Single Crystal X-ray Diffraction Report for IMesN^Imine.HCl (3a)

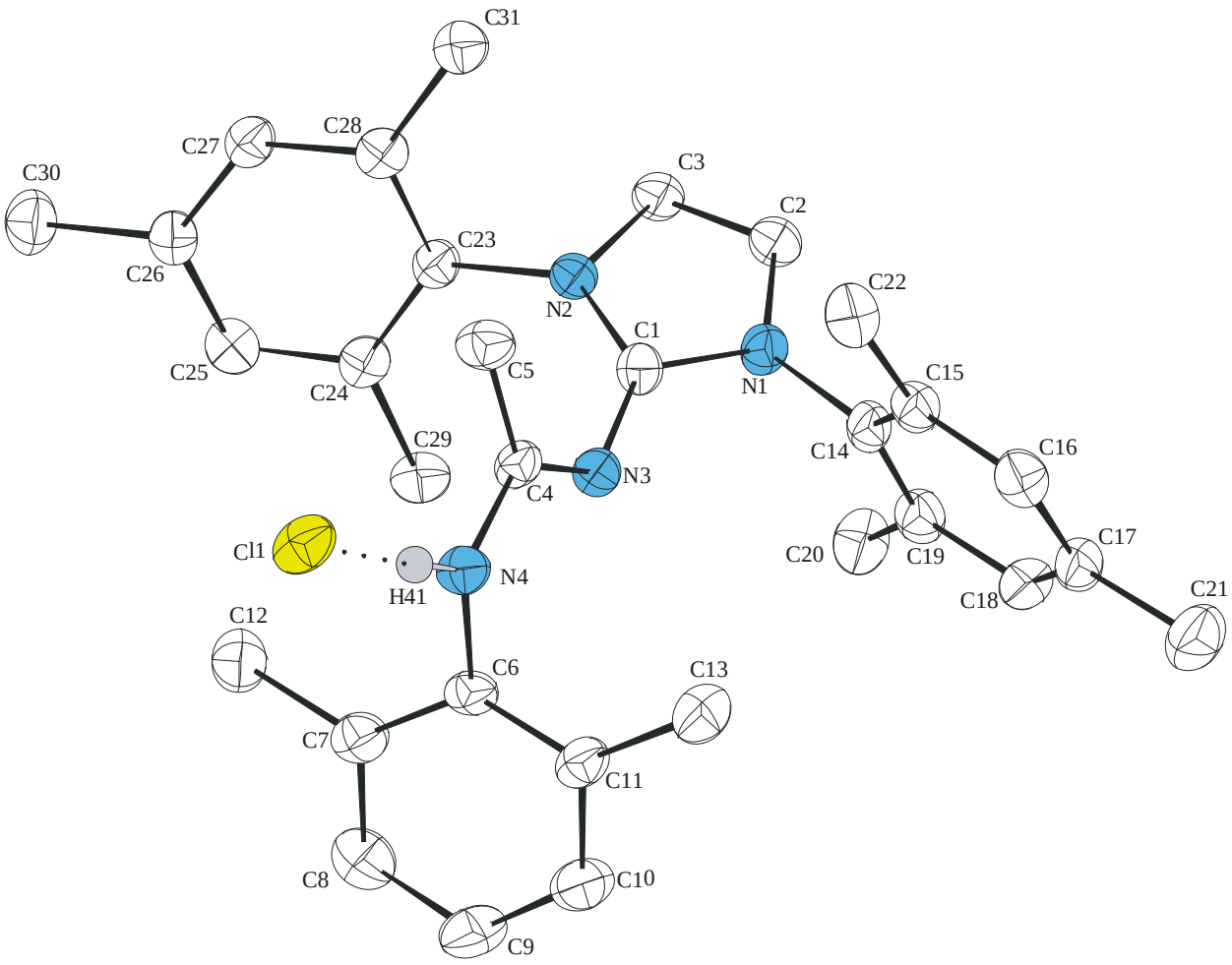

Table 1. Crystal data and structure refinement for IMesN^Imine.HCl (3a)

Identification code	k09163a	
Empirical formula	C33 H41 Cl5 N4	
Formula weight	670.95	
Temperature	150(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 15.8893(8) Å	α= 90°.
	b = 15.8157(5) Å	β= 90.3420(18)°.
	c = 13.8555(9) Å	γ = 90°.
Volume	3481.8(3) $Å^3$	
Z	4	
Density (calculated)	1.280 Mg/m^3	
Absorption coefficient	0.445 mm^{-1}	
F(000)	1408	
Crystal size	0.32 x 0.12 x 0.12 mm^3	
Theta range for data collection	2.56 to 25.00°.	
Index ranges	-18<=h<=18, -18<=k<=17, -16<=l<=16	
Reflections collected	19493	
Independent reflections	6120 [R(int) = 0.0743]	
Completeness to theta = 25.00°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.989 and 0.780	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6120 / 0 / 392	
Goodness-of-fit on F^2	1.018	
Final R indices [I>2sigma(I)]	R1 = 0.0590, wR2 = 0.1379	
R indices (all data)	R1 = 0.1251, wR2 = 0.1736	
Largest diff. peak and hole	0.493 and -0.362 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for k09163a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	3757(2)	5610(2)	1745(2)	30(1)
N(2)	4587(2)	4948(2)	2740(2)	26(1)
N(3)	3198(2)	4354(2)	2417(2)	27(1)
N(4)	2681(2)	3024(2)	2603(2)	31(1)
C(1)	3828(2)	4904(2)	2290(2)	27(1)
C(2)	4486(2)	6094(2)	1852(3)	32(1)
C(3)	5001(2)	5686(2)	2460(3)	30(1)
C(4)	3290(2)	3537(2)	2305(3)	27(1)
C(5)	4031(2)	3111(2)	1840(3)	34(1)
C(6)	1954(2)	3281(2)	3142(3)	30(1)
C(7)	1928(2)	3022(2)	4109(3)	34(1)
C(8)	1210(3)	3234(2)	4634(3)	46(1)
C(9)	554(3)	3668(2)	4211(3)	51(1)
C(10)	598(3)	3917(2)	3248(3)	48(1)
C(11)	1311(2)	3724(2)	2697(3)	33(1)
C(12)	2629(3)	2525(2)	4570(3)	45(1)
C(13)	1338(3)	3982(2)	1646(3)	45(1)
C(14)	3037(2)	5834(2)	1152(3)	31(1)
C(15)	2959(2)	5473(2)	237(3)	32(1)
C(16)	2287(2)	5738(2)	-338(3)	36(1)
C(17)	1717(2)	6343(2)	-24(3)	37(1)
C(18)	1810(2)	6660(2)	903(3)	38(1)
C(19)	2464(2)	6412(2)	1511(3)	34(1)
C(20)	2532(3)	6742(2)	2526(3)	44(1)
C(21)	1010(3)	6643(3)	-668(3)	50(1)
C(22)	3560(3)	4797(2)	-107(3)	41(1)
C(23)	4915(2)	4342(2)	3433(3)	27(1)
C(24)	4483(2)	4219(2)	4297(3)	28(1)
C(25)	4819(2)	3623(2)	4939(3)	32(1)
C(26)	5556(2)	3181(2)	4746(3)	29(1)
C(27)	5976(2)	3350(2)	3892(3)	30(1)

C(28)	5664(2)	3921(2)	3211(2)	28(1)
C(29)	3709(2)	4700(2)	4572(3)	34(1)
C(30)	5914(3)	2554(2)	5460(3)	43(1)
C(31)	6135(2)	4076(2)	2294(3)	32(1)
Cl(1)	2889(1)	1132(1)	2097(1)	41(1)
Cl(2)	1684(1)	5994(1)	6832(1)	62(1)
Cl(3)	1734(1)	5846(1)	4747(1)	85(1)
C(32)	1655(3)	5301(3)	5847(3)	58(1)
Cl(4)	-42(1)	3739(1)	7013(1)	70(1)
Cl(5)	594(1)	4258(1)	8891(1)	80(1)
C(33)	711(3)	3557(3)	7920(3)	55(1)

Table 3. Bond lengths [Å] and angles [°] for k09163a.

N(1)-C(1)	1.354(4)	C(13)-H(13B)	0.9800	C(29)-H(29C)	0.9800
N(1)-C(2)	1.396(4)	C(13)-H(13C)	0.9800	C(30)-H(30A)	0.9800
N(1)-C(14)	1.448(4)	C(14)-C(19)	1.385(5)	C(30)-H(30B)	0.9800
N(2)-C(1)	1.356(4)	C(14)-C(15)	1.396(5)	C(30)-H(30C)	0.9800
N(2)-C(3)	1.397(4)	C(15)-C(16)	1.392(5)	C(31)-H(31A)	0.9800
N(2)-C(23)	1.450(4)	C(15)-C(22)	1.512(5)	C(31)-H(31B)	0.9800
N(3)-C(4)	1.311(4)	C(16)-C(17)	1.389(5)	C(31)-H(31C)	0.9800
N(3)-C(1)	1.338(4)	C(16)-H(16A)	0.9500	Cl(2)-C(32)	1.752(4)
N(4)-C(4)	1.330(4)	C(17)-C(18)	1.386(5)	Cl(3)-C(32)	1.756(4)
N(4)-C(6)	1.438(4)	C(17)-C(21)	1.507(5)	C(32)-H(32A)	0.9900
N(4)-H(4N)	0.86(3)	C(18)-C(19)	1.389(5)	C(32)-H(32B)	0.9900
C(2)-C(3)	1.336(5)	C(18)-H(18A)	0.9500	Cl(4)-C(33)	1.754(4)
C(2)-H(2A)	0.9500	C(19)-C(20)	1.503(5)	Cl(5)-C(33)	1.755(4)
C(3)-H(3A)	0.9500	C(20)-H(20A)	0.9800	C(33)-H(33A)	0.9900
C(4)-C(5)	1.504(5)	C(20)-H(20B)	0.9800	C(33)-H(33B)	0.9900
C(5)-H(5A)	0.9800	C(20)-H(20C)	0.9800		
C(5)-H(5B)	0.9800	C(21)-H(21A)	0.9800		
C(5)-H(5C)	0.9800	C(21)-H(21B)	0.9800		
C(6)-C(11)	1.382(5)	C(21)-H(21C)	0.9800		
C(6)-C(7)	1.401(5)	C(22)-H(22A)	0.9800		
C(7)-C(8)	1.397(5)	C(22)-H(22B)	0.9800		
C(7)-C(12)	1.503(5)	C(22)-H(22C)	0.9800		
C(8)-C(9)	1.377(6)	C(23)-C(24)	1.397(5)		
C(8)-H(8A)	0.9500	C(23)-C(28)	1.400(5)		
C(9)-C(10)	1.394(6)	C(24)-C(25)	1.399(5)		
C(9)-H(9A)	0.9500	C(24)-C(29)	1.498(5)		
C(10)-C(11)	1.403(5)	C(25)-C(26)	1.391(5)		
C(10)-H(10A)	0.9500	C(25)-H(25A)	0.9500		
C(11)-C(13)	1.512(5)	C(26)-C(27)	1.388(5)		
C(12)-H(12A)	0.9800	C(26)-C(30)	1.509(5)		
C(12)-H(12B)	0.9800	C(27)-C(28)	1.395(5)		
C(12)-H(12C)	0.9800	C(27)-H(27A)	0.9500		
C(13)-H(13A)	0.9800	C(28)-C(31)	1.498(5)		

C(1)-N(1)-C(2)	109.0(3)	C(9)-C(8)-H(8A)	119.5
C(1)-N(1)-C(14)	125.6(3)	C(7)-C(8)-H(8A)	119.5
C(2)-N(1)-C(14)	125.4(3)	C(8)-C(9)-C(10)	120.4(4)
C(1)-N(2)-C(3)	109.5(3)	C(8)-C(9)-H(9A)	119.8
C(1)-N(2)-C(23)	125.8(3)	C(10)-C(9)-H(9A)	119.8
C(3)-N(2)-C(23)	124.6(3)	C(9)-C(10)-C(11)	120.4(4)
C(4)-N(3)-C(1)	122.7(3)	C(9)-C(10)-H(10A)	119.8
C(4)-N(4)-C(6)	125.3(3)	C(11)-C(10)-H(10A)	119.8
C(4)-N(4)-H(4N)	116(2)	C(6)-C(11)-C(10)	117.7(4)
C(6)-N(4)-H(4N)	118(2)	C(6)-C(11)-C(13)	122.7(3)
N(3)-C(1)-N(1)	123.3(3)	C(10)-C(11)-C(13)	119.6(3)
N(3)-C(1)-N(2)	129.6(3)	C(7)-C(12)-H(12A)	109.5
N(1)-C(1)-N(2)	106.6(3)	C(7)-C(12)-H(12B)	109.5
C(3)-C(2)-N(1)	107.9(3)	H(12A)-C(12)-H(12B)	109.5
C(3)-C(2)-H(2A)	126.0	C(7)-C(12)-H(12C)	109.5
N(1)-C(2)-H(2A)	126.0	H(12A)-C(12)-H(12C)	109.5
C(2)-C(3)-N(2)	106.9(3)	H(12B)-C(12)-H(12C)	109.5
C(2)-C(3)-H(3A)	126.5	C(11)-C(13)-H(13A)	109.5
N(2)-C(3)-H(3A)	126.5	C(11)-C(13)-H(13B)	109.5
N(3)-C(4)-N(4)	118.8(3)	H(13A)-C(13)-H(13B)	109.5
N(3)-C(4)-C(5)	125.5(3)	C(11)-C(13)-H(13C)	109.5
N(4)-C(4)-C(5)	115.7(3)	H(13A)-C(13)-H(13C)	109.5
C(4)-C(5)-H(5A)	109.5	H(13B)-C(13)-H(13C)	109.5
C(4)-C(5)-H(5B)	109.5	C(19)-C(14)-C(15)	122.7(3)
H(5A)-C(5)-H(5B)	109.5	C(19)-C(14)-N(1)	118.5(3)
C(4)-C(5)-H(5C)	109.5	C(15)-C(14)-N(1)	118.7(3)
H(5A)-C(5)-H(5C)	109.5	C(16)-C(15)-C(14)	117.4(3)
H(5B)-C(5)-H(5C)	109.5	C(16)-C(15)-C(22)	121.1(3)
C(11)-C(6)-C(7)	123.3(3)	C(14)-C(15)-C(22)	121.5(3)
C(11)-C(6)-N(4)	120.4(3)	C(17)-C(16)-C(15)	121.8(3)
C(7)-C(6)-N(4)	116.2(3)	C(17)-C(16)-H(16A)	119.1
C(8)-C(7)-C(6)	117.2(3)	C(15)-C(16)-H(16A)	119.1
C(8)-C(7)-C(12)	120.5(4)	C(18)-C(17)-C(16)	118.3(3)
C(6)-C(7)-C(12)	122.3(3)	C(18)-C(17)-C(21)	120.7(4)
C(9)-C(8)-C(7)	121.0(4)	C(16)-C(17)-C(21)	121.1(4)
C(17)-C(18)-C(19)	122.4(4)	C(25)-C(26)-C(30)	121.3(3)

C(17)-C(18)-H(18A)	118.8	C(26)-C(27)-C(28)	122.0(3)
C(19)-C(18)-H(18A)	118.8	C(26)-C(27)-H(27A)	119.0
C(14)-C(19)-C(18)	117.4(3)	C(28)-C(27)-H(27A)	119.0
C(14)-C(19)-C(20)	121.3(3)	C(27)-C(28)-C(23)	117.3(3)
C(18)-C(19)-C(20)	121.3(3)	C(27)-C(28)-C(31)	120.2(3)
C(19)-C(20)-H(20A)	109.5	C(23)-C(28)-C(31)	122.5(3)
C(19)-C(20)-H(20B)	109.5	C(24)-C(29)-H(29A)	109.5
H(20A)-C(20)-H(20B)	109.5	C(24)-C(29)-H(29B)	109.5
C(19)-C(20)-H(20C)	109.5	H(29A)-C(29)-H(29B)	109.5
H(20A)-C(20)-H(20C)	109.5	C(24)-C(29)-H(29C)	109.5
H(20B)-C(20)-H(20C)	109.5	H(29A)-C(29)-H(29C)	109.5
C(17)-C(21)-H(21A)	109.5	H(29B)-C(29)-H(29C)	109.5
C(17)-C(21)-H(21B)	109.5	C(26)-C(30)-H(30A)	109.5
H(21A)-C(21)-H(21B)	109.5	C(26)-C(30)-H(30B)	109.5
C(17)-C(21)-H(21C)	109.5	H(30A)-C(30)-H(30B)	109.5
H(21A)-C(21)-H(21C)	109.5	C(26)-C(30)-H(30C)	109.5
H(21B)-C(21)-H(21C)	109.5	H(30A)-C(30)-H(30C)	109.5
C(15)-C(22)-H(22A)	109.5	H(30B)-C(30)-H(30C)	109.5
C(15)-C(22)-H(22B)	109.5	C(28)-C(31)-H(31A)	109.5
H(22A)-C(22)-H(22B)	109.5	C(28)-C(31)-H(31B)	109.5
C(15)-C(22)-H(22C)	109.5	H(31A)-C(31)-H(31B)	109.5
H(22A)-C(22)-H(22C)	109.5	C(28)-C(31)-H(31C)	109.5
H(22B)-C(22)-H(22C)	109.5	H(31A)-C(31)-H(31C)	109.5
C(24)-C(23)-C(28)	123.0(3)	H(31B)-C(31)-H(31C)	109.5
C(24)-C(23)-N(2)	118.9(3)	Cl(2)-C(32)-Cl(3)	111.6(2)
C(28)-C(23)-N(2)	118.1(3)	Cl(2)-C(32)-H(32A)	109.3
C(23)-C(24)-C(25)	116.8(3)	Cl(3)-C(32)-H(32A)	109.3
C(23)-C(24)-C(29)	123.8(3)	Cl(2)-C(32)-H(32B)	109.3
C(25)-C(24)-C(29)	119.4(3)	Cl(3)-C(32)-H(32B)	109.3
C(26)-C(25)-C(24)	122.3(3)	H(32A)-C(32)-H(32B)	108.0
C(26)-C(25)-H(25A)	118.8	Cl(4)-C(33)-Cl(5)	111.7(2)
C(24)-C(25)-H(25A)	118.8	Cl(4)-C(33)-H(33A)	109.3
C(27)-C(26)-C(25)	118.5(3)	Cl(5)-C(33)-H(33A)	109.3
C(27)-C(26)-C(30)	120.2(3)	Cl(4)-C(33)-H(33B)	109.3
Cl(5)-C(33)-H(33B)	109.3	H(33A)-C(33)-H(33B)	107.9

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for k09163a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	27(2)	28(2)	35(2)	4(1)	-6(1)	-3(1)
N(2)	24(2)	23(1)	32(2)	2(1)	-1(1)	-3(1)
N(3)	26(2)	22(2)	35(2)	1(1)	-4(1)	-3(1)
N(4)	28(2)	22(2)	42(2)	-2(1)	3(2)	0(1)
C(1)	30(2)	24(2)	27(2)	0(2)	-1(2)	0(2)
C(2)	29(2)	27(2)	38(2)	2(2)	-1(2)	-6(2)
C(3)	27(2)	28(2)	35(2)	2(2)	-1(2)	-4(2)
C(4)	23(2)	25(2)	33(2)	0(2)	-5(2)	-1(2)
C(5)	28(2)	31(2)	44(2)	-4(2)	2(2)	-3(2)
C(6)	24(2)	23(2)	43(3)	-1(2)	3(2)	-4(2)
C(7)	29(2)	26(2)	49(3)	0(2)	1(2)	-3(2)
C(8)	49(3)	49(2)	40(3)	1(2)	8(2)	-3(2)
C(9)	34(3)	55(3)	64(3)	2(2)	11(2)	13(2)
C(10)	29(3)	43(2)	71(3)	7(2)	3(2)	2(2)
C(11)	26(2)	27(2)	47(3)	0(2)	-5(2)	0(2)
C(12)	45(3)	42(2)	47(3)	7(2)	-4(2)	0(2)
C(13)	36(3)	51(2)	49(3)	5(2)	-8(2)	3(2)
C(14)	29(2)	25(2)	38(2)	9(2)	-6(2)	-5(2)
C(15)	32(2)	28(2)	36(2)	5(2)	-1(2)	-4(2)
C(16)	39(3)	36(2)	32(2)	2(2)	-5(2)	-9(2)
C(17)	30(2)	39(2)	40(3)	12(2)	-7(2)	-3(2)
C(18)	30(2)	39(2)	46(3)	7(2)	0(2)	4(2)
C(19)	35(2)	30(2)	36(2)	4(2)	-2(2)	-4(2)
C(20)	49(3)	42(2)	42(3)	2(2)	-4(2)	7(2)
C(21)	43(3)	60(3)	48(3)	5(2)	-11(2)	7(2)
C(22)	48(3)	37(2)	39(2)	3(2)	-1(2)	-1(2)
C(23)	26(2)	20(2)	35(2)	1(2)	-3(2)	-2(2)
C(24)	28(2)	24(2)	33(2)	-3(2)	-6(2)	-4(2)
C(25)	37(2)	30(2)	30(2)	-3(2)	2(2)	-2(2)
C(26)	33(2)	25(2)	29(2)	0(2)	-6(2)	-4(2)
C(27)	28(2)	27(2)	34(2)	-1(2)	-4(2)	1(2)

C(28)	28(2)	24(2)	31(2)	-5(2)	-4(2)	-4(2)
C(29)	31(2)	33(2)	37(2)	-6(2)	2(2)	-1(2)
C(30)	48(3)	36(2)	46(3)	9(2)	-4(2)	4(2)
C(31)	32(2)	31(2)	35(2)	-2(2)	1(2)	0(2)
Cl(1)	33(1)	28(1)	61(1)	-6(1)	-6(1)	2(1)
Cl(2)	47(1)	71(1)	70(1)	-6(1)	-10(1)	5(1)
Cl(3)	68(1)	124(1)	63(1)	40(1)	18(1)	39(1)
C(32)	60(3)	61(3)	52(3)	8(2)	3(2)	15(2)
Cl(4)	56(1)	88(1)	67(1)	6(1)	-8(1)	-1(1)
Cl(5)	89(1)	78(1)	73(1)	-12(1)	-1(1)	-15(1)
C(33)	42(3)	50(2)	73(3)	6(2)	-3(2)	9(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for k09163a.

	x	y	z	U(eq)
H(4N)	2740(20)	2490(20)	2480(20)	33(10)
H(2A)	4598	6619	1546	38
H(3A)	5545	5865	2664	36
H(5A)	4369	3533	1499	51
H(5B)	3830	2684	1380	51
H(5C)	4377	2838	2338	51
H(8A)	1175	3075	5294	55
H(9A)	69	3800	4578	61
H(10A)	143	4218	2963	57
H(12A)	3167	2805	4444	68
H(12B)	2638	1953	4300	68
H(12C)	2538	2494	5269	68
H(13A)	1590	3525	1266	68
H(13B)	1677	4496	1579	68
H(13C)	765	4091	1412	68
H(16A)	2217	5499	-962	43
H(18A)	1413	7060	1132	46
H(20A)	2576	6265	2976	67
H(20B)	2032	7077	2678	67
H(20C)	3035	7097	2587	67
H(21A)	514	6767	-275	75
H(21B)	872	6201	-1138	75
H(21C)	1185	7156	-1009	75
H(22A)	4137	5014	-79	62
H(22B)	3419	4641	-772	62
H(22C)	3513	4299	310	62
H(25A)	4534	3517	5527	39
H(27A)	6492	3068	3768	36
H(29A)	3642	4682	5275	50
H(29B)	3216	4443	4261	50

H(29C)	3763	5288	4362	50
H(30A)	5769	2730	6117	65
H(30B)	6528	2534	5396	65
H(30C)	5678	1993	5332	65
H(31A)	5734	4157	1762	49
H(31B)	6496	3589	2155	49
H(31C)	6484	4583	2365	49
H(32A)	1121	4978	5856	69
H(32B)	2125	4892	5903	69
H(33A)	1281	3622	7646	66
H(33B)	656	2969	8156	66

Table 6. Hydrogen bonds for k09163a [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(4)-H(4N)...Cl(1)	0.86(3)	2.23(3)	3.091(3)	178(3)

Symmetry transformations used to generate equivalent atoms:

Supplementary Material (ESI) for Dalton Transactions

Single Crystal X-ray Diffraction Report for IPrN^Imine.HCl (3b)

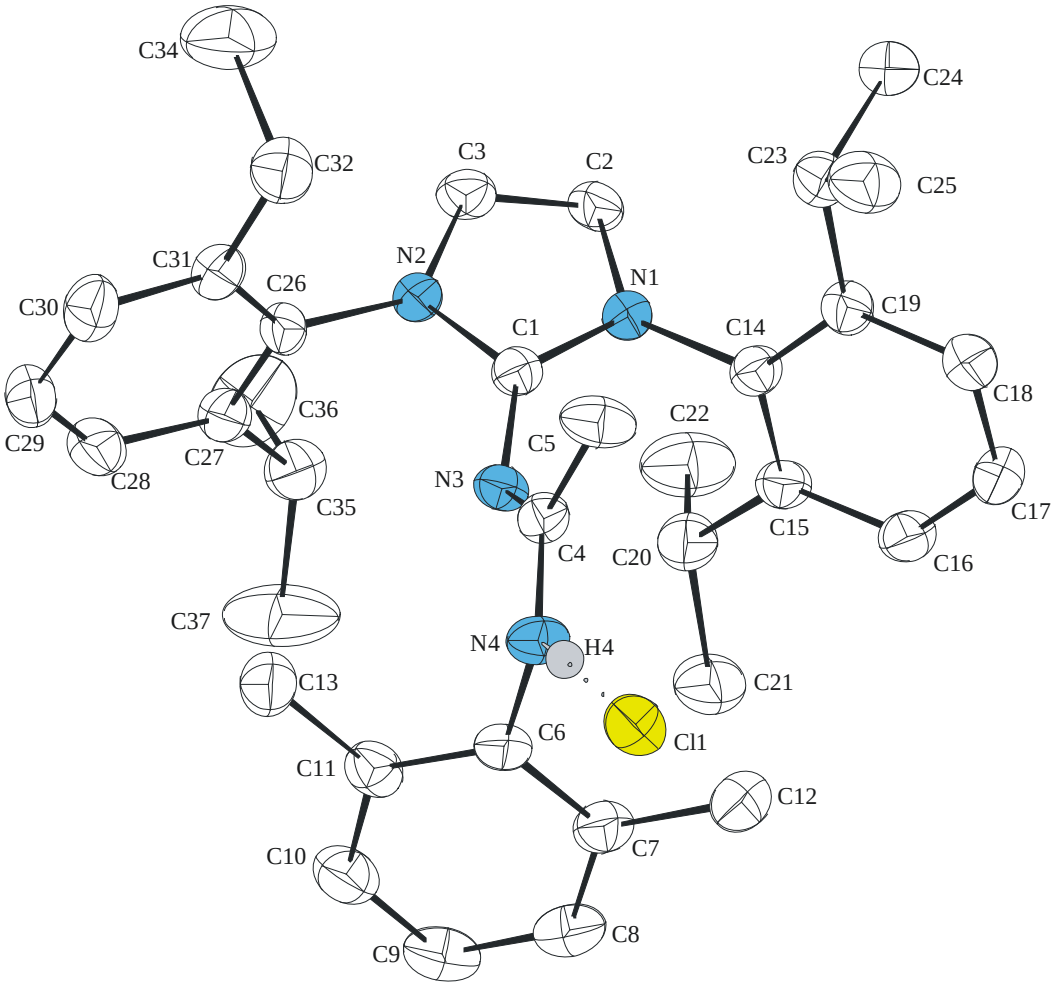

Table 1. Crystal data and structure refinement for IPrN^Imine.HCl (3b)

Identification code	k09161	
Empirical formula	C39 H53 Cl5 N4	
Formula weight	755.10	
Temperature	150(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 10.9207(3) Å	α= 90°.
	b = 23.5718(6) Å	β= 108.0720(12)°.
	c = 16.7583(4) Å	γ = 90°.
Volume	4101.11(18) $Å^3$	
Z	4	
Density (calculated)	1.223 Mg/m^3	
Absorption coefficient	0.385 mm^{-1}	
F(000)	1600	
Crystal size	0.60 x 0.40 x 0.20 mm^3	
Theta range for data collection	2.56 to 25.00°.	
Index ranges	-12<=h<=12, -27<=k<=28, -19<=l<=19	
Reflections collected	17529	
Independent reflections	7134 [R(int) = 0.0516]	
Completeness to theta = 25.00°	99.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.935 and 0.522	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7134 / 18 / 473	
Goodness-of-fit on F^2	1.094	
Final R indices [I>2sigma(I)]	R1 = 0.0720, wR2 = 0.1850	
R indices (all data)	R1 = 0.1010, wR2 = 0.2027	
Largest diff. peak and hole	0.955 and -0.438 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for k09161. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	4623(3)	6615(1)	1753(2)	29(1)
N(2)	5171(3)	6758(1)	3101(2)	30(1)
N(3)	4129(3)	5882(1)	2626(2)	30(1)
N(4)	3807(3)	4925(1)	2517(2)	34(1)
C(1)	4667(3)	6370(2)	2492(2)	28(1)
C(2)	5096(4)	7168(2)	1903(2)	33(1)
C(3)	5438(4)	7260(2)	2736(2)	35(1)
C(4)	4499(3)	5379(2)	2467(2)	30(1)
C(5)	5708(4)	5262(2)	2233(3)	43(1)
C(6)	2554(4)	4955(2)	2632(2)	33(1)
C(7)	1488(4)	4853(2)	1931(3)	39(1)
C(8)	279(4)	4882(2)	2044(3)	49(1)
C(9)	143(5)	4999(2)	2819(3)	54(1)
C(10)	1201(4)	5095(2)	3497(3)	48(1)
C(11)	2446(4)	5068(2)	3423(2)	36(1)
C(12)	1646(4)	4719(2)	1093(3)	48(1)
C(13)	3613(4)	5158(2)	4172(3)	45(1)
C(14)	4024(3)	6371(2)	930(2)	30(1)
C(15)	2675(4)	6311(2)	656(2)	32(1)
C(16)	2129(4)	6066(2)	-130(2)	39(1)
C(17)	2882(4)	5905(2)	-623(2)	43(1)
C(18)	4190(4)	5989(2)	-349(2)	38(1)
C(19)	4799(4)	6219(2)	437(2)	34(1)
C(20)	1841(4)	6547(2)	1160(3)	42(1)
C(21)	526(4)	6273(2)	961(3)	51(1)
C(22)	1691(5)	7189(2)	1050(4)	67(2)
C(23)	6246(4)	6322(2)	705(2)	38(1)
C(24)	6552(4)	6828(2)	222(3)	44(1)
C(25)	6986(4)	5799(2)	571(3)	51(1)
C(26)	5310(4)	6671(2)	3974(2)	31(1)
C(27)	4236(4)	6778(2)	4244(2)	36(1)

C(28)	4381(4)	6671(2)	5081(3)	45(1)
C(29)	5531(4)	6463(2)	5623(3)	46(1)
C(30)	6574(4)	6375(2)	5338(2)	44(1)
C(31)	6494(4)	6481(2)	4510(2)	36(1)
C(32)	7675(4)	6407(2)	4214(3)	46(1)
C(33)	8310(15)	5833(4)	4427(9)	74(3)
C(34)	8634(10)	6879(6)	4559(11)	82(4)
C(33A)	7910(50)	5774(5)	4200(30)	35(13)
C(34A)	8820(30)	6680(30)	4850(30)	54(15)
C(35)	2989(4)	7013(2)	3660(3)	43(1)
C(36)	2882(6)	7638(2)	3828(4)	77(2)
C(37)	1821(5)	6687(3)	3707(5)	88(2)
Cl(1)	4572(1)	3709(1)	2153(1)	42(1)
Cl(2)	8464(2)	7629(2)	2021(2)	69(1)
Cl(3)	9382(3)	8239(1)	3578(1)	84(1)
C(38)	8366(6)	8246(4)	2557(3)	54(2)
Cl(2A)	8898(14)	8001(8)	3748(8)	92(4)
Cl(3A)	8529(11)	7387(6)	2249(8)	69(4)
C(38A)	8430(60)	8050(10)	2665(9)	80(20)
Cl(4)	7896(2)	4315(1)	4076(1)	85(1)
Cl(5)	8793(3)	3644(1)	2934(2)	80(1)
C(39)	7763(5)	3687(2)	3527(3)	69(2)
Cl(5A)	9199(15)	3499(10)	3380(20)	99(8)

Table 3. Bond lengths [Å] and angles [°] for k09161.

N(1)-C(1)	1.353(5)
N(1)-C(2)	1.397(5)
N(1)-C(14)	1.450(5)
N(2)-C(1)	1.354(5)
N(2)-C(3)	1.403(5)
N(2)-C(26)	1.438(5)
N(3)-C(4)	1.307(5)
N(3)-C(1)	1.343(5)
N(4)-C(4)	1.328(5)
N(4)-C(6)	1.441(5)
C(2)-C(3)	1.345(5)
C(4)-C(5)	1.515(5)
C(6)-C(11)	1.394(5)
C(6)-C(7)	1.394(5)
C(7)-C(8)	1.392(6)
C(7)-C(12)	1.501(6)
C(8)-C(9)	1.381(7)
C(9)-C(10)	1.365(7)
C(10)-C(11)	1.404(6)
C(11)-C(13)	1.501(6)
C(14)-C(19)	1.399(5)
C(14)-C(15)	1.407(5)
C(15)-C(16)	1.392(5)
C(15)-C(20)	1.527(6)
C(16)-C(17)	1.388(6)
C(17)-C(18)	1.372(6)
C(18)-C(19)	1.389(5)
C(19)-C(23)	1.522(5)
C(20)-C(21)	1.515(6)
C(20)-C(22)	1.527(7)
C(23)-C(25)	1.528(6)
C(23)-C(24)	1.536(6)
C(26)-C(31)	1.399(5)
C(26)-C(27)	1.404(5)

C(27)-C(28)	1.386(6)
C(27)-C(35)	1.515(6)
C(28)-C(29)	1.391(6)
C(29)-C(30)	1.380(6)
C(30)-C(31)	1.387(6)
C(31)-C(32)	1.528(6)
C(32)-C(33)	1.511(5)
C(32)-C(34)	1.516(5)
C(35)-C(36)	1.512(7)
C(35)-C(37)	1.512(7)
Cl(2)-C(38)	1.730(6)
Cl(3)-C(38)	1.727(5)
Cl(2A)-C(38A)	1.729(7)
Cl(3A)-C(38A)	1.729(7)
Cl(4)-C(39)	1.724(4)
Cl(5)-C(39)	1.721(4)

C(1)-N(1)-C(2)	109.1(3)
C(1)-N(1)-C(14)	125.3(3)
C(2)-N(1)-C(14)	125.1(3)
C(1)-N(2)-C(3)	109.4(3)
C(1)-N(2)-C(26)	124.1(3)
C(3)-N(2)-C(26)	126.4(3)
C(4)-N(3)-C(1)	124.4(3)
C(4)-N(4)-C(6)	123.5(3)
N(3)-C(1)-N(1)	128.7(3)
N(3)-C(1)-N(2)	123.4(3)
N(1)-C(1)-N(2)	107.0(3)
C(3)-C(2)-N(1)	107.7(3)
C(2)-C(3)-N(2)	106.8(3)
N(3)-C(4)-N(4)	120.0(3)
N(3)-C(4)-C(5)	124.6(3)
N(4)-C(4)-C(5)	115.4(3)
C(11)-C(6)-C(7)	122.6(4)
C(11)-C(6)-N(4)	120.1(3)
C(7)-C(6)-N(4)	117.3(3)

C(8)-C(7)-C(6)	117.2(4)
C(8)-C(7)-C(12)	121.7(4)
C(6)-C(7)-C(12)	121.1(4)
C(9)-C(8)-C(7)	121.4(4)
C(10)-C(9)-C(8)	120.4(4)
C(9)-C(10)-C(11)	120.8(4)
C(6)-C(11)-C(10)	117.6(4)
C(6)-C(11)-C(13)	121.5(4)
C(10)-C(11)-C(13)	121.0(4)
C(19)-C(14)-C(15)	123.0(3)
C(19)-C(14)-N(1)	119.0(3)
C(15)-C(14)-N(1)	117.9(3)
C(16)-C(15)-C(14)	116.7(3)
C(16)-C(15)-C(20)	121.4(3)
C(14)-C(15)-C(20)	121.8(3)
C(17)-C(16)-C(15)	121.2(4)
C(18)-C(17)-C(16)	120.6(4)
C(17)-C(18)-C(19)	121.1(4)
C(18)-C(19)-C(14)	117.4(4)
C(18)-C(19)-C(23)	119.3(3)
C(14)-C(19)-C(23)	123.2(3)
C(21)-C(20)-C(15)	114.2(4)
C(21)-C(20)-C(22)	109.7(4)
C(15)-C(20)-C(22)	110.8(4)
C(19)-C(23)-C(25)	112.1(3)
C(19)-C(23)-C(24)	110.1(3)
C(25)-C(23)-C(24)	109.7(3)
C(31)-C(26)-C(27)	123.2(3)
C(31)-C(26)-N(2)	118.9(3)
C(27)-C(26)-N(2)	117.8(3)
C(28)-C(27)-C(26)	116.7(4)
C(28)-C(27)-C(35)	121.2(4)
C(26)-C(27)-C(35)	122.1(3)
C(27)-C(28)-C(29)	121.3(4)
C(30)-C(29)-C(28)	120.2(4)
C(29)-C(30)-C(31)	121.1(4)

C(30)-C(31)-C(26)	117.3(4)
C(30)-C(31)-C(32)	120.4(4)
C(26)-C(31)-C(32)	122.2(3)
C(33)-C(32)-C(34)	110.8(6)
C(33)-C(32)-C(31)	113.5(5)
C(34)-C(32)-C(31)	110.1(4)
C(36)-C(35)-C(37)	111.7(4)
C(36)-C(35)-C(27)	110.0(4)
C(37)-C(35)-C(27)	112.6(4)
Cl(3)-C(38)-Cl(2)	112.4(5)
Cl(3A)-C(38A)-Cl(2A)	109.0(11)
Cl(5)-C(39)-Cl(4)	113.4(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for k09161. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	30(2)	29(2)	29(2)	-1(1)	9(1)	-2(1)
N(2)	33(2)	29(2)	29(2)	-4(1)	11(1)	-5(1)
N(3)	31(2)	27(2)	34(2)	0(1)	14(1)	-4(1)
N(4)	33(2)	25(2)	47(2)	-5(2)	16(2)	-3(1)
C(1)	26(2)	28(2)	31(2)	-4(2)	11(2)	0(1)
C(2)	38(2)	29(2)	35(2)	3(2)	15(2)	-5(2)
C(3)	38(2)	26(2)	40(2)	1(2)	12(2)	-6(2)
C(4)	27(2)	32(2)	30(2)	0(2)	8(2)	0(2)
C(5)	34(2)	36(2)	68(3)	0(2)	27(2)	2(2)
C(6)	32(2)	29(2)	39(2)	0(2)	13(2)	-5(2)
C(7)	38(2)	36(2)	41(2)	-1(2)	10(2)	-7(2)
C(8)	35(2)	51(3)	58(3)	-3(2)	10(2)	-11(2)
C(9)	43(3)	58(3)	69(3)	3(2)	27(2)	-9(2)
C(10)	50(3)	50(3)	53(3)	-2(2)	29(2)	-7(2)
C(11)	44(2)	29(2)	39(2)	3(2)	18(2)	-1(2)
C(12)	49(3)	48(3)	42(2)	-5(2)	9(2)	-10(2)
C(13)	52(3)	45(2)	35(2)	0(2)	11(2)	-3(2)
C(14)	31(2)	28(2)	31(2)	-1(2)	8(2)	-3(2)
C(15)	31(2)	32(2)	34(2)	3(2)	9(2)	-4(2)
C(16)	33(2)	42(2)	37(2)	3(2)	5(2)	-8(2)
C(17)	48(3)	47(2)	30(2)	-4(2)	7(2)	-11(2)
C(18)	40(2)	42(2)	36(2)	-2(2)	15(2)	-4(2)
C(19)	37(2)	33(2)	32(2)	-2(2)	12(2)	-2(2)
C(20)	33(2)	51(3)	42(2)	-2(2)	11(2)	0(2)
C(21)	34(2)	63(3)	58(3)	1(2)	17(2)	-2(2)
C(22)	51(3)	53(3)	104(4)	-9(3)	33(3)	-2(2)
C(23)	32(2)	46(2)	35(2)	-3(2)	13(2)	-2(2)
C(24)	43(2)	50(3)	42(2)	-4(2)	16(2)	-13(2)
C(25)	44(3)	53(3)	64(3)	-4(2)	28(2)	0(2)
C(26)	39(2)	31(2)	27(2)	-5(2)	14(2)	-5(2)
C(27)	40(2)	35(2)	36(2)	-7(2)	15(2)	-6(2)

C(28)	51(3)	48(3)	44(2)	-8(2)	26(2)	-10(2)
C(29)	61(3)	47(3)	30(2)	-1(2)	16(2)	-10(2)
C(30)	48(3)	45(2)	32(2)	1(2)	5(2)	1(2)
C(31)	37(2)	34(2)	34(2)	-4(2)	10(2)	-2(2)
C(32)	38(2)	56(3)	44(2)	-2(2)	14(2)	5(2)
C(33)	65(7)	73(5)	82(6)	4(4)	22(5)	22(4)
C(34)	61(5)	86(7)	115(8)	-25(7)	49(5)	-23(4)
C(32A)	38(2)	56(3)	44(2)	-2(2)	14(2)	5(2)
C(35)	41(2)	44(2)	47(2)	-8(2)	17(2)	0(2)
C(36)	81(4)	57(3)	83(4)	-2(3)	8(3)	17(3)
C(37)	31(3)	82(4)	139(6)	36(4)	9(3)	-1(3)
Cl(1)	52(1)	32(1)	46(1)	-2(1)	24(1)	0(1)
Cl(2)	62(1)	80(2)	62(1)	-17(1)	16(1)	-10(1)
Cl(3)	94(2)	74(2)	57(1)	-12(1)	-16(1)	11(1)
C(38)	32(3)	70(5)	55(4)	6(3)	9(3)	11(3)
Cl(4)	118(1)	66(1)	81(1)	-8(1)	42(1)	8(1)
Cl(5)	88(2)	86(1)	83(2)	-9(1)	52(2)	-7(1)
C(39)	57(3)	60(3)	96(4)	-3(3)	32(3)	0(3)
Cl(4A)	118(1)	66(1)	81(1)	-8(1)	42(1)	8(1)
C(39A)	57(3)	60(3)	96(4)	-3(3)	32(3)	0(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for k09161.

	x	y	z	U(eq)
H(4N)	4060(40)	4596(19)	2420(30)	37(11)
H(2A)	5163	7433	1491	40
H(3A)	5791	7599	3021	42
H(5A)	6334	5566	2452	65
H(5B)	5493	5245	1620	65
H(5C)	6078	4898	2475	65
H(8A)	-468	4821	1577	59
H(9A)	-693	5012	2881	65
H(10A)	1094	5181	4025	58
H(12A)	797	4697	669	72
H(12B)	2089	4354	1125	72
H(12C)	2156	5018	940	72
H(13A)	4265	4872	4173	67
H(13B)	3372	5123	4687	67
H(13C)	3965	5537	4145	67
H(16A)	1224	6008	-332	46
H(17A)	2488	5735	-1155	52
H(18A)	4687	5888	-703	46
H(20A)	2306	6473	1767	51
H(21A)	623	5859	996	76
H(21B)	1	6380	393	76
H(21C)	103	6402	1366	76
H(22A)	1236	7338	1426	101
H(22B)	1196	7276	467	101
H(22C)	2543	7365	1186	101
H(23A)	6542	6417	1317	45
H(24A)	6088	7164	317	67
H(24B)	6282	6740	-380	67
H(24C)	7480	6902	418	67
H(25A)	6743	5471	848	77

H(25B)	7913	5867	811	77
H(25C)	6777	5723	-31	77
H(28A)	3679	6742	5290	54
H(29A)	5599	6382	6190	55
H(30A)	7360	6240	5716	52
H(32)	7378	6442	3588	55
H(33A)	8741	5810	5034	111
H(33B)	8947	5783	4130	111
H(33C)	7656	5535	4257	111
H(34A)	8832	6898	5170	123
H(34B)	8264	7241	4311	123
H(34C)	9426	6805	4418	123
H(32A)	7524	6576	3644	55
H(33D)	8132	5624	4775	52
H(33E)	8625	5703	3976	52
H(33F)	7133	5586	3848	52
H(34D)	8540	7032	5060	82
H(34E)	9478	6771	4586	82
H(34F)	9175	6420	5321	82
H(35A)	3026	6975	3073	52
H(36A)	3676	7831	3828	116
H(36B)	2748	7688	4376	116
H(36C)	2151	7801	3389	116
H(37A)	1868	6296	3522	132
H(37B)	1038	6868	3343	132
H(37C)	1799	6687	4287	132
H(38A)	8588	8573	2257	64
H(38B)	7469	8298	2561	64
H(38C)	7532	8192	2452	100
H(38D)	8994	8320	2493	100
H(39A)	7941	3368	3930	83
H(39B)	6866	3647	3153	83
H(39C)	7487	3382	3840	83
H(39D)	7094	3728	2975	83

Table 6. Hydrogen bonds for k09161 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(4)-H(4N)...Cl(1)	0.86(4)	2.24(5)	3.098(4)	175(4)

Symmetry transformations used to generate equivalent atoms:

Single Crystal X-ray Diffraction Report for Ti(IMesN^Imine)Cl_4 (4a)

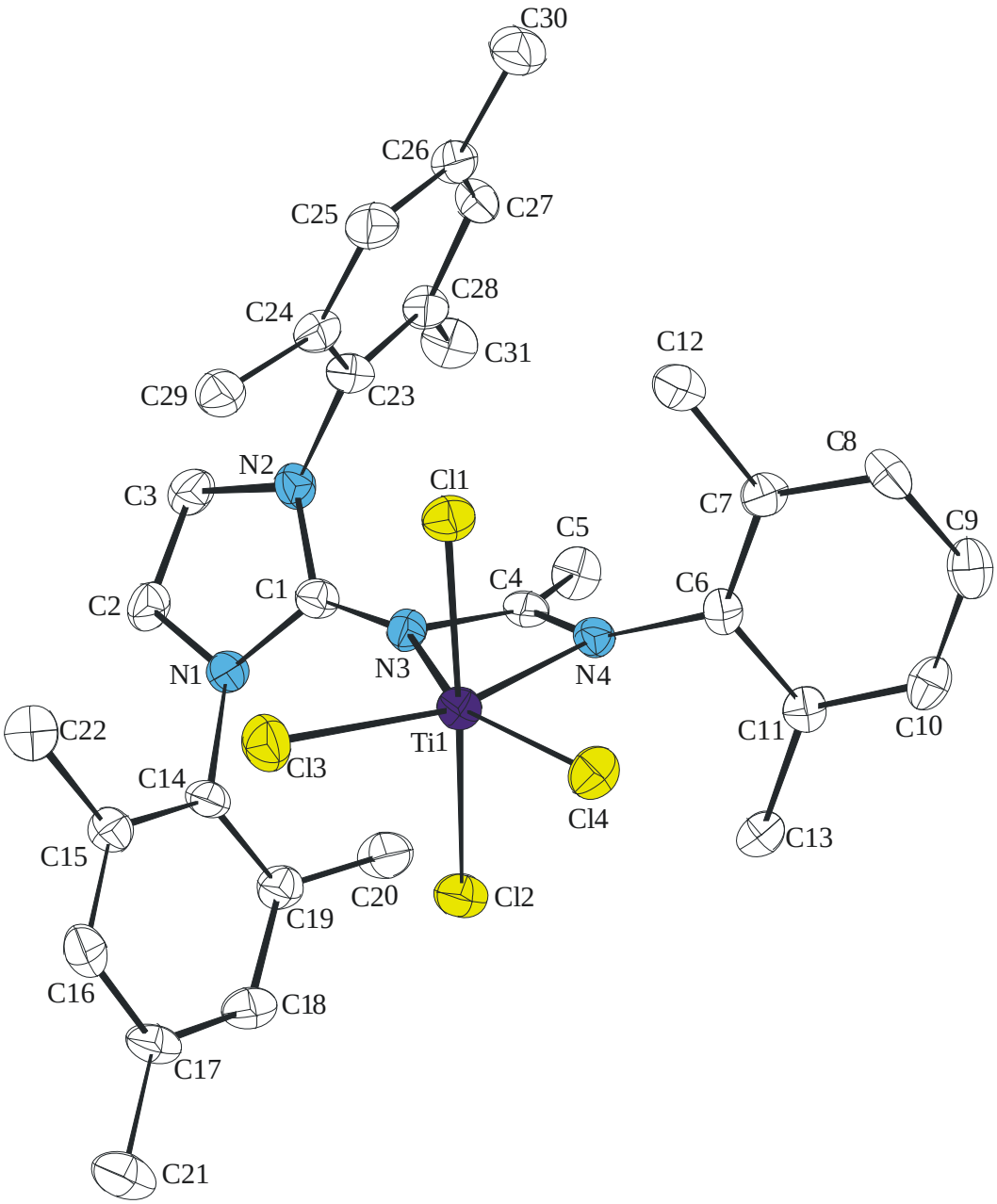

Table 1. Crystal data and structure refinement for Ti(IMesN^Imine)Cl_4 (4a)

Identification code	k09228	
Empirical formula	C32 H37 Cl7 N4 Ti	
Formula weight	773.71	
Temperature	150(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 31.2113(7) Å	α= 90°.
	b = 9.2685(4) Å	β= 105.3630(18)°.
	c = 25.6275(8) Å	γ = 90°.
Volume	7148.7(4) $Å^3$	
Z	8	
Density (calculated)	1.438 Mg/m^3	
Absorption coefficient	0.792 mm^{-1}	
F(000)	3184	
Crystal size	0.30 x 0.30 x 0.15 mm^3	
Theta range for data collection	2.72 to 27.48°.	
Index ranges	-40<=h<=38, -12<=k<=12, -23<=l<=33	
Reflections collected	22260	
Independent reflections	8106 [R(int) = 0.0735]	
Completeness to theta = 27.48°	99.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.886 and 0.751	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8106 / 0 / 406	
Goodness-of-fit on F^2	1.019	
Final R indices [I>2sigma(I)]	R1 = 0.0631, wR2 = 0.1441	
R indices (all data)	R1 = 0.1526, wR2 = 0.1909	
Largest diff. peak and hole	0.787 and -0.660 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for k09228. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ti(1)	6255(1)	2029(1)	6538(1)	24(1)
Cl(1)	6845(1)	1482(1)	6180(1)	32(1)
Cl(2)	5691(1)	2603(1)	6922(1)	32(1)
Cl(3)	6747(1)	1927(1)	7378(1)	38(1)
Cl(4)	5958(1)	-167(1)	6313(1)	32(1)
N(1)	6763(1)	6549(4)	6354(1)	25(1)
N(2)	6512(1)	6298(4)	7064(1)	24(1)
N(3)	6321(1)	4409(4)	6396(1)	23(1)
N(4)	5926(1)	2930(4)	5784(1)	22(1)
C(1)	6514(1)	5678(5)	6588(2)	24(1)
C(2)	6912(1)	7718(5)	6691(2)	29(1)
C(3)	6758(1)	7579(5)	7130(2)	28(1)
C(4)	6944(1)	6144(5)	5906(2)	25(1)
C(5)	6802(1)	6869(5)	5411(2)	28(1)
C(6)	6985(1)	6394(5)	4998(2)	31(1)
C(7)	7286(1)	5290(5)	5069(2)	30(1)
C(8)	7440(1)	4669(5)	5582(2)	32(1)
C(9)	7277(1)	5101(5)	6011(2)	28(1)
C(10)	6486(1)	8145(5)	5312(2)	33(1)
C(11)	7455(2)	4752(6)	4605(2)	41(1)
C(12)	7472(1)	4516(5)	6569(2)	32(1)
C(13)	6301(1)	5790(5)	7469(2)	25(1)
C(14)	6574(1)	5265(5)	7953(2)	29(1)
C(15)	6380(2)	4883(5)	8357(2)	32(1)
C(16)	5926(1)	4998(5)	8297(2)	30(1)
C(17)	5668(1)	5515(5)	7807(2)	30(1)
C(18)	5843(1)	5924(5)	7382(2)	27(1)
C(19)	7077(1)	5126(5)	8046(2)	40(1)
C(20)	5718(2)	4608(6)	8746(2)	41(1)
C(21)	5548(1)	6484(5)	6858(2)	36(1)
C(22)	6038(1)	4282(5)	5893(2)	24(1)

C(23)	5835(1)	5492(5)	5530(2)	30(1)
C(24)	5672(1)	2470(4)	5259(2)	22(1)
C(25)	5870(1)	2318(5)	4838(2)	28(1)
C(26)	5617(1)	1806(5)	4340(2)	31(1)
C(27)	5179(1)	1439(5)	4266(2)	34(1)
C(28)	4979(1)	1623(5)	4678(2)	29(1)
C(29)	5217(1)	2139(4)	5184(2)	24(1)
C(30)	6351(1)	2747(6)	4893(2)	38(1)
C(31)	4994(1)	2375(5)	5630(2)	34(1)
Cl(5)	5454(1)	1083(2)	8191(1)	57(1)
Cl(6)	6057(1)	-976(2)	7946(1)	65(1)
Cl(7)	6376(1)	1042(2)	8811(1)	64(1)
C(32)	6003(2)	783(5)	8167(2)	40(1)

Table 3. Bond lengths [Å] and angles [°] for k09228.

Ti(1)-N(4)	2.106(3)
Ti(1)-Cl(4)	2.2480(13)
Ti(1)-N(3)	2.253(3)
Ti(1)-Cl(3)	2.2913(13)
Ti(1)-Cl(2)	2.2944(12)
Ti(1)-Cl(1)	2.3182(12)
Ti(1)-C(22)	2.637(4)
N(1)-C(1)	1.365(5)
N(1)-C(2)	1.386(5)
N(1)-C(4)	1.455(5)
N(2)-C(1)	1.349(5)
N(2)-C(3)	1.400(5)
N(2)-C(13)	1.449(5)
N(3)-C(1)	1.354(5)
N(3)-C(22)	1.361(5)
N(4)-C(22)	1.312(5)
N(4)-C(24)	1.433(5)
C(2)-C(3)	1.341(6)
C(4)-C(9)	1.393(6)
C(4)-C(5)	1.400(6)
C(5)-C(6)	1.401(6)
C(5)-C(10)	1.517(6)
C(6)-C(7)	1.369(6)
C(7)-C(8)	1.398(6)
C(7)-C(11)	1.507(6)
C(8)-C(9)	1.388(6)
C(9)-C(12)	1.500(6)
C(13)-C(18)	1.393(5)
C(13)-C(14)	1.394(6)
C(14)-C(15)	1.378(6)
C(14)-C(19)	1.528(6)
C(15)-C(16)	1.390(6)
C(16)-C(17)	1.385(6)
C(16)-C(20)	1.509(6)

C(17)-C(18)	1.394(6)
C(18)-C(21)	1.505(6)
C(22)-C(23)	1.487(6)
C(24)-C(25)	1.387(6)
C(24)-C(29)	1.415(5)
C(25)-C(26)	1.395(6)
C(25)-C(30)	1.522(6)
C(26)-C(27)	1.374(6)
C(27)-C(28)	1.373(6)
C(28)-C(29)	1.398(6)
C(29)-C(31)	1.504(6)
Cl(5)-C(32)	1.754(5)
Cl(6)-C(32)	1.749(5)
Cl(7)-C(32)	1.765(5)

N(4)-Ti(1)-Cl(4)	93.22(10)
N(4)-Ti(1)-N(3)	60.50(12)
Cl(4)-Ti(1)-N(3)	153.42(9)
N(4)-Ti(1)-Cl(3)	157.13(10)
Cl(4)-Ti(1)-Cl(3)	109.33(5)
N(3)-Ti(1)-Cl(3)	97.18(9)
N(4)-Ti(1)-Cl(2)	93.33(9)
Cl(4)-Ti(1)-Cl(2)	90.43(5)
N(3)-Ti(1)-Cl(2)	87.45(9)
Cl(3)-Ti(1)-Cl(2)	90.33(5)
N(4)-Ti(1)-Cl(1)	88.31(9)
Cl(4)-Ti(1)-Cl(1)	91.05(5)
N(3)-Ti(1)-Cl(1)	91.99(9)
Cl(3)-Ti(1)-Cl(1)	87.54(5)
Cl(2)-Ti(1)-Cl(1)	177.72(5)
N(4)-Ti(1)-C(22)	29.49(12)
Cl(4)-Ti(1)-C(22)	122.46(10)
N(3)-Ti(1)-C(22)	31.07(12)
Cl(3)-Ti(1)-C(22)	128.21(10)
Cl(2)-Ti(1)-C(22)	89.21(9)
Cl(1)-Ti(1)-C(22)	91.45(9)

C(1)-N(1)-C(2)	108.9(3)
C(1)-N(1)-C(4)	125.4(3)
C(2)-N(1)-C(4)	123.8(3)
C(1)-N(2)-C(3)	109.8(3)
C(1)-N(2)-C(13)	128.4(3)
C(3)-N(2)-C(13)	121.9(3)
C(1)-N(3)-C(22)	122.3(4)
C(1)-N(3)-Ti(1)	147.5(3)
C(22)-N(3)-Ti(1)	90.3(3)
C(22)-N(4)-C(24)	122.3(3)
C(22)-N(4)-Ti(1)	98.3(2)
C(24)-N(4)-Ti(1)	139.3(3)
N(2)-C(1)-N(3)	126.2(4)
N(2)-C(1)-N(1)	106.5(3)
N(3)-C(1)-N(1)	127.2(4)
C(3)-C(2)-N(1)	108.3(4)
C(2)-C(3)-N(2)	106.6(4)
C(9)-C(4)-C(5)	123.3(4)
C(9)-C(4)-N(1)	116.9(4)
C(5)-C(4)-N(1)	119.7(4)
C(4)-C(5)-C(6)	116.0(4)
C(4)-C(5)-C(10)	124.1(4)
C(6)-C(5)-C(10)	119.8(4)
C(7)-C(6)-C(5)	122.6(4)
C(6)-C(7)-C(8)	119.0(4)
C(6)-C(7)-C(11)	120.9(4)
C(8)-C(7)-C(11)	120.1(4)
C(9)-C(8)-C(7)	121.3(4)
C(8)-C(9)-C(4)	117.4(4)
C(8)-C(9)-C(12)	120.6(4)
C(4)-C(9)-C(12)	121.9(4)
C(18)-C(13)-C(14)	122.3(4)
C(18)-C(13)-N(2)	119.9(4)
C(14)-C(13)-N(2)	117.7(3)
C(15)-C(14)-C(13)	118.1(4)
C(15)-C(14)-C(19)	120.0(4)

C(13)-C(14)-C(19)	121.9(4)
C(14)-C(15)-C(16)	122.4(4)
C(17)-C(16)-C(15)	117.2(4)
C(17)-C(16)-C(20)	120.8(4)
C(15)-C(16)-C(20)	122.0(4)
C(16)-C(17)-C(18)	123.4(4)
C(13)-C(18)-C(17)	116.5(4)
C(13)-C(18)-C(21)	122.3(4)
C(17)-C(18)-C(21)	121.1(4)
N(4)-C(22)-N(3)	110.7(4)
N(4)-C(22)-C(23)	122.8(4)
N(3)-C(22)-C(23)	126.1(4)
N(4)-C(22)-Ti(1)	52.2(2)
N(3)-C(22)-Ti(1)	58.7(2)
C(23)-C(22)-Ti(1)	170.0(3)
C(25)-C(24)-C(29)	120.8(4)
C(25)-C(24)-N(4)	120.7(4)
C(29)-C(24)-N(4)	118.5(3)
C(24)-C(25)-C(26)	119.1(4)
C(24)-C(25)-C(30)	122.3(4)
C(26)-C(25)-C(30)	118.6(4)
C(27)-C(26)-C(25)	120.7(4)
C(28)-C(27)-C(26)	120.3(4)
C(27)-C(28)-C(29)	121.2(4)
C(28)-C(29)-C(24)	117.8(4)
C(28)-C(29)-C(31)	121.1(4)
C(24)-C(29)-C(31)	121.1(4)
Cl(6)-C(32)-Cl(5)	109.7(3)
Cl(6)-C(32)-Cl(7)	109.5(3)
Cl(5)-C(32)-Cl(7)	110.8(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for k09228. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ti(1)	26(1)	22(1)	24(1)	1(1)	7(1)	0(1)
Cl(1)	30(1)	32(1)	36(1)	-1(1)	13(1)	2(1)
Cl(2)	34(1)	34(1)	31(1)	0(1)	15(1)	0(1)
Cl(3)	38(1)	45(1)	28(1)	1(1)	2(1)	2(1)
Cl(4)	34(1)	23(1)	39(1)	-2(1)	9(1)	-3(1)
N(1)	30(2)	23(2)	22(2)	-4(2)	6(2)	-3(2)
N(2)	23(2)	23(2)	25(2)	-2(2)	8(2)	-1(2)
N(3)	22(2)	23(2)	22(2)	-1(2)	4(1)	-3(2)
N(4)	27(2)	21(2)	21(2)	-1(2)	9(2)	-4(2)
C(1)	26(2)	23(2)	24(2)	-1(2)	10(2)	0(2)
C(2)	27(2)	27(3)	33(3)	-2(2)	8(2)	-7(2)
C(3)	28(2)	24(2)	32(2)	-9(2)	8(2)	-7(2)
C(4)	27(2)	24(2)	26(2)	1(2)	12(2)	0(2)
C(5)	29(2)	29(3)	26(2)	3(2)	8(2)	-4(2)
C(6)	35(2)	37(3)	21(2)	-2(2)	8(2)	-6(2)
C(7)	28(2)	34(3)	30(3)	-7(2)	12(2)	-7(2)
C(8)	26(2)	36(3)	36(3)	-3(2)	12(2)	4(2)
C(9)	25(2)	29(3)	31(3)	1(2)	9(2)	-6(2)
C(10)	39(3)	27(3)	35(3)	4(2)	13(2)	4(2)
C(11)	35(3)	57(4)	35(3)	-5(3)	16(2)	7(2)
C(12)	26(2)	40(3)	30(2)	1(2)	8(2)	3(2)
C(13)	31(2)	26(2)	22(2)	-3(2)	14(2)	-5(2)
C(14)	30(2)	30(3)	27(2)	-5(2)	10(2)	-2(2)
C(15)	38(3)	33(3)	23(2)	-3(2)	4(2)	-2(2)
C(16)	39(3)	27(3)	30(3)	-2(2)	21(2)	0(2)
C(17)	28(2)	29(3)	39(3)	0(2)	17(2)	1(2)
C(18)	30(2)	23(2)	29(2)	-2(2)	11(2)	-4(2)
C(19)	39(3)	44(3)	37(3)	-2(2)	9(2)	-3(2)
C(20)	56(3)	40(3)	35(3)	-1(2)	25(2)	-1(3)
C(21)	29(2)	42(3)	38(3)	9(2)	12(2)	2(2)
C(22)	23(2)	29(3)	24(2)	-2(2)	12(2)	0(2)

C(23)	33(2)	20(2)	35(3)	1(2)	7(2)	2(2)
C(24)	27(2)	17(2)	20(2)	1(2)	2(2)	-1(2)
C(25)	26(2)	28(3)	29(2)	0(2)	9(2)	-1(2)
C(26)	38(3)	35(3)	18(2)	-1(2)	6(2)	5(2)
C(27)	39(3)	25(3)	32(3)	-4(2)	0(2)	2(2)
C(28)	26(2)	21(2)	36(3)	-3(2)	3(2)	-2(2)
C(29)	27(2)	19(2)	25(2)	1(2)	5(2)	0(2)
C(30)	35(3)	54(3)	28(3)	0(2)	12(2)	-2(2)
C(31)	25(2)	42(3)	36(3)	-4(2)	10(2)	-8(2)
Cl(5)	62(1)	57(1)	60(1)	3(1)	30(1)	3(1)
Cl(6)	97(1)	41(1)	70(1)	-19(1)	43(1)	-4(1)
Cl(7)	83(1)	51(1)	47(1)	0(1)	-2(1)	-2(1)
C(32)	58(3)	31(3)	36(3)	-5(2)	20(2)	-2(2)

Table 5. Hydrogen coordinates (x 104) and isotropic displacement parameters (Å2x 10 3) for k09228.

	x	y	z	U(eq)
H(2A)	7091	8485	6622	35
H(3A)	6807	8225	7428	34
H(6A)	6897	6857	4655	37
H(8A)	7661	3937	5638	38
H(10A)	6356	8251	5619	50
H(10B)	6249	7982	4980	50
H(10C)	6649	9024	5274	50
H(11A)	7713	4128	4744	62
H(11B)	7541	5575	4415	62
H(11C)	7220	4203	4354	62
H(12A)	7571	5317	6822	48
H(12B)	7726	3897	6568	48
H(12C)	7247	3951	6682	48
H(15A)	6564	4528	8689	39
H(17A)	5357	5595	7758	37
H(19A)	7142	4757	7717	60
H(19B)	7195	4458	8346	60
H(19C)	7216	6075	8135	60
H(20A)	5433	4125	8594	62
H(20B)	5669	5487	8935	62
H(20C)	5916	3959	9002	62
H(21A)	5270	6846	6919	54
H(21B)	5481	5702	6591	54
H(21C)	5699	7268	6722	54
H(23A)	5986	5596	5242	45
H(23B)	5865	6389	5739	45
H(23C)	5519	5290	5369	45
H(26A)	5750	1709	4048	37
H(27A)	5014	1057	3929	41
H(28A)	4673	1395	4618	35

H(30A)	6508	2837	5277	57
H(30B)	6359	3673	4712	57
H(30C)	6496	2006	4726	57
H(31A)	4678	2127	5500	51
H(31B)	5023	3390	5742	51
H(31C)	5134	1762	5940	51
H(32B)	6078	1479	7906	48

Supplementary Material (ESI) for Dalton Transactions

Single Crystal X-ray Diffraction Report for $[Pd(IMesN^Imine)Cl_2]_2$ (5b)

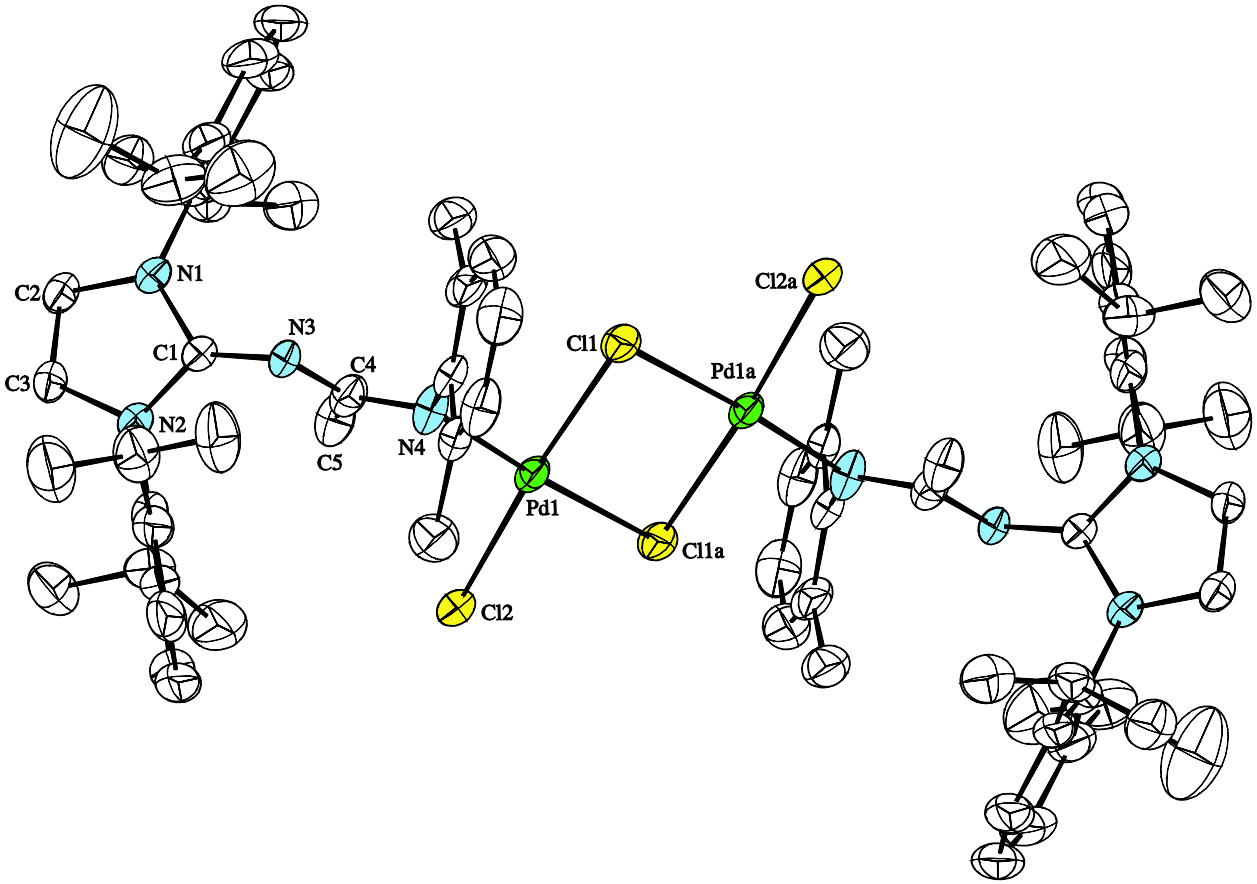

Table 1. Crystal data and structure refinement for $[Pd(IPrN^Imine)Cl_2]_2$ (5b)

Identification code	k09220	
Empirical formula	C76 H100 Cl8 N8 Pd2	
Formula weight	1622.04	
Temperature	150(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 14.0092(3) Å	α= 90°.
	b = 21.2077(6) Å	β= 94.8230(16)°.
	c = 14.3841(4) Å	γ = 90°.
Volume	4258.43(19) $Å^3$	
Z	2	
Density (calculated)	1.265 Mg/m^3	
Absorption coefficient	0.716 mm^{-1}	
F(000)	1680	
Crystal size	0.60 x 0.35 x 0.12 mm^3	
Theta range for data collection	2.74 to 27.49°.	
Index ranges	-18<=h<=18, -27<=k<=27, -18<=l<=18	
Reflections collected	28275	
Independent reflections	9700 [R(int) = 0.0629]	
Completeness to theta = 27.49°	99.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.921 and 0.662	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9700 / 12 / 469	
Goodness-of-fit on F^2	1.033	
Final R indices [I>2sigma(I)]	R1 = 0.0863, wR2 = 0.2379	
R indices (all data)	R1 = 0.1276, wR2 = 0.2769	
Largest diff. peak and hole	1.514 and -1.118 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for k09220. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pd(1)	5991(1)	185(1)	732(1)	39(1)
Cl(1)	4874(1)	-632(1)	568(1)	53(1)
Cl(2)	6708(1)	-318(1)	2017(1)	53(1)
N(1)	8051(3)	2722(2)	2175(3)	44(1)
N(2)	8659(4)	1918(2)	2967(4)	55(1)
N(3)	7809(3)	1725(2)	1452(3)	44(1)
N(4)	6943(3)	901(2)	764(4)	51(1)
C(1)	8107(4)	2082(2)	2163(4)	42(1)
C(2)	8579(4)	2959(3)	2965(4)	51(1)
C(3)	8948(5)	2470(3)	3445(5)	58(2)
C(4)	7116(4)	1303(3)	1470(4)	48(1)
C(5)	6461(5)	1270(3)	2241(5)	61(2)
C(6)	7465(4)	971(2)	-49(4)	43(1)
C(7)	8205(4)	542(3)	-180(4)	49(1)
C(8)	8669(5)	582(4)	-1001(5)	65(2)
C(9)	8394(6)	1043(4)	-1658(5)	74(2)
C(10)	7681(6)	1459(4)	-1479(5)	72(2)
C(11)	7215(4)	1439(3)	-681(5)	56(2)
C(12)	8503(5)	41(4)	542(6)	71(2)
C(13)	6468(5)	1936(3)	-475(6)	68(2)
C(14)	7530(5)	3082(3)	1453(4)	50(1)
C(15)	6588(5)	3228(3)	1552(4)	57(2)
C(16)	6088(6)	3555(3)	827(5)	69(2)
C(17)	6528(7)	3749(3)	58(5)	79(2)
C(18)	7475(8)	3603(3)	-13(5)	85(3)
C(19)	8011(6)	3265(3)	687(5)	65(2)
C(20)	6083(5)	3062(3)	2430(4)	58(2)
C(21)	6038(6)	3629(4)	3055(5)	73(2)
C(22)	5080(6)	2771(4)	2203(7)	87(2)
C(23)	9041(7)	3108(4)	603(7)	88(3)
C(24)	9661(10)	3708(7)	845(12)	167(6)

C(25)	9259(10)	2862(6)	-332(9)	125(4)
C(26)	9084(5)	1303(3)	3148(5)	64(2)
C(27)	8685(7)	892(3)	3797(5)	76(2)
C(28)	9136(8)	313(4)	3946(7)	90(3)
C(29)	9906(9)	161(4)	3437(7)	94(3)
C(30)	10304(7)	557(4)	2829(6)	87(3)
C(31)	9863(7)	1156(3)	2664(5)	74(2)
C(32)	10326(6)	1606(4)	2029(6)	81(2)
C(33)	11364(8)	1794(6)	2369(8)	114(4)
C(34)	10315(8)	1369(5)	1009(6)	103(3)
C(35)	7876(6)	1075(4)	4366(6)	79(2)
C(36)	8250(7)	1328(5)	5328(6)	91(3)
C(37)	7168(8)	528(5)	4490(8)	111(4)
C(1S)	7264(9)	-1682(9)	-183(12)	110(7)
C(2S)	6250(15)	-21(7)	-2304(8)	100(6)
Pd(1A)	4567(2)	-742(1)	-201(2)	41(1)
Cl(1A)	6053(7)	-277(5)	157(7)	60(2)
Cl(2A)	5342(7)	-1694(5)	-257(7)	63(2)
Cl(3)	6243(8)	-1935(6)	-759(8)	207(3)
Cl(4)	7955(8)	-2307(6)	152(8)	207(3)
Cl(5)	6354(4)	-711(4)	-1723(7)	149(3)
Cl(6)	6796(7)	-39(4)	-3303(5)	162(3)

Table 3. Bond lengths [Å] and angles [°] for k09220.

Pd(1)-N(4)	2.019(5)
Pd(1)-Cl(2)	2.2920(18)
Pd(1)-Cl(1)	2.3335(16)
Pd(1)-Cl(1)#1	2.3413(18)
Cl(1)-Pd(1)#1	2.3413(18)
N(1)-C(1)	1.360(7)
N(1)-C(2)	1.395(7)
N(1)-C(14)	1.438(7)
N(2)-C(1)	1.381(7)
N(2)-C(3)	1.401(7)
N(2)-C(26)	1.447(8)
N(3)-C(1)	1.313(7)
N(3)-C(4)	1.321(7)
N(4)-C(4)	1.332(7)
N(4)-C(6)	1.439(7)
N(4)-Pd(1A)#1	2.226(5)
C(2)-C(3)	1.327(9)
C(4)-C(5)	1.499(9)
C(6)-C(11)	1.370(9)
C(6)-C(7)	1.404(8)
C(7)-C(8)	1.398(9)
C(7)-C(12)	1.520(10)
C(8)-C(9)	1.392(11)
C(9)-C(10)	1.373(12)
C(10)-C(11)	1.368(11)
C(11)-C(13)	1.532(10)
C(14)-C(15)	1.375(10)
C(14)-C(19)	1.395(9)
C(15)-C(16)	1.391(9)
C(15)-C(20)	1.540(10)
C(16)-C(17)	1.374(11)
C(17)-C(18)	1.375(13)
C(18)-C(19)	1.402(11)
C(19)-C(23)	1.495(12)

C(20)-C(21)	1.507(9)
C(20)-C(22)	1.544(11)
C(23)-C(25)	1.498(14)
C(23)-C(24)	1.564(15)
C(26)-C(31)	1.378(12)
C(26)-C(27)	1.425(11)
C(27)-C(28)	1.390(11)
C(27)-C(35)	1.502(13)
C(28)-C(29)	1.391(15)
C(29)-C(30)	1.365(15)
C(30)-C(31)	1.423(11)
C(31)-C(32)	1.506(13)
C(32)-C(33)	1.547(13)
C(32)-C(34)	1.550(11)
C(35)-C(36)	1.536(11)
C(35)-C(37)	1.546(12)
C(1S)-Cl(3)	1.681(10)
C(1S)-Cl(4)	1.687(10)
C(2S)-Cl(6)	1.684(10)
C(2S)-Cl(5)	1.686(10)
Pd(1A)-N(4)#1	2.226(5)
Pd(1A)-Cl(2A)	2.296(11)
Pd(1A)-Cl(1A)	2.322(10)
Pd(1A)-Cl(1A)#1	2.332(10)
Cl(1A)-Pd(1A)#1	2.332(10)
Cl(2A)-Cl(3)	1.590(15)

N(4)-Pd(1)-Cl(2)	95.07(16)
N(4)-Pd(1)-Cl(1)	175.48(16)
Cl(2)-Pd(1)-Cl(1)	88.89(6)
N(4)-Pd(1)-Cl(1)#1	90.60(16)
Cl(2)-Pd(1)-Cl(1)#1	174.20(6)
Cl(1)-Pd(1)-Cl(1)#1	85.50(6)
Pd(1)-Cl(1)-Pd(1)#1	94.50(6)
C(1)-N(1)-C(2)	110.0(5)
C(1)-N(1)-C(14)	123.2(5)

C(2)-N(1)-C(14)	126.8(5)
C(1)-N(2)-C(3)	108.5(5)
C(1)-N(2)-C(26)	124.8(5)
C(3)-N(2)-C(26)	124.6(5)
C(1)-N(3)-C(4)	124.2(5)
C(4)-N(4)-C(6)	118.8(5)
C(4)-N(4)-Pd(1)	125.2(4)
C(6)-N(4)-Pd(1)	116.0(3)
C(4)-N(4)-Pd(1A)#1	118.7(4)
C(6)-N(4)-Pd(1A)#1	104.6(3)
Pd(1)-N(4)-Pd(1A)#1	43.31(11)
N(3)-C(1)-N(1)	124.8(5)
N(3)-C(1)-N(2)	128.7(5)
N(1)-C(1)-N(2)	105.7(4)
C(3)-C(2)-N(1)	107.4(5)
C(2)-C(3)-N(2)	108.4(5)
N(3)-C(4)-N(4)	120.3(5)
N(3)-C(4)-C(5)	122.9(5)
N(4)-C(4)-C(5)	116.7(5)
C(11)-C(6)-C(7)	122.1(6)
C(11)-C(6)-N(4)	119.7(5)
C(7)-C(6)-N(4)	118.2(5)
C(8)-C(7)-C(6)	118.3(6)
C(8)-C(7)-C(12)	120.0(6)
C(6)-C(7)-C(12)	121.7(6)
C(9)-C(8)-C(7)	119.6(7)
C(10)-C(9)-C(8)	119.2(7)
C(11)-C(10)-C(9)	122.9(7)
C(10)-C(11)-C(6)	117.8(6)
C(10)-C(11)-C(13)	121.4(6)
C(6)-C(11)-C(13)	120.7(6)
C(15)-C(14)-C(19)	123.4(6)
C(15)-C(14)-N(1)	118.6(6)
C(19)-C(14)-N(1)	118.0(6)
C(14)-C(15)-C(16)	117.5(7)
C(14)-C(15)-C(20)	122.9(5)

C(16)-C(15)-C(20)	119.5(6)
C(17)-C(16)-C(15)	121.4(8)
C(16)-C(17)-C(18)	119.6(7)
C(17)-C(18)-C(19)	121.6(8)
C(14)-C(19)-C(18)	116.4(8)
C(14)-C(19)-C(23)	122.4(7)
C(18)-C(19)-C(23)	121.2(7)
C(21)-C(20)-C(15)	110.5(6)
C(21)-C(20)-C(22)	111.2(6)
C(15)-C(20)-C(22)	112.9(6)
C(19)-C(23)-C(25)	114.9(9)
C(19)-C(23)-C(24)	108.8(8)
C(25)-C(23)-C(24)	109.4(9)
C(31)-C(26)-C(27)	124.3(7)
C(31)-C(26)-N(2)	116.4(7)
C(27)-C(26)-N(2)	119.3(7)
C(28)-C(27)-C(26)	116.2(10)
C(28)-C(27)-C(35)	119.9(8)
C(26)-C(27)-C(35)	123.7(7)
C(27)-C(28)-C(29)	119.1(10)
C(30)-C(29)-C(28)	124.8(8)
C(29)-C(30)-C(31)	117.4(10)
C(26)-C(31)-C(30)	118.0(8)
C(26)-C(31)-C(32)	124.2(7)
C(30)-C(31)-C(32)	117.6(9)
C(31)-C(32)-C(33)	114.4(8)
C(31)-C(32)-C(34)	113.5(8)
C(33)-C(32)-C(34)	108.5(8)
C(27)-C(35)-C(36)	111.4(7)
C(27)-C(35)-C(37)	113.0(8)
C(36)-C(35)-C(37)	109.3(8)
Cl(3)-C(1S)-Cl(4)	109.5(12)
Cl(6)-C(2S)-Cl(5)	112.1(10)
N(4)#1-Pd(1A)-Cl(2A)	107.0(3)
N(4)#1-Pd(1A)-Cl(1A)	162.1(3)
Cl(2A)-Pd(1A)-Cl(1A)	87.9(4)

N(4)#1-Pd(1A)-Cl(1A)#1	78.8(3)
Cl(2A)-Pd(1A)-Cl(1A)#1	173.6(4)
Cl(1A)-Pd(1A)-Cl(1A)#1	85.9(4)
Pd(1A)-Cl(1A)-Pd(1A)#1	94.1(4)
Cl(3)-Cl(2A)-Pd(1A)	134.0(8)
Cl(2A)-Cl(3)-C(1S)	110.4(10)

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for k09220. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pd(1)	39(1)	28(1)	50(1)	-3(1)	2(1)	-6(1)
Cl(1)	48(1)	41(1)	67(1)	11(1)	-6(1)	-15(1)
Cl(2)	65(1)	33(1)	60(1)	2(1)	-7(1)	-6(1)
N(1)	56(3)	29(2)	47(2)	-5(2)	-1(2)	0(2)
N(2)	68(3)	31(2)	64(3)	-5(2)	-20(3)	2(2)
N(3)	51(3)	32(2)	48(2)	-2(2)	-8(2)	-12(2)
N(4)	46(3)	48(3)	61(3)	-21(2)	12(2)	-14(2)
C(1)	47(3)	31(3)	47(3)	1(2)	-3(2)	-5(2)
C(2)	55(3)	35(3)	60(3)	-9(3)	-5(3)	-3(3)
C(3)	67(4)	40(3)	62(4)	-13(3)	-22(3)	2(3)
C(4)	42(3)	37(3)	64(3)	-12(3)	3(3)	0(2)
C(5)	56(4)	59(4)	68(4)	-22(3)	14(3)	-10(3)
C(6)	46(3)	31(3)	54(3)	-12(2)	7(2)	-11(2)
C(7)	48(3)	42(3)	56(3)	-14(3)	0(3)	-9(3)
C(8)	54(3)	68(4)	77(4)	-32(4)	17(3)	-13(3)
C(9)	84(5)	84(5)	56(4)	-8(4)	21(4)	-29(4)
C(10)	76(5)	67(5)	72(5)	14(4)	-4(4)	-15(4)
C(11)	52(3)	40(3)	77(4)	3(3)	3(3)	-17(3)
C(12)	57(4)	69(5)	86(5)	2(4)	-1(4)	5(4)
C(13)	62(4)	51(4)	89(5)	9(4)	-4(4)	-5(3)
C(14)	73(4)	30(3)	47(3)	-5(2)	-1(3)	3(3)
C(15)	81(4)	36(3)	52(3)	-2(3)	-10(3)	12(3)
C(16)	89(5)	51(4)	65(4)	-2(3)	-8(4)	25(4)
C(17)	129(7)	49(4)	55(4)	4(3)	-8(4)	28(4)
C(18)	160(9)	45(4)	51(4)	7(3)	16(5)	10(5)
C(19)	95(5)	41(3)	59(4)	4(3)	8(4)	-2(3)
C(20)	65(4)	52(4)	55(3)	1(3)	1(3)	15(3)
C(21)	86(5)	64(4)	71(4)	-14(4)	15(4)	16(4)
C(22)	90(6)	71(5)	98(6)	7(5)	-2(5)	3(5)
C(23)	95(6)	77(5)	97(6)	18(5)	39(5)	0(5)
C(24)	119(10)	164(13)	225(17)	-68(13)	57(10)	-50(10)

C(25)	153(10)	105(8)	125(9)	-16(7)	51(8)	11(8)
C(26)	81(5)	41(3)	64(4)	-16(3)	-21(4)	8(3)
C(27)	113(6)	38(3)	69(4)	8(3)	-37(4)	-8(4)
C(28)	118(7)	50(4)	92(6)	2(4)	-39(6)	1(5)
C(29)	150(10)	47(4)	77(5)	-6(4)	-44(6)	21(5)
C(30)	111(7)	68(5)	74(5)	-31(4)	-40(5)	28(5)
C(31)	108(6)	50(4)	58(4)	-8(3)	-24(4)	10(4)
C(32)	76(5)	83(6)	81(5)	-32(5)	-6(4)	24(4)
C(33)	109(7)	123(9)	104(7)	-39(7)	-31(6)	19(7)
C(34)	104(7)	125(8)	79(6)	-40(6)	-8(5)	-7(6)
C(35)	88(5)	55(4)	90(5)	16(4)	-12(5)	0(4)
C(36)	99(6)	100(7)	70(5)	11(5)	-17(4)	-6(5)
C(37)	113(8)	86(7)	129(8)	36(6)	-18(7)	-29(6)
C(1S)	100(11)	149(15)	85(10)	3(11)	36(9)	-36(11)
C(2S)	98(13)	85(12)	117(16)	-49(12)	14(12)	-7(11)
Cl(3)	187(6)	225(8)	213(7)	-42(6)	40(5)	-50(6)
Cl(4)	187(6)	225(8)	213(7)	-42(6)	40(5)	-50(6)
Cl(5)	89(4)	143(6)	225(8)	-36(6)	60(4)	-3(4)
Cl(6)	186(7)	202(7)	107(4)	-79(5)	63(5)	-15(6)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for k09220.

	x	y	z	U(eq)
H(2A)	8659	3391	3128	61
H(3A)	9340	2491	4016	69
H(5A)	6529	1654	2619	91
H(5B)	6628	902	2635	91
H(5C)	5797	1231	1973	91
H(8A)	9168	295	-1111	79
H(9A)	8696	1070	-2224	88
H(10A)	7504	1775	-1929	87
H(12A)	8510	223	1169	107
H(12B)	9145	-113	440	107
H(12C)	8047	-310	484	107
H(13A)	6158	2097	-1064	102
H(13B)	6783	2284	-123	102
H(13C)	5985	1745	-108	102
H(16A)	5428	3647	864	83
H(17A)	6180	3983	-422	94
H(18A)	7774	3734	-550	102
H(20A)	6485	2737	2783	69
H(21A)	6687	3792	3211	110
H(21B)	5755	3508	3629	110
H(21C)	5644	3957	2732	110
H(22A)	4862	2577	2765	130
H(22B)	5112	2450	1716	130
H(22C)	4629	3103	1981	130
H(23A)	9233	2777	1079	105
H(24A)	10044	3644	1440	250
H(24B)	9240	4074	896	250
H(24C)	10089	3784	351	250
H(25A)	8836	2505	-506	188
H(25B)	9928	2722	-303	188

H(25C)	9156	3197	-799	188
H(28A)	8923	25	4389	107
H(29A)	10174	-249	3518	113
H(30A)	10853	437	2526	105
H(32A)	9937	2002	2012	97
H(33A)	11370	1993	2985	171
H(33B)	11611	2092	1927	171
H(33C)	11769	1417	2412	171
H(34A)	9655	1275	769	155
H(34B)	10705	986	990	155
H(34C)	10578	1696	622	155
H(35A)	7511	1422	4027	95
H(36A)	8657	1697	5250	136
H(36B)	8624	1000	5672	136
H(36C)	7707	1450	5677	136
H(37A)	7022	315	3891	166
H(37B)	6577	696	4712	166
H(37C)	7458	226	4947	166
H(1S1)	7116	-1436	372	132
H(1S2)	7612	-1404	-592	132
H(2S1)	5562	77	-2449	120
H(2S2)	6534	320	-1899	120

Supplementary Material (ESI) for Dalton Transactions