-C(9)	1.370(4)
C(8)-H(8)	0.93
C(9)-C(12)	1.511(4)
C(10)-H(10A)	0.96
C(10)-H(10B)	0.96
C(10)-H(10C)	0.96
C(11)-H(11A)	0.96
C(11)-H(11B)	0.96
C(11)-H(11C)	0.96
C(12)-H(12A)	0.96
C(12)-H(12B)	0.96
C(12)-H(12C)	0.96
C(13)-C(18)	1.375(4)
C(13)-C(14)	1.396(4)
C(13)-N(2)	1.436(4)
C(14)-C(15)	1.381(4)
C(14)-C(19)	1.500(4)
C(15)-C(16)	1.371(4)
C(15)-H(15)	0.93
C(16)-C(17)	1.387(4)
C(16)-C(20)	1.513(4)
C(17)-C(18)	1.386(4)
C(17)-H(17)	0.93
C(18)-C(21)	1.506(4)
C(19)-H(19A)	0.96
C(19)-H(19B)	0.96
C(19)-H(19C)	0.96
C(20)-H(20A)	0.96
C(20)-H(20B)	0.96
C(20)-H(20C)	0.96
C(21)-H(21A)	0.96
C(21)-H(21B)	0.96
C(21)-H(21C)	0.96
C(22)-N(4)	1.322(4)
C(22)-N(3)	1.330(4)
C(22)-H(22)	0.93
C(23)-C(24)	1.336(4)
C(23)-N(3)	1.380(4)
C(23)-H(23)	0.93
C(24)-N(4)	1.366(4)
C(24)-H(24)	0.93
C(25)-C(30)	1.376(5)
C(25)-C(26)	1.380(5)
C(25)-N(3)	1.441(4)

C(26)-C(27)	1.383(5)
C(26)-C(31)	1.502(5)
C(27)-C(28)	1.366(5)
C(27)-H(27)	0.93
C(28)-C(29)	1.377(5)
C(28)-C(32)	1.531(5)
C(29)-C(30)	1.381(5)
C(29)-H(29)	0.93
C(30)-C(33)	1.506(5)
C(31)-H(31A)	0.96
C(31)-H(31B)	0.96
C(31)-H(31C)	0.96
C(32)-H(32A)	0.96
C(32)-H(32B)	0.96
C(32)-H(32C)	0.96
C(33)-H(33A)	0.96
C(33)-H(33B)	0.96
C(33)-H(33C)	0.96
C(34)-C(39)	1.383(5)
C(34)-C(35)	1.389(5)
C(34)-N(4)	1.442(4)
C(35)-C(36)	1.372(5)
C(35)-C(40)	1.503(4)
C(36)-C(37)	1.371(5)
C(36)-H(36)	0.93
C(37)-C(38)	1.382(5)
C(37)-C(41)	1.516(5)
C(38)-C(39)	1.368(5)
C(38)-H(38)	0.93
C(39)-C(42)	1.510(4)
C(40)-H(40A)	0.96
C(40)-H(40B)	0.96
C(40)-H(40C)	0.96
C(41)-H(41A)	0.96
C(41)-H(41B)	0.96
C(41)-H(41C)	0.96
C(42)-H(42A)	0.96
C(42)-H(42B)	0.96
C(42)-H(42C)	0.96
C(43)-N(6)	1.327(4)
C(43)-N(5)	1.328(4)
C(43)-H(43)	0.93
C(44)-C(45)	1.337(4)
C(44)-N(5)	1.376(4)
C(44)-H(44)	0.93
C(45)-N(6)	1.378(4)
C(45)-H(45)	0.93
C(46)-C(47)	1.373(4)
C(46)-C(51)	1.379(4)
C(46)-N(5)	1.447(4)
C(47)-C(48)	1.393(4)
C(47)-C(52)	1.499(4)
C(48)-C(49)	1.387(4)
C(48)-H(48)	0.93
C(49)-C(50)	1.376(4)
C(49)-C(53)	1.504(4)
C(50)-C(51)	1.385(4)
C(50)-H(50)	0.93
C(51)-C(54)	1.511(4)
C(52)-H(52A)	0.96
C(52)-H(52B)	0.96
C(52)-H(52C)	0.96
C(53)-H(53A)	0.96
C(53)-H(53B)	0.96
C(53)-H(53C)	0.96
C(54)-H(54A)	0.96
C(54)-H(54B)	0.96
C(54)-H(54C)	0.96

C(55)-C(56)	1.374(4)
C(55)-C(60)	1.377(4)
C(55)-N(6)	1.450(4)
C(56)-C(57)	1.392(4)
C(56)-C(61)	1.502(4)
C(57)-C(58)	1.378(4)
C(57)-H(57)	0.93
C(58)-C(59)	1.371(4)
C(58)-C(62)	1.510(4)
C(59)-C(60)	1.386(4)
C(59)-H(59)	0.93
C(60)-C(63)	1.503(4)
C(61)-H(61A)	0.96
C(61)-H(61B)	0.96
C(61)-H(61C)	0.96
C(62)-H(62A)	0.96
C(62)-H(62B)	0.96
C(62)-H(62C)	0.96
C(63)-H(63A)	0.96
C(63)-H(63B)	0.96
C(63)-H(63C)	0.96
C(64)-N(8)	1.319(4)
C(64)-N(7)	1.332(4)
C(64)-H(64)	0.93
C(65)-C(66)	1.342(4)
C(65)-N(7)	1.373(4)
C(65)-H(65)	0.93
C(66)-N(8)	1.382(4)
C(66)-H(66)	0.93
C(67)-C(72)	1.365(4)
C(67)-C(68)	1.386(5)
C(67)-N(7)	1.447(4)
C(68)-C(69)	1.381(5)
C(68)-C(73)	1.494(5)
C(69)-C(70)	1.366(5)
C(69)-H(69)	0.93
C(70)-C(71)	1.369(6)
C(70)-C(74)	1.520(6)
C(71)-C(72)	1.392(5)
C(71)-H(71)	0.93
C(72)-C(75)	1.49672
C(73)-H(73A)	0.96
C(73)-H(73B)	0.96
C(73)-H(73C)	0.96
C(74)-H(74A)	0.9579
C(74)-H(74B)	0.9589
C(74)-H(74C)	0.9613
C(75)-H(75A)	0.96
C(75)-H(75B)	0.96
C(75)-H(75C)	0.96
C(76)-C(81)	1.361(4)
C(76)-C(77)	1.389(4)
C(76)-N(8)	1.445(4)
C(77)-C(78)	1.369(4)
C(77)-C(82)	1.514(4)
C(78)-C(79)	1.365(5)
C(78)-H(78)	0.93
C(79)-C(80)	1.390(5)
C(79)-C(83)	1.513(4)
C(80)-C(81)	1.396(4)
C(80)-H(80)	0.93
C(81)-C(84)	1.509(4)
C(82)-H(82A)	0.96
C(82)-H(82B)	0.96
C(82)-H(82C)	0.96
C(83)-H(83A)	0.96
C(83)-H(83B)	0.96
C(83)-H(83C)	0.96

C(84)-H(84A)	0.96
C(84)-H(84B)	0.96
C(84)-H(84C)	0.96
N(2)-C(1)-N(1)	108.0(3)
N(2)-C(1)-H(1)	126
N(1)-C(1)-H(1)	126
C(3)-C(2)-N(1)	106.9(3)
C(3)-C(2)-H(2)	126.5
N(1)-C(2)-H(2)	126.5
C(2)-C(3)-N(2)	107.3(3)
C(2)-C(3)-H(3)	126.3
N(2)-C(3)-H(3)	126.3
C(9)-C(4)-C(5)	123.4(4)
C(9)-C(4)-N(1)	119.4(3)
C(5)-C(4)-N(1)	117.1(3)
C(6)-C(5)-C(4)	116.6(3)
C(6)-C(5)-C(10)	120.6(4)
C(4)-C(5)-C(10)	122.8(3)
C(5)-C(6)-C(7)	122.5(4)
C(5)-C(6)-H(6)	118.8
C(7)-C(6)-H(6)	118.8
C(6)-C(7)-C(8)	117.7(4)
C(6)-C(7)-C(11)	121.8(4)
C(8)-C(7)-C(11)	120.5(4)
C(9)-C(8)-C(7)	123.0(4)
C(9)-C(8)-H(8)	118.5
C(7)-C(8)-H(8)	118.5
C(8)-C(9)-C(4)	116.6(4)
C(8)-C(9)-C(12)	120.8(3)
C(4)-C(9)-C(12)	122.5(3)
C(5)-C(10)-H(10A)	109.5
C(5)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(5)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(7)-C(11)-H(11A)	109.5
C(7)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(7)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(9)-C(12)-H(12A)	109.5
C(9)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(9)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(18)-C(13)-C(14)	123.9(3)
C(18)-C(13)-N(2)	117.7(3)
C(14)-C(13)-N(2)	118.4(3)
C(15)-C(14)-C(13)	116.3(3)
C(15)-C(14)-C(19)	122.8(3)
C(13)-C(14)-C(19)	120.9(3)
C(16)-C(15)-C(14)	122.6(4)
C(16)-C(15)-H(15)	118.7
C(14)-C(15)-H(15)	118.7
C(15)-C(16)-C(17)	118.6(4)
C(15)-C(16)-C(20)	120.5(4)
C(17)-C(16)-C(20)	120.9(4)
C(18)-C(17)-C(16)	121.9(4)
C(18)-C(17)-H(17)	119.1
C(16)-C(17)-H(17)	119.1
C(13)-C(18)-C(17)	116.8(3)
C(13)-C(18)-C(21)	122.9(3)
C(17)-C(18)-C(21)	120.3(3)
C(14)-C(19)-H(19A)	109.5

C(14)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(14)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(16)-C(20)-H(20A)	109.5
C(16)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(16)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(18)-C(21)-H(21A)	109.5
C(18)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(18)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
N(4)-C(22)-N(3)	108.0(3)
N(4)-C(22)-H(22)	126
N(3)-C(22)-H(22)	126
C(24)-C(23)-N(3)	106.3(4)
C(24)-C(23)-H(23)	126.8
N(3)-C(23)-H(23)	126.8
C(23)-C(24)-N(4)	108.0(4)
C(23)-C(24)-H(24)	126
N(4)-C(24)-H(24)	126
C(30)-C(25)-C(26)	123.0(4)
C(30)-C(25)-N(3)	117.8(4)
C(26)-C(25)-N(3)	119.0(4)
C(25)-C(26)-C(27)	118.0(4)
C(25)-C(26)-C(31)	122.0(4)
C(27)-C(26)-C(31)	119.9(4)
C(28)-C(27)-C(26)	120.2(4)
C(28)-C(27)-H(27)	119.9
C(26)-C(27)-H(27)	119.9
C(27)-C(28)-C(29)	120.5(5)
C(27)-C(28)-C(32)	119.4(5)
C(29)-C(28)-C(32)	120.2(5)
C(28)-C(29)-C(30)	121.0(4)
C(28)-C(29)-H(29)	119.5
C(30)-C(29)-H(29)	119.5
C(25)-C(30)-C(29)	117.2(4)
C(25)-C(30)-C(33)	121.7(4)
C(29)-C(30)-C(33)	121.0(4)
C(26)-C(31)-H(31A)	109.5
C(26)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(26)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(28)-C(32)-H(32A)	109.5
C(28)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(28)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(30)-C(33)-H(33A)	109.5
C(30)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(30)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(39)-C(34)-C(35)	123.0(4)
C(39)-C(34)-N(4)	119.4(4)
C(35)-C(34)-N(4)	117.6(4)
C(36)-C(35)-C(34)	117.4(4)
C(36)-C(35)-C(40)	121.2(4)
C(34)-C(35)-C(40)	121.5(4)

C(37)-C(36)-C(35)	121.8(4)
C(37)-C(36)-H(36)	119.1
C(35)-C(36)-H(36)	119.1
C(36)-C(37)-C(38)	118.5(4)
C(36)-C(37)-C(41)	120.8(4)
C(38)-C(37)-C(41)	120.7(4)
C(39)-C(38)-C(37)	122.5(4)
C(39)-C(38)-H(38)	118.7
C(37)-C(38)-H(38)	118.7
C(38)-C(39)-C(34)	116.7(4)
C(38)-C(39)-C(42)	121.9(4)
C(34)-C(39)-C(42)	121.4(4)
C(35)-C(40)-H(40A)	109.5
C(35)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(35)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
C(37)-C(41)-H(41A)	109.5
C(37)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
C(37)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
C(39)-C(42)-H(42A)	109.5
C(39)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(39)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
N(6)-C(43)-N(5)	107.3(3)
N(6)-C(43)-H(43)	126.4
N(5)-C(43)-H(43)	126.4
C(45)-C(44)-N(5)	107.8(3)
C(45)-C(44)-H(44)	126.1
N(5)-C(44)-H(44)	126.1
C(44)-C(45)-N(6)	106.1(3)
C(44)-C(45)-H(45)	127
N(6)-C(45)-H(45)	127
C(47)-C(46)-C(51)	124.2(4)
C(47)-C(46)-N(5)	118.2(4)
C(51)-C(46)-N(5)	117.5(4)
C(46)-C(47)-C(48)	116.8(4)
C(46)-C(47)-C(52)	122.0(4)
C(48)-C(47)-C(52)	121.2(4)
C(49)-C(48)-C(47)	121.3(4)
C(49)-C(48)-H(48)	119.4
C(47)-C(48)-H(48)	119.4
C(50)-C(49)-C(48)	119.2(3)
C(50)-C(49)-C(53)	120.7(4)
C(48)-C(49)-C(53)	120.1(4)
C(49)-C(50)-C(51)	121.6(4)
C(49)-C(50)-H(50)	119.2
C(51)-C(50)-H(50)	119.2
C(46)-C(51)-C(50)	117.0(4)
C(46)-C(51)-C(54)	121.7(3)
C(50)-C(51)-C(54)	121.3(4)
C(47)-C(52)-H(52A)	109.5
C(47)-C(52)-H(52B)	109.5
H(52A)-C(52)-H(52B)	109.5
C(47)-C(52)-H(52C)	109.5
H(52A)-C(52)-H(52C)	109.5
H(52B)-C(52)-H(52C)	109.5
C(49)-C(53)-H(53A)	109.5
C(49)-C(53)-H(53B)	109.5
H(53A)-C(53)-H(53B)	109.5
C(49)-C(53)-H(53C)	109.5
H(53A)-C(53)-H(53C)	109.5

H(53B)-C(53)-H(53C)	109.5
C(51)-C(54)-H(54A)	109.5
C(51)-C(54)-H(54B)	109.5
H(54A)-C(54)-H(54B)	109.5
C(51)-C(54)-H(54C)	109.5
H(54A)-C(54)-H(54C)	109.5
H(54B)-C(54)-H(54C)	109.5
C(56)-C(55)-C(60)	124.5(4)
C(56)-C(55)-N(6)	117.4(4)
C(60)-C(55)-N(6)	118.1(4)
C(55)-C(56)-C(57)	116.4(4)
C(55)-C(56)-C(61)	122.6(4)
C(57)-C(56)-C(61)	121.0(4)
C(58)-C(57)-C(56)	122.1(4)
C(58)-C(57)-H(57)	119
C(56)-C(57)-H(57)	119
C(59)-C(58)-C(57)	118.2(4)
C(59)-C(58)-C(62)	120.3(4)
C(57)-C(58)-C(62)	121.5(4)
C(58)-C(59)-C(60)	122.8(4)
C(58)-C(59)-H(59)	118.6
C(60)-C(59)-H(59)	118.6
C(55)-C(60)-C(59)	116.1(4)
C(55)-C(60)-C(63)	123.0(4)
C(59)-C(60)-C(63)	120.9(4)
C(56)-C(61)-H(61A)	109.5
C(56)-C(61)-H(61B)	109.5
H(61A)-C(61)-H(61B)	109.5
C(56)-C(61)-H(61C)	109.5
H(61A)-C(61)-H(61C)	109.5
H(61B)-C(61)-H(61C)	109.5
C(58)-C(62)-H(62A)	109.5
C(58)-C(62)-H(62B)	109.5
H(62A)-C(62)-H(62B)	109.5
C(58)-C(62)-H(62C)	109.5
H(62A)-C(62)-H(62C)	109.5
H(62B)-C(62)-H(62C)	109.5
C(60)-C(63)-H(63A)	109.5
C(60)-C(63)-H(63B)	109.5
H(63A)-C(63)-H(63B)	109.5
C(60)-C(63)-H(63C)	109.5
H(63A)-C(63)-H(63C)	109.5
H(63B)-C(63)-H(63C)	109.5
N(8)-C(64)-N(7)	108.7(3)
N(8)-C(64)-H(64)	125.7
N(7)-C(64)-H(64)	125.7
C(66)-C(65)-N(7)	107.6(3)
C(66)-C(65)-H(65)	126.2
N(7)-C(65)-H(65)	126.2
C(65)-C(66)-N(8)	106.6(3)
C(65)-C(66)-H(66)	126.7
N(8)-C(66)-H(66)	126.7
C(72)-C(67)-C(68)	124.2(4)
C(72)-C(67)-N(7)	118.6(4)
C(68)-C(67)-N(7)	117.2(4)
C(69)-C(68)-C(67)	115.8(4)
C(69)-C(68)-C(73)	120.6(5)
C(67)-C(68)-C(73)	123.6(4)
C(70)-C(69)-C(68)	122.9(5)
C(70)-C(69)-H(69)	118.5
C(68)-C(69)-H(69)	118.5
C(69)-C(70)-C(71)	118.5(5)
C(69)-C(70)-C(74)	121.6(6)
C(71)-C(70)-C(74)	119.8(6)
C(70)-C(71)-C(72)	121.8(5)
C(70)-C(71)-H(71)	119.1
C(72)-C(71)-H(71)	119.1
C(67)-C(72)-C(71)	116.8(4)

C(67)-C(72)-C(75)	121.14
C(71)-C(72)-C(75)	122.02
C(68)-C(73)-H(73A)	109.5
C(68)-C(73)-H(73B)	109.5
H(73A)-C(73)-H(73B)	109.5
C(68)-C(73)-H(73C)	109.5
H(73A)-C(73)-H(73C)	109.5
H(73B)-C(73)-H(73C)	109.5
C(70)-C(74)-H(74A)	109.4
C(70)-C(74)-H(74B)	109.4
H(74A)-C(74)-H(74B)	109.7
C(70)-C(74)-H(74C)	109.3
H(74A)-C(74)-H(74C)	109.5
H(74B)-C(74)-H(74C)	109.5
C(72)-C(75)-H(75A)	109.5
C(72)-C(75)-H(75B)	109.5
H(75A)-C(75)-H(75B)	109.5
C(72)-C(75)-H(75C)	109.5
H(75A)-C(75)-H(75C)	109.5
H(75B)-C(75)-H(75C)	109.5
C(81)-C(76)-C(77)	123.9(4)
C(81)-C(76)-N(8)	119.3(4)
C(77)-C(76)-N(8)	116.8(4)
C(78)-C(77)-C(76)	117.1(4)
C(78)-C(77)-C(82)	120.7(4)
C(76)-C(77)-C(82)	122.3(4)
C(79)-C(78)-C(77)	122.0(4)
C(79)-C(78)-H(78)	119
C(77)-C(78)-H(78)	119
C(78)-C(79)-C(80)	119.1(4)
C(78)-C(79)-C(83)	122.1(4)
C(80)-C(79)-C(83)	118.8(4)
C(79)-C(80)-C(81)	121.0(4)
C(79)-C(80)-H(80)	119.5
C(81)-C(80)-H(80)	119.5
C(76)-C(81)-C(80)	116.8(4)
C(76)-C(81)-C(84)	122.3(4)
C(80)-C(81)-C(84)	120.8(4)
C(77)-C(82)-H(82A)	109.5
C(77)-C(82)-H(82B)	109.5
H(82A)-C(82)-H(82B)	109.5
C(77)-C(82)-H(82C)	109.5
H(82A)-C(82)-H(82C)	109.5
H(82B)-C(82)-H(82C)	109.5
C(79)-C(83)-H(83A)	109.5
C(79)-C(83)-H(83B)	109.5
H(83A)-C(83)-H(83B)	109.5
C(79)-C(83)-H(83C)	109.5
H(83A)-C(83)-H(83C)	109.5
H(83B)-C(83)-H(83C)	109.5
C(81)-C(84)-H(84A)	109.5
C(81)-C(84)-H(84B)	109.5
H(84A)-C(84)-H(84B)	109.5
C(81)-C(84)-H(84C)	109.5
H(84A)-C(84)-H(84C)	109.5
H(84B)-C(84)-H(84C)	109.5
C(1)-N(1)-C(2)	108.9(3)
C(1)-N(1)-C(4)	123.0(3)
C(2)-N(1)-C(4)	128.1(3)
C(1)-N(2)-C(3)	108.9(3)
C(1)-N(2)-C(13)	125.1(3)
C(3)-N(2)-C(13)	125.9(3)
C(22)-N(3)-C(23)	108.8(3)
C(22)-N(3)-C(25)	125.9(3)
C(23)-N(3)-C(25)	125.3(3)
C(22)-N(4)-C(24)	108.8(3)
C(22)-N(4)-C(34)	125.4(3)
C(24)-N(4)-C(34)	125.7(3)

C(43)-N(5)-C(44)	109.0(3)
C(43)-N(5)-C(46)	126.1(3)
C(44)-N(5)-C(46)	124.9(3)
C(43)-N(6)-C(45)	109.9(3)
C(43)-N(6)-C(55)	125.2(3)
C(45)-N(6)-C(55)	124.8(3)
C(64)-N(7)-C(65)	108.2(3)
C(64)-N(7)-C(67)	127.0(3)
C(65)-N(7)-C(67)	124.7(3)
C(64)-N(8)-C(66)	108.8(3)
C(64)-N(8)-C(76)	126.8(3)
C(66)-N(8)-C(76)	124.3(3)

Table 48. Anisotropic displacement parameters (A^2 x 10^3) for **IMes.HCl**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	31(2)	41(3)	28(2)	9(2)	15(2)	0(2)
C(2)	39(3)	51(3)	33(3)	4(2)	20(2)	3(2)
C(3)	36(3)	58(3)	24(2)	4(2)	15(2)	7(2)
C(4)	30(2)	36(3)	31(2)	-5(2)	15(2)	-7(2)
C(5)	29(2)	44(3)	34(2)	11(2)	10(2)	8(2)
C(6)	44(3)	38(3)	45(3)	2(2)	20(2)	-7(2)
C(7)	35(3)	47(3)	43(3)	3(2)	13(2)	4(2)
C(8)	33(3)	43(3)	41(3)	5(2)	15(2)	7(2)
C(9)	24(2)	41(3)	31(2)	2(2)	9(2)	4(2)
C(10)	49(3)	42(3)	59(3)	14(2)	23(2)	4(2)
C(11)	36(3)	62(3)	62(3)	2(2)	1(2)	-7(2)
C(12)	46(3)	38(3)	55(3)	12(2)	21(2)	7(2)
C(13)	30(2)	31(3)	24(2)	1(2)	8(2)	-11(2)
C(14)	31(2)	30(3)	25(2)	-3(2)	5(2)	-3(2)
C(15)	27(2)	45(3)	39(2)	-4(2)	10(2)	-6(2)
C(16)	39(3)	38(3)	37(2)	1(2)	18(2)	-9(2)
C(17)	45(3)	34(3)	35(2)	2(2)	10(2)	4(2)
C(18)	29(2)	35(3)	36(2)	-1(2)	12(2)	-6(2)
C(19)	42(3)	47(3)	43(3)	5(2)	11(2)	5(2)
C(20)	45(3)	55(3)	77(3)	10(2)	30(2)	-12(2)
C(21)	39(3)	47(3)	54(3)	14(2)	17(2)	12(2)
C(22)	53(3)	62(3)	17(2)	-2(2)	19(2)	4(2)
C(23)	46(3)	103(4)	31(3)	-3(2)	18(2)	-6(3)
C(24)	55(3)	118(4)	22(3)	9(3)	24(3)	10(3)
C(25)	37(3)	56(3)	23(2)	-3(2)	12(2)	-5(3)
C(26)	42(3)	67(3)	24(2)	7(2)	7(2)	3(3)
C(27)	34(3)	87(4)	31(3)	5(3)	7(2)	1(3)
C(28)	60(4)	79(4)	31(3)	-14(3)	19(3)	-19(3)
C(29)	81(4)	45(3)	47(3)	-11(2)	29(3)	-13(3)
C(30)	57(3)	50(3)	30(3)	-5(2)	20(2)	-5(3)
C(31)	62(3)	83(4)	53(3)	16(3)	27(2)	21(3)
C(32)	69(4)	141(5)	74(4)	-7(3)	29(3)	-48(3)
C(33)	76(3)	65(3)	51(3)	4(2)	25(3)	23(3)
C(34)	36(3)	62(3)	32(3)	5(2)	24(2)	1(3)
C(35)	40(3)	67(4)	47(3)	21(3)	23(2)	12(3)
C(36)	51(3)	61(3)	65(3)	6(3)	35(3)	9(3)
C(37)	43(3)	61(4)	65(3)	-14(3)	28(3)	-2(3)
C(38)	36(3)	81(4)	46(3)	3(3)	23(2)	20(3)
C(39)	37(3)	57(3)	41(3)	3(2)	22(2)	10(3)
C(40)	57(3)	84(4)	80(3)	35(3)	30(3)	9(3)
C(41)	56(3)	90(4)	103(4)	-26(3)	31(3)	6(3)
C(42)	58(3)	62(3)	67(3)	16(3)	27(3)	19(3)
C(43)	29(2)	44(3)	25(2)	6(2)	13(2)	5(2)
C(44)	53(3)	52(3)	18(2)	6(2)	18(2)	3(2)
C(45)	44(3)	53(3)	35(3)	3(2)	24(2)	5(2)
C(46)	28(2)	44(3)	29(2)	2(2)	11(2)	13(2)
C(47)	34(3)	36(3)	38(2)	-4(2)	9(2)	0(2)
C(48)	39(3)	31(3)	43(3)	-2(2)	15(2)	-2(2)
C(49)	35(3)	39(3)	37(2)	4(2)	17(2)	9(2)
C(50)	32(2)	43(3)	37(2)	4(2)	13(2)	1(2)
C(51)	35(3)	36(3)	34(2)	1(2)	15(2)	2(2)
C(52)	38(3)	50(3)	87(3)	-4(2)	22(3)	-8(2)
C(53)	41(3)	51(3)	66(3)	-3(2)	19(2)	7(2)
C(54)	38(3)	50(3)	49(3)	2(2)	15(2)	1(2)
C(55)	39(3)	34(3)	31(2)	0(2)	17(2)	9(2)
C(56)	36(3)	44(3)	39(3)	-3(2)	15(2)	-6(2)
C(57)	45(3)	48(3)	68(3)	11(3)	34(3)	6(3)
C(58)	35(3)	47(3)	62(3)	13(3)	22(3)	6(2)
C(59)	28(3)	56(3)	48(3)	7(3)	15(2)	1(2)

C(60)	41(3)	39(3)	39(3)	5(2)	24(2)	5(2)
C(61)	52(3)	54(3)	55(3)	5(2)	18(2)	-4(2)
C(62)	43(3)	72(4)	131(4)	38(3)	22(3)	25(3)
C(63)	39(3)	52(3)	57(3)	-2(2)	12(2)	-8(2)
C(64)	37(3)	53(3)	20(2)	0(2)	6(2)	-1(2)
C(65)	40(3)	83(3)	20(2)	13(2)	12(2)	12(3)
C(66)	47(3)	87(4)	25(3)	9(2)	19(2)	10(3)
C(67)	39(3)	57(3)	28(2)	5(2)	16(2)	1(3)
C(68)	45(3)	79(4)	22(2)	3(2)	17(2)	-1(3)
C(69)	35(3)	138(5)	26(3)	18(3)	13(2)	6(4)
C(70)	62(4)	144(6)	32(3)	30(3)	23(3)	59(4)
C(71)	83(4)	84(4)	43(3)	21(3)	25(3)	47(4)
C(72)	45(3)	55(3)	33(3)	8(2)	11(2)	10(3)
C(73)	66(3)	91(4)	48(3)	-7(3)	21(3)	-27(3)
C(74)	90(4)	233(6)	85(4)	63(4)	57(3)	109(4)
C(75)	81	51	47	2	20	-3
C(76)	29(3)	56(3)	23(2)	0(2)	12(2)	2(2)
C(77)	43(3)	49(3)	37(3)	-2(2)	20(2)	-1(3)
C(78)	46(3)	52(3)	53(3)	17(2)	25(2)	5(3)
C(79)	39(3)	65(4)	62(3)	29(3)	26(3)	4(3)
C(80)	36(3)	69(3)	32(2)	27(2)	9(2)	-1(3)
C(81)	42(3)	43(3)	25(2)	-1(2)	14(2)	-5(2)
C(82)	62(3)	60(3)	61(3)	-4(2)	19(3)	-3(3)
C(83)	45(3)	84(4)	83(3)	42(3)	13(3)	13(3)
C(84)	58(3)	55(3)	51(3)	-1(2)	22(2)	-7(2)
N(1)	36(2)	47(2)	20(2)	6(2)	12(2)	-1(2)
N(2)	33(2)	35(2)	27(2)	2(2)	13(2)	0(2)
N(3)	49(2)	61(2)	29(2)	5(2)	25(2)	1(2)
N(4)	45(2)	65(3)	23(2)	10(2)	19(2)	4(2)
N(5)	29(2)	42(2)	23(2)	6(2)	8(2)	1(2)
N(6)	29(2)	42(2)	29(2)	5(2)	12(2)	6(2)
N(7)	32(2)	51(2)	28(2)	-3(2)	18(2)	0(2)
N(8)	35(2)	56(2)	30(2)	0(2)	18(2)	5(2)
Cl(1)	50(1)	60(1)	34(1)	7(1)	21(1)	4(1)
Cl(2)	45(1)	61(1)	33(1)	10(1)	20(1)	10(1)
Cl(3)	59(1)	61(1)	34(1)	10(1)	21(1)	5(1)
Cl(4)	44(1)	46(1)	33(1)	6(1)	19(1)	5(1)

X-ray Data for Complex $[VCl_2(CH_3CN)_4]_2[HIMes]$

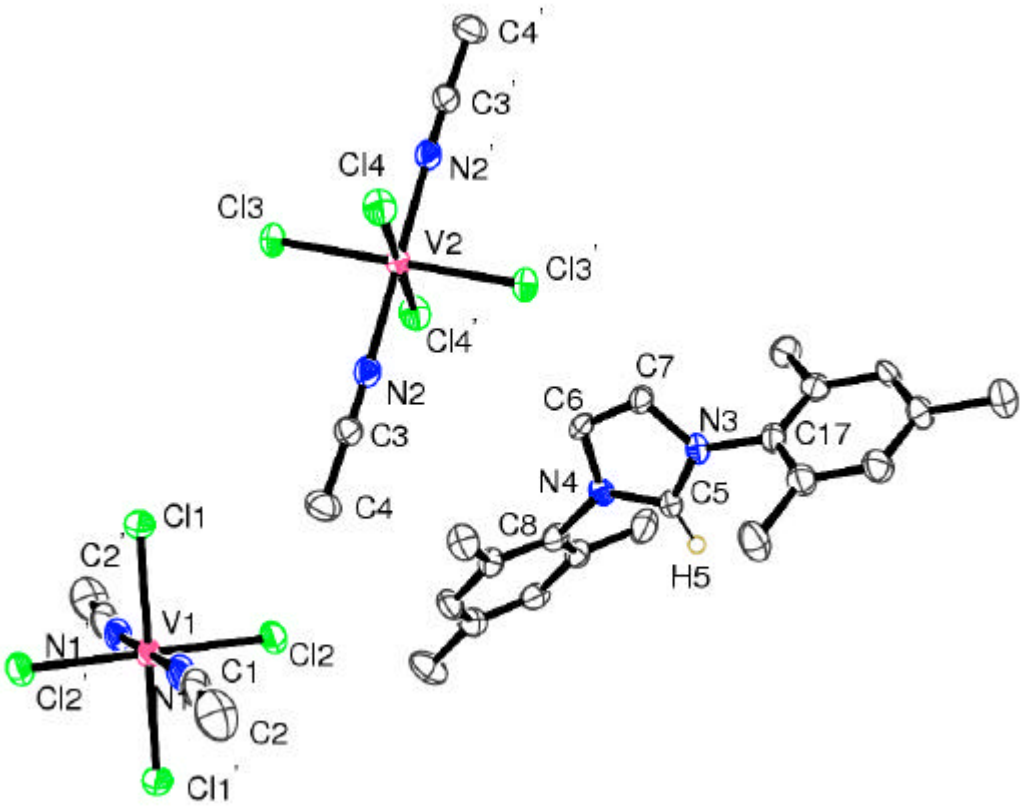

Table 49. Crystal data and structure refinement for $[VCl_2(CH_3CN)_4]_2[HIMes]$.

Empirical formula	C25 H31 Cl4 N4 V
Formula weight	580.28
Temperature	180 K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 8.5259(15) A alpha = 63.734(16) deg. b = 13.090(3) A beta = 79.869(13) deg. c = 14.3003(19) A gamma = 81.140(15) deg.
Volume	1403.6(5) A^3
Z, Calculated density	2, 1.373 Mg/m^3
Absorption coefficient	0.755 mm^-1
F(000)	600
Crystal size	0.15 x 0.09 x 0.03 mm
Theta range for data collection	2.74 to 26.31 deg.
Limiting indices	-10<=h<=10, -16<=k<=16, -14<=l<=17
Reflections collected / unique	10991 / 5722 [R(int) = 0.0691]
Completeness to theta = 26.31	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.978 and 0.8617
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5722 / 0 / 318
Goodness-of-fit on F^2	0.824
Final R indices [I>2sigma(I)]	R1 = 0.043, wR2 = 0.0713
R indices (all data)	R1 = 0.1308, wR2 = 0.0893
Largest diff. peak and hole	0.358 and -0.409 e.A^-3

Table 50. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for $[VCl_2(CH_3CN)_4]_2[HIMes]$.

	x	y	z	U(eq)
C(1)	-2933(6)	6212(3)	-1365(3)	37(1)
C(2)	-4376(5)	6676(3)	-1877(3)	57(1)
C(3)	1799(5)	8872(3)	-3541(3)	29(1)
C(4)	380(4)	8332(3)	-2892(3)	39(1)
C(5)	1971(4)	13056(3)	-2078(3)	28(1)
C(6)	3360(4)	11982(3)	-2811(3)	31(1)
C(7)	3085(4)	13023(3)	-3555(3)	32(1)
C(8)	2687(4)	11071(3)	-843(3)	27(1)
C(9)	2097(4)	10049(3)	-658(3)	26(1)
C(10)	2154(4)	9184(3)	342(3)	35(1)
C(11)	2721(4)	9300(3)	1122(3)	31(1)
C(12)	3295(4)	10319(3)	901(3)	31(1)
C(13)	3307(4)	11222(3)	-87(3)	27(1)
C(14)	3984(5)	12302(3)	-277(3)	41(1)
C(15)	1472(5)	9877(3)	-1485(3)	40(1)
C(16)	2709(5)	8321(3)	2212(3)	48(1)
C(17)	1747(5)	14893(3)	-3667(3)	26(1)
C(18)	157(5)	15227(3)	-3816(3)	32(1)
C(19)	-240(5)	16389(3)	-4391(3)	36(1)
C(20)	885(5)	17169(3)	-4799(3)	29(1)
C(21)	2455(4)	16805(3)	-4612(3)	28(1)
C(22)	2910(4)	15661(3)	-4033(3)	27(1)
C(23)	-1103(4)	14377(3)	-3355(3)	45(1)
C(24)	391(4)	18416(3)	-5435(3)	38(1)
C(25)	4578(4)	15271(3)	-3751(3)	35(1)
N(1)	-1866(4)	5823(2)	-933(2)	36(1)
N(2)	2889(4)	9287(2)	-4063(2)	30(1)
N(3)	2226(3)	13692(2)	-3102(2)	25(1)
N(4)	2654(3)	12011(2)	-1879(2)	24(1)
Cl(1)	1846(1)	5341(1)	-1488(1)	37(1)
Cl(2)	501(1)	6731(1)	-21(1)	38(1)
Cl(3)	6098(1)	8169(1)	-4726(1)	34(1)
Cl(4)	4032(1)	10203(1)	-6520(1)	35(1)
V(1)	0	5000	0	29(1)
V(2)	5000	10000	-5000	26(1)

Table 51. Bond lengths [A] and angles [deg] for $[VCl_2(CH_3CN)_4]_2[HIMes]$.

C(1)-N(1)	1.116(4)
C(1)-C(2)	1.454(5)
C(2)-H(2A)	0.96
C(2)-H(2B)	0.96
C(2)-H(2C)	0.96
C(3)-N(2)	1.126(4)
C(3)-C(4)	1.454(5)
C(4)-H(4A)	0.96
C(4)-H(4B)	0.96
C(4)-H(4C)	0.96
C(5)-N(3)	1.323(4)
C(5)-N(4)	1.326(4)
C(5)-H(5)	0.93
C(6)-C(7)	1.324(4)
C(6)-N(4)	1.377(4)
C(6)-H(6)	0.93
C(7)-N(3)	1.365(4)
C(7)-H(7)	0.93
C(8)-C(13)	1.382(5)
C(8)-C(9)	1.400(5)
C(8)-N(4)	1.449(4)
C(9)-C(10)	1.380(4)
C(9)-C(15)	1.492(4)
C(10)-C(11)	1.366(5)
C(10)-H(10)	0.93
C(11)-C(12)	1.376(5)
C(11)-C(16)	1.517(4)
C(12)-C(13)	1.383(4)
C(12)-H(12)	0.93
C(13)-C(14)	1.503(5)
C(14)-H(14A)	0.96
C(14)-H(14B)	0.96
C(14)-H(14C)	0.96
C(15)-H(15A)	0.96
C(15)-H(15B)	0.96
C(15)-H(15C)	0.96
C(16)-H(16A)	0.96
C(16)-H(16B)	0.96
C(16)-H(16C)	0.96
C(17)-C(18)	1.382(5)
C(17)-C(22)	1.388(5)
C(17)-N(3)	1.444(4)
C(18)-C(19)	1.391(4)
C(18)-C(23)	1.515(5)
C(19)-C(20)	1.372(5)
C(19)-H(19)	0.93
C(20)-C(21)	1.381(5)
C(20)-C(24)	1.509(4)
C(21)-C(22)	1.385(4)
C(21)-H(21)	0.93
C(22)-C(25)	1.497(4)
C(23)-H(23A)	0.96
C(23)-H(23B)	0.96
C(23)-H(23C)	0.96
C(24)-H(24A)	0.96
C(24)-H(24B)	0.96
C(24)-H(24C)	0.96
C(25)-H(25A)	0.96
C(25)-H(25B)	0.96
C(25)-H(25C)	0.96
N(1)-V(1)	2.102(3)
N(2)-V(2)	2.114(3)
Cl(1)-V(1)	2.3238(10)
Cl(2)-V(1)	2.3556(10)
Cl(3)-V(2)	2.3199(10)

Cl(4)-V(2)	2.3510(9)
V(1)-N(1)#1	2.102(3)
V(1)-Cl(1)#1	2.3238(10)
V(1)-Cl(2)#1	2.3556(10)
V(2)-N(2)#2	2.114(3)
V(2)-Cl(3)#2	2.3199(10)
V(2)-Cl(4)#2	2.3510(9)

N(1)-C(1)-C(2)	176.8(4)
C(1)-C(2)-H(2A)	109.5
C(1)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
C(1)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
N(2)-C(3)-C(4)	178.4(4)
C(3)-C(4)-H(4A)	109.5
C(3)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(3)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
N(3)-C(5)-N(4)	108.3(3)
N(3)-C(5)-H(5)	125.9
N(4)-C(5)-H(5)	125.9
C(7)-C(6)-N(4)	106.2(3)
C(7)-C(6)-H(6)	126.9
N(4)-C(6)-H(6)	126.9
C(6)-C(7)-N(3)	108.7(3)
C(6)-C(7)-H(7)	125.6
N(3)-C(7)-H(7)	125.6
C(13)-C(8)-C(9)	123.1(3)
C(13)-C(8)-N(4)	118.6(3)
C(9)-C(8)-N(4)	118.3(3)
C(10)-C(9)-C(8)	115.9(3)
C(10)-C(9)-C(15)	121.1(3)
C(8)-C(9)-C(15)	123.0(3)
C(11)-C(10)-C(9)	123.2(4)
C(11)-C(10)-H(10)	118.4
C(9)-C(10)-H(10)	118.4
C(10)-C(11)-C(12)	118.7(3)
C(10)-C(11)-C(16)	120.4(4)
C(12)-C(11)-C(16)	120.9(3)
C(11)-C(12)-C(13)	121.7(3)
C(11)-C(12)-H(12)	119.2
C(13)-C(12)-H(12)	119.2
C(8)-C(13)-C(12)	117.4(3)
C(8)-C(13)-C(14)	123.9(3)
C(12)-C(13)-C(14)	118.7(3)
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(9)-C(15)-H(15A)	109.5
C(9)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(9)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(11)-C(16)-H(16A)	109.5
C(11)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(11)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(18)-C(17)-C(22)	123.0(3)

C(18)-C(17)-N(3)	118.8(3)
C(22)-C(17)-N(3)	118.2(3)
C(17)-C(18)-C(19)	116.7(4)
C(17)-C(18)-C(23)	121.8(3)
C(19)-C(18)-C(23)	121.5(3)
C(20)-C(19)-C(18)	122.0(4)
C(20)-C(19)-H(19)	119
C(18)-C(19)-H(19)	119
C(19)-C(20)-C(21)	119.5(3)
C(19)-C(20)-C(24)	119.7(3)
C(21)-C(20)-C(24)	120.8(3)
C(20)-C(21)-C(22)	120.8(3)
C(20)-C(21)-H(21)	119.6
C(22)-C(21)-H(21)	119.6
C(21)-C(22)-C(17)	117.8(3)
C(21)-C(22)-C(25)	121.2(3)
C(17)-C(22)-C(25)	120.9(3)
C(18)-C(23)-H(23A)	109.5
C(18)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(18)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(20)-C(24)-H(24A)	109.5
C(20)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(20)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(22)-C(25)-H(25A)	109.5
C(22)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(22)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(1)-N(1)-V(1)	174.7(3)
C(3)-N(2)-V(2)	177.4(3)
C(5)-N(3)-C(7)	108.0(3)
C(5)-N(3)-C(17)	127.5(3)
C(7)-N(3)-C(17)	124.5(3)
C(5)-N(4)-C(6)	108.8(3)
C(5)-N(4)-C(8)	125.2(3)
C(6)-N(4)-C(8)	126.0(3)
N(1)#1-V(1)-N(1)	180.00(18)
N(1)#1-V(1)-Cl(1)#1	91.00(9)
N(1)-V(1)-Cl(1)#1	89.00(9)
N(1)#1-V(1)-Cl(1)	89.00(9)
N(1)-V(1)-Cl(1)	91.00(9)
Cl(1)#1-V(1)-Cl(1)	180
N(1)#1-V(1)-Cl(2)	88.53(9)
N(1)-V(1)-Cl(2)	91.47(9)
Cl(1)#1-V(1)-Cl(2)	90.17(4)
Cl(1)-V(1)-Cl(2)	89.83(4)
N(1)#1-V(1)-Cl(2)#1	91.47(9)
N(1)-V(1)-Cl(2)#1	88.53(9)
Cl(1)#1-V(1)-Cl(2)#1	89.83(4)
Cl(1)-V(1)-Cl(2)#1	90.17(4)
Cl(2)-V(1)-Cl(2)#1	180.00(5)
N(2)-V(2)-N(2)#2	180.0000(10)
N(2)-V(2)-Cl(3)#2	91.41(8)
N(2)#2-V(2)-Cl(3)#2	88.59(8)
N(2)-V(2)-Cl(3)	88.59(8)
N(2)#2-V(2)-Cl(3)	91.41(8)
Cl(3)#2-V(2)-Cl(3)	180
N(2)-V(2)-Cl(4)#2	89.07(8)
N(2)#2-V(2)-Cl(4)#2	90.93(8)
Cl(3)#2-V(2)-Cl(4)#2	89.81(4)
Cl(3)-V(2)-Cl(4)#2	90.19(4)

N(2)-V(2)-Cl(4)	90.93(8)
N(2)#2-V(2)-Cl(4)	89.07(8)
Cl(3)#2-V(2)-Cl(4)	90.19(4)
Cl(3)-V(2)-Cl(4)	89.81(4)
Cl(4)#2-V(2)-Cl(4)	180

Table 53. Anisotropic displacement parameters (A^2 x 10^3) for $[VCl_2(CH_3CN)_4]_2$[HIMes]. The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	59(3)	19(2)	25(2)	-2(2)	-9(2)	0(2)
C(2)	71(4)	48(3)	46(3)	-9(2)	-22(3)	-4(3)
C(3)	36(3)	22(2)	26(2)	-8(2)	-7(2)	1(2)
C(4)	41(3)	38(3)	30(2)	-7(2)	3(2)	-9(2)
C(5)	30(2)	19(2)	26(2)	-7(2)	2(2)	0(2)
C(6)	38(3)	22(2)	29(2)	-14(2)	4(2)	4(2)
C(7)	45(3)	20(2)	23(2)	-6(2)	-1(2)	5(2)
C(8)	25(2)	25(2)	25(2)	-8(2)	-7(2)	8(2)
C(9)	27(2)	27(2)	27(2)	-15(2)	-6(2)	1(2)
C(10)	36(3)	21(2)	36(2)	-2(2)	-2(2)	-3(2)
C(11)	30(2)	32(2)	24(2)	-7(2)	-5(2)	1(2)
C(12)	32(2)	34(3)	26(2)	-15(2)	-2(2)	3(2)
C(13)	26(2)	22(2)	32(2)	-11(2)	-7(2)	2(2)
C(14)	52(3)	33(2)	40(3)	-20(2)	-7(2)	6(2)
C(15)	45(3)	33(2)	38(3)	-12(2)	-6(2)	-5(2)
C(16)	55(3)	40(3)	32(2)	1(2)	-4(2)	-9(2)
C(17)	34(3)	20(2)	24(2)	-8(2)	-6(2)	3(2)
C(18)	30(3)	28(2)	35(2)	-11(2)	-5(2)	-1(2)
C(19)	31(2)	29(2)	37(2)	-5(2)	-8(2)	3(2)
C(20)	32(3)	21(2)	27(2)	-3(2)	-9(2)	-1(2)
C(21)	31(2)	17(2)	28(2)	-4(2)	1(2)	-7(2)
C(22)	29(2)	29(2)	22(2)	-10(2)	-2(2)	-1(2)
C(23)	36(3)	30(2)	59(3)	-6(2)	-14(2)	-5(2)
C(24)	38(3)	26(2)	46(3)	-10(2)	-11(2)	-3(2)
C(25)	27(2)	33(2)	35(2)	-9(2)	-6(2)	3(2)
N(1)	53(2)	20(2)	25(2)	-3(2)	-4(2)	1(2)
N(2)	35(2)	21(2)	27(2)	-7(2)	-1(2)	1(2)
N(3)	29(2)	18(2)	28(2)	-9(2)	-5(2)	0(2)
N(4)	29(2)	21(2)	18(2)	-4(1)	-6(2)	-1(2)
Cl(1)	49(1)	30(1)	28(1)	-12(1)	8(1)	-6(1)
Cl(2)	53(1)	25(1)	34(1)	-12(1)	5(1)	-11(1)
Cl(3)	37(1)	21(1)	39(1)	-11(1)	-4(1)	3(1)
Cl(4)	45(1)	32(1)	30(1)	-12(1)	-11(1)	-3(1)
V(1)	39(1)	22(1)	23(1)	-7(1)	1(1)	-5(1)
V(2)	28(1)	20(1)	26(1)	-8(1)	-1(1)	-2(1)