Supplementary Material for:

First Aryl-Substituted Acyclic Imino-*N*-Heterocyclic Carbene Ligand Precursor: Synthesis and Characterisation and Coordination with Silver(I) and Copper(I)

by

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Table of Contents

Crystallographic Data

X-Ray crystallographic data for **1–3** were collected on a Bruker-Nonius Kappa-CCD diffractometer using monochromated Mo-Kα radiation (k = 0.71073 Å) at 150K and were measured using a combination of ϕ scans and ω scans with κ offsets, to fill the Ewald sphere. Intensity data were processed using the Denzo-SMN package.[3] Absorption corrections were carried out using SORTAV.[4] The structure was solved and refined using SHELXTL V6.1[5] for full-matrix least-squares refinement that was based on F^2. All H atoms were included in calculated positions and allowed to refine in riding-motion approximation with U_{iso}-tied to the carrier atom. Crystallographic data for the compounds are given below.

1-(1-(2,6-Dimethylphenylimino)ethyl)-3-(2,4,6-trimethylphenyl)imidazolium Chloride (1), C^imine·HCl

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

CCDC Deposition Number	759030	
Identification code	k09132	
Empirical formula	C23 H28 Cl3 N3	
Formula weight	452.83	
Temperature	150(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 9.0219(2) Å	a= 90°.
	b = 26.6329(7) Å	b= 113.6980(14)°.
	c = 10.7548(3) Å	g = 90°.
Volume	2366.25(10) $Å^3$	
Z	4	
Density (calculated)	1.271 Mg/m^3	
Absorption coefficient	0.401 mm^{-1}	
F(000)	952	
Crystal size	0.30 x 0.22 x 0.12 mm^3	
Theta range for data collection	2.57 to 25.00°.	
Index ranges	-10<=h<=9, -31<=k<=31, -10<=l<=12	
Reflections collected	20220	
Independent reflections	4151 [R(int) = 0.1302]	
Completeness to theta = 25.00°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.955 and 0.475	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4151 / 0 / 268	
Goodness-of-fit on F^2	1.076	
Final R indices [I>2sigma(I)]	R1 = 0.0582, wR2 = 0.1383	
R indices (all data)	R1 = 0.1043, wR2 = 0.1799	
Largest diff. peak and hole	0.334 and -0.422 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for k09132. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	3966(1)	4902(1)	6914(1)	36(1)
N(1)	1479(3)	5418(1)	3147(3)	30(1)
N(2)	1637(3)	4626(1)	3587(3)	28(1)
N(3)	1287(3)	3817(1)	4094(3)	33(1)
C(1)	2445(4)	5023(1)	3414(4)	29(1)
C(2)	90(4)	4776(1)	3417(4)	30(1)
C(3)	-9(4)	5270(1)	3142(4)	32(1)
C(4)	2271(4)	4123(1)	3950(3)	28(1)
C(5)	3964(4)	4048(1)	4108(4)	36(1)
C(6)	1747(4)	3303(1)	4417(4)	32(1)
C(7)	2602(4)	3157(1)	5768(4)	36(1)
C(8)	2930(5)	2643(1)	6007(5)	46(1)
C(9)	2418(5)	2297(1)	4967(4)	45(1)
C(10)	1532(5)	2453(1)	3651(4)	42(1)
C(11)	1170(4)	2958(1)	3351(4)	36(1)
C(12)	3132(5)	3528(2)	6923(4)	50(1)
C(13)	160(5)	3134(2)	1931(4)	50(1)
C(14)	1867(4)	5920(1)	2841(4)	30(1)
C(15)	1989(4)	6000(1)	1609(4)	32(1)
C(16)	2322(4)	6487(1)	1330(4)	35(1)
C(17)	2510(4)	6881(1)	2228(4)	35(1)
C(18)	2405(4)	6776(1)	3461(4)	36(1)
C(19)	2086(4)	6295(1)	3797(4)	30(1)
C(20)	1793(5)	5583(1)	602(4)	41(1)
C(21)	2783(5)	7409(1)	1860(4)	46(1)
C(22)	2004(5)	6197(1)	5142(4)	38(1)
Cl(2)	2423(1)	4188(1)	107(1)	54(1)
Cl(3)	5649(1)	3753(1)	1068(1)	54(1)
C(23)	4441(5)	4283(1)	303(4)	45(1)

Table 3. Bond lengths [Å] and angles [°] for k09132.

	N(1)-C(1)	1.323(4)
	N(1)-C(3)	1.398(4)
	N(1)-C(14)	1.452(4)
	N(2)-C(1)	1.338(4)
	N(2)-C(2)	1.391(4)
	N(2)-C(4)	1.447(4)
	N(3)-C(4)	1.262(4)
	N(3)-C(6)	1.432(4)
	C(2)-C(3)	1.344(5)
	C(4)-C(5)	1.480(5)
	C(6)-C(11)	1.395(5)
	C(6)-C(7)	1.399(5)
	C(7)-C(8)	1.402(5)
	C(7)-C(12)	1.506(5)
	C(8)-C(9)	1.378(6)
	C(9)-C(10)	1.381(6)
	C(10)-C(11)	1.391(5)
	C(11)-C(13)	1.505(5)
	C(14)-C(15)	1.389(5)
	C(14)-C(19)	1.390(5)
	C(15)-C(16)	1.389(5)
	C(15)-C(20)	1.513(5)
	C(16)-C(17)	1.390(5)
	C(17)-C(18)	1.395(5)
	C(17)-C(21)	1.509(5)
	C(18)-C(19)	1.393(5)
	C(19)-C(22)	1.501(5)
	Cl(2)-C(23)	1.765(4)
	Cl(3)-C(23)	1.773(4)
	C(1)-N(1)-C(3)	108.9(3)
	C(1)-N(1)-C(14)	125.8(3)

	C(3)-N(1)-C(14)	125.3(3)
	C(1)-N(2)-C(2)	109.3(3)
	C(1)-N(2)-C(4)	126.1(3)
	C(2)-N(2)-C(4)	124.6(3)
	C(4)-N(3)-C(6)	120.0(3)
	N(1)-C(1)-N(2)	108.1(3)
	C(3)-C(2)-N(2)	106.5(3)
	C(2)-C(3)-N(1)	107.3(3)
	N(3)-C(4)-N(2)	114.3(3)
	N(3)-C(4)-C(5)	130.0(3)
	N(2)-C(4)-C(5)	115.8(3)
	C(11)-C(6)-C(7)	122.6(3)
	C(11)-C(6)-N(3)	116.9(3)
	C(7)-C(6)-N(3)	120.2(3)
	C(6)-C(7)-C(8)	116.7(4)
	C(6)-C(7)-C(12)	122.3(3)
	C(8)-C(7)-C(12)	121.0(4)
	C(9)-C(8)-C(7)	121.8(4)
	C(8)-C(9)-C(10)	119.8(3)
	C(9)-C(10)-C(11)	121.0(4)
	C(10)-C(11)-C(6)	118.0(4)
	C(10)-C(11)-C(13)	121.8(4)
	C(6)-C(11)-C(13)	120.2(3)
	C(15)-C(14)-C(19)	123.5(3)
	C(15)-C(14)-N(1)	118.5(3)
	C(19)-C(14)-N(1)	118.0(3)
	C(16)-C(15)-C(14)	117.2(3)
	C(16)-C(15)-C(20)	120.3(3)
	C(14)-C(15)-C(20)	122.5(3)
	C(15)-C(16)-C(17)	122.0(4)
	C(16)-C(17)-C(18)	118.3(3)
	C(16)-C(17)-C(21)	120.6(3)
	C(18)-C(17)-C(21)	121.0(3)
	C(19)-C(18)-C(17)	122.0(3)
	C(14)-C(19)-C(18)	116.9(3)
	C(14)-C(19)-C(22)	122.7(3)

C(18)-C(19)-C(22)	120.3(3)
Cl(2)-C(23)-Cl(3)	110.7(2)

Symmetry transformations used to generate equivalent atoms:

5

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for k09132. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

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

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for k09132.

	x	y	z	U(eq)
H(1A)	3524	5020	3473	35
H(2A)	-734	4569	3483	36
H(3A)	-921	5480	2976	38
H(5A)	4229	3690	4227	54
H(5B)	4696	4234	4905	54
H(5C)	4087	4171	3296	54
H(8A)	3521	2531	6911	56
H(9A)	2673	1951	5156	54
H(10A)	1164	2212	2940	50
H(12A)	3762	3796	6744	75
H(12B)	3802	3356	7769	75
H(12C)	2177	3672	7008	75
H(13A)	-753	3333	1932	76
H(13B)	-249	2843	1333	76
H(13C)	825	3342	1601	76
H(16A)	2423	6552	499	42
H(18A)	2556	7042	4091	43
H(20A)	881	5368	536	61
H(20B)	2785	5381	909	61
H(20C)	1585	5727	-290	61
H(21A)	3332	7605	2691	69
H(21B)	1739	7565	1313	69
H(21C)	3456	7401	1337	69
H(22A)	2535	6472	5769	57
H(22B)	2554	5880	5517	57
H(22C)	869	6175	5019	57
H(23A)	4889	4583	874	55
H(23B)	4465	4344	-597	55

Chloro[1-(1-(2,6-dimethylphenylimino)ethyl)-3-(2,4,6-trimethylphenyl)imidazol-2-ylidene]silver(I), Ag(C^imine)Cl (2)

Table 6. Crystal data and structure refinement for Compound **2**.

CCDC Deposition Number	759031	
Identification code	k09165	
Empirical formula	C23 H27 Ag Cl3 N3	
Formula weight	559.70	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 9.1037(2) Å	a= 90°.
	b = 15.7675(3) Å	b= 90°.
	c = 17.1993(3) Å	g = 90°.
Volume	2468.83(8) $Å^3$	
Z	4	
Density (calculated)	1.506 Mg/m^3	
Absorption coefficient	1.156 mm^{-1}	
F(000)	1136	
Crystal size	0.30 x 0.26 x 0.22 mm^3	
Theta range for data collection	2.58 to 27.49°.	
Index ranges	-11<=h<=11, -20<=k<=20, -22<=l<=22	
Reflections collected	22758	
Independent reflections	5650 [R(int) = 0.0371]	
Completeness to theta = 27.49°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.773 and 0.724	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5650 / 6 / 305	
Goodness-of-fit on F^2	1.075	
Final R indices [I>2sigma(I)]	R1 = 0.0349, wR2 = 0.0770	
R indices (all data)	R1 = 0.0439, wR2 = 0.0824	
Absolute structure parameter	-0.08(3)	
Largest diff. peak and hole	1.169 and -0.560 e.$Å^{-3}$	

Table 7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for k09165. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ag(1)	6348(1)	8051(1)	6550(1)	29(1)
Cl(1)	6751(1)	9474(1)	6239(1)	35(1)
N(1)	5688(3)	6407(2)	7448(2)	27(1)
N(2)	5953(3)	6117(2)	6242(2)	30(1)
N(3)	5628(4)	7662(2)	8132(2)	30(1)
C(1)	5998(4)	6770(2)	6751(2)	28(1)
C(2)	5604(4)	5358(2)	6617(2)	32(1)
C(3)	5448(4)	5537(2)	7366(2)	33(1)
C(4)	5647(4)	6863(2)	8173(2)	27(1)
C(5)	5653(5)	6313(2)	8882(2)	38(1)
C(6)	5616(4)	8167(2)	8821(2)	30(1)
C(7)	4349(5)	8244(2)	9271(2)	34(1)
C(8)	4397(5)	8803(3)	9907(2)	40(1)
C(9)	5651(5)	9261(2)	10080(2)	42(1)
C(10)	6891(5)	9180(2)	9627(2)	39(1)
C(11)	6893(5)	8633(2)	8983(2)	36(1)
C(12)	2954(5)	7787(3)	9079(2)	44(1)
C(13)	8251(5)	8538(3)	8488(3)	54(1)
C(14)	6207(4)	6195(2)	5410(2)	28(1)
C(15)	5120(4)	6544(2)	4946(2)	32(1)
C(16)	5409(5)	6602(3)	4147(2)	36(1)
C(17)	6697(5)	6304(3)	3826(2)	39(1)
C(18)	7756(5)	5959(3)	4313(2)	37(1)
C(19)	7536(4)	5895(2)	5111(2)	34(1)
C(20)	3668(4)	6820(2)	5269(2)	36(1)
C(21)	6995(6)	6387(4)	2963(2)	61(1)
C(22)	8713(5)	5530(3)	5627(2)	47(1)
Cl(2)	5759(8)	3720(5)	2835(4)	74(2)
Cl(3)	3205(11)	3577(9)	2078(6)	106(3)

C(24)	4180(13)	4293(13)	2642(14)	109(11)
Cl(2A)	5866(8)	4140(13)	2846(4)	112(4)
Cl(3A)	3131(7)	3969(7)	1969(4)	71(2)
C(24A)	3968(9)	4106(15)	2865(8)	53(4)

Table 8. Bond lengths [Å] and angles [°] for k09165.

	Ag(1)-C(1)	2.074(3)
	Ag(1)-Cl(1)	2.3346(9)
	N(1)-C(1)	1.359(4)
	N(1)-C(3)	1.397(5)
	N(1)-C(4)	1.439(4)
	N(2)-C(1)	1.352(4)
	N(2)-C(2)	1.397(4)
	N(2)-C(14)	1.455(4)
	N(3)-C(4)	1.263(5)
	N(3)-C(6)	1.426(4)
	C(2)-C(3)	1.327(5)
	C(4)-C(5)	1.497(5)
	C(6)-C(7)	1.395(5)
	C(6)-C(11)	1.403(5)
	C(7)-C(8)	1.404(5)
	C(7)-C(12)	1.497(6)
	C(8)-C(9)	1.383(6)
	C(9)-C(10)	1.378(6)
	C(10)-C(11)	1.403(5)
	C(11)-C(13)	1.509(6)
	C(14)-C(15)	1.385(5)
	C(14)-C(19)	1.397(5)
	C(15)-C(16)	1.402(5)
	C(15)-C(20)	1.499(6)
	C(16)-C(17)	1.378(6)
	C(17)-C(18)	1.388(6)
	C(17)-C(21)	1.516(5)
	C(18)-C(19)	1.390(5)
	C(19)-C(22)	1.506(6)
	Cl(2)-C(24)	1.731(8)
	Cl(3)-C(24)	1.733(8)
	Cl(2A)-C(24A)	1.729(8)
	Cl(3A)-C(24A)	1.733(8)

	C(1)-Ag(1)-Cl(1)	176.29(9)
	C(1)-N(1)-C(3)	110.9(3)
	C(1)-N(1)-C(4)	124.0(3)
	C(3)-N(1)-C(4)	125.1(3)
	C(1)-N(2)-C(2)	111.2(3)
	C(1)-N(2)-C(14)	124.6(3)
	C(2)-N(2)-C(14)	124.2(3)
	C(4)-N(3)-C(6)	120.7(3)
	N(2)-C(1)-N(1)	104.1(3)
	N(2)-C(1)-Ag(1)	129.7(2)
	N(1)-C(1)-Ag(1)	126.1(2)
	C(3)-C(2)-N(2)	106.8(3)
	C(2)-C(3)-N(1)	106.9(3)
	N(3)-C(4)-N(1)	116.8(3)
	N(3)-C(4)-C(5)	128.5(3)
	N(1)-C(4)-C(5)	114.7(3)
	C(7)-C(6)-C(11)	121.9(3)
	C(7)-C(6)-N(3)	121.1(3)
	C(11)-C(6)-N(3)	116.8(3)
	C(6)-C(7)-C(8)	117.5(4)
	C(6)-C(7)-C(12)	122.4(3)
	C(8)-C(7)-C(12)	120.1(4)
	C(9)-C(8)-C(7)	121.4(4)
	C(10)-C(9)-C(8)	120.4(3)
	C(9)-C(10)-C(11)	120.3(4)
	C(10)-C(11)-C(6)	118.5(4)
	C(10)-C(11)-C(13)	120.5(4)
	C(6)-C(11)-C(13)	121.0(3)
	C(15)-C(14)-C(19)	122.7(3)
	C(15)-C(14)-N(2)	119.2(3)
	C(19)-C(14)-N(2)	118.1(3)
	C(14)-C(15)-C(16)	117.2(4)
	C(14)-C(15)-C(20)	122.1(3)
	C(16)-C(15)-C(20)	120.6(4)
	C(17)-C(16)-C(15)	121.9(4)

C(16)-C(17)-C(18)	118.9(3)
C(16)-C(17)-C(21)	121.0(4)
C(18)-C(17)-C(21)	120.1(4)
C(17)-C(18)-C(19)	121.6(4)
C(18)-C(19)-C(14)	117.6(4)
C(18)-C(19)-C(22)	120.4(4)
C(14)-C(19)-C(22)	121.9(3)
Cl(2)-C(24)-Cl(3)	101.1(11)
Cl(2A)-C(24A)-Cl(3A)	115.2(8)

Symmetry transformations used to generate equivalent atoms:

Table 9. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for k09165. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ag(1)	35(1)	26(1)	28(1)	0(1)	2(1)	-3(1)
Cl(1)	40(1)	27(1)	37(1)	0(1)	6(1)	-3(1)
N(1)	36(2)	24(1)	22(1)	2(1)	-1(1)	-3(1)
N(2)	36(2)	28(1)	25(1)	-4(1)	6(1)	-7(1)
N(3)	35(2)	33(2)	23(1)	-2(1)	1(1)	-2(1)
C(1)	28(2)	30(2)	26(2)	-2(1)	-1(1)	-1(1)
C(2)	41(2)	24(2)	31(2)	2(2)	-3(2)	-7(2)
C(3)	43(2)	26(2)	29(2)	0(1)	-3(2)	-5(2)
C(4)	27(2)	32(2)	22(1)	-4(1)	-2(1)	-2(2)
C(5)	55(3)	32(2)	25(2)	1(2)	-6(2)	-2(2)
C(6)	42(2)	27(2)	22(2)	1(1)	0(2)	0(2)
C(7)	42(2)	37(2)	24(2)	3(1)	-1(2)	-3(2)
C(8)	57(3)	40(2)	22(2)	1(2)	5(2)	8(2)
C(9)	71(3)	32(2)	21(2)	-2(2)	-6(2)	0(2)
C(10)	51(2)	31(2)	35(2)	0(2)	-9(2)	-1(2)
C(11)	44(2)	33(2)	30(2)	0(2)	-4(2)	-2(2)
C(12)	46(2)	51(2)	34(2)	0(2)	5(2)	-5(2)
C(13)	48(3)	61(3)	54(3)	-14(2)	2(2)	-14(2)
C(14)	37(2)	27(2)	21(2)	-5(1)	0(2)	-6(2)
C(15)	35(2)	30(2)	30(2)	-1(2)	-3(2)	-2(2)
C(16)	38(2)	41(2)	29(2)	1(2)	-4(2)	-2(2)
C(17)	43(3)	47(2)	26(2)	-3(2)	4(2)	-5(2)
C(18)	36(2)	41(2)	34(2)	-7(2)	6(2)	-2(2)
C(19)	35(2)	32(2)	33(2)	-4(2)	0(2)	1(2)
C(20)	34(2)	44(2)	30(2)	-3(2)	-4(2)	4(2)
C(21)	62(3)	90(4)	30(2)	5(2)	9(2)	-3(3)
C(22)	44(2)	57(2)	40(2)	2(2)	-3(2)	10(2)
Cl(2)	47(3)	112(4)	64(2)	0(2)	-16(2)	33(3)
Cl(3)	83(4)	135(6)	100(4)	-34(4)	-12(3)	-37(4)
C(24)	71(11)	150(20)	111(16)	-73(16)	20(10)	24(11)

Cl(2A)	50(3)	234(11)	53(2)	-25(5)	6(2)	-44(5)
Cl(3A)	37(2)	127(6)	49(2)	-9(3)	-10(1)	5(3)
C(24A)	25(6)	98(10)	36(5)	-19(6)	1(5)	6(6)

Table 10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for k09165.

	x	y	z	U(eq)
H(2A)	5499	4816	6380	39
H(3A)	5217	5147	7769	39
H(5A)	5698	6671	9348	56
H(5B)	6510	5938	8869	56
H(5C)	4754	5972	8895	56
H(8A)	3550	8867	10224	47
H(9A)	5657	9634	10513	50
H(10A)	7748	9495	9750	47
H(12A)	2917	7676	8518	66
H(12B)	2112	8137	9229	66
H(12C)	2922	7248	9362	66
H(13A)	8013	8675	7947	82
H(13B)	8608	7953	8519	82
H(13C)	9014	8925	8676	82
H(16A)	4696	6854	3817	43
H(18A)	8652	5761	4096	44
H(20A)	3825	7131	5755	54
H(20B)	3057	6320	5370	54
H(20C)	3173	7189	4892	54
H(21A)	6131	6630	2705	91
H(21B)	7202	5826	2744	91
H(21C)	7843	6759	2881	91
H(22A)	9647	5516	5344	71
H(22B)	8439	4953	5781	71
H(22C)	8819	5885	6092	71
H(24A)	4399	4820	2352	131
H(24B)	3644	4437	3126	131
H(24C)	3603	4641	3097	64
H(24D)	3661	3636	3211	64

Chlorobis[1-(1-(2,6-dimethylphenylimino)ethyl)-3-(2,4,6-trimethylphenyl)-imidazol-2-ylidene]copper(I), Cu(C^imine)$_2$Cl (3)

Table 11. Crystal data and structure refinement for Compound **3**.

CCDC Deposition Number	759032	
Identification code	k09221	
Empirical formula	C47 H56 Cl7 Cu N6	
Formula weight	1016.67	
Temperature	150(1) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 11.1810(3) Å	a= 98.178(2)°.
	b = 11.2363(3) Å	b= 90.697(2)°.
	c = 24.0984(9) Å	g = 116.143(2)°.
Volume	2680.63(14) Å^3	
Z	2	
Density (calculated)	1.260 Mg/m^3	
Absorption coefficient	0.792 mm^{-1}	
F(000)	1056	
Crystal size	0.40 x 0.18 x 0.14 mm^3	
Theta range for data collection	2.55 to 25.00°.	
Index ranges	-13<=h<=13, -13<=k<=13, -28<=l<=28	
Reflections collected	24919	
Independent reflections	9381 [R(int) = 0.063]	
Completeness to theta = 25.00°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.695 and 0.566	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9381 / 0 / 561	
Goodness-of-fit on F^2	1.082	
Final R indices [I>2sigma(I)]	R1 = 0.0582, wR2 = 0.1631	
R indices (all data)	R1 = 0.0775, wR2 = 0.1759	
Largest diff. peak and hole	1.091 and -1.022 e.Å^{-3}	

Table 12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for k09221. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cu(1)	7555(1)	4858(1)	2495(1)	28(1)
Cl(1)	8952(1)	3723(1)	2287(1)	43(1)
N(1)	5115(3)	3404(3)	1747(1)	28(1)
N(2)	4864(3)	2397(3)	2455(1)	27(1)
N(3)	4007(3)	996(3)	3098(1)	30(1)
N(4)	9245(3)	7090(3)	3369(1)	30(1)
N(5)	9905(3)	7634(3)	2572(1)	27(1)
N(6)	11075(3)	8631(3)	1864(1)	33(1)
C(1)	5746(3)	3514(3)	2246(2)	26(1)
C(2)	3735(3)	1625(3)	2076(2)	32(1)
C(3)	3892(3)	2249(3)	1634(2)	33(1)
C(4)	5608(3)	4326(3)	1351(2)	29(1)
C(5)	6212(3)	3992(4)	890(2)	32(1)
C(6)	6620(4)	4854(4)	497(2)	40(1)
C(7)	6455(4)	6023(4)	559(2)	40(1)
C(8)	5892(4)	6337(4)	1029(2)	40(1)
C(9)	5439(3)	5498(4)	1440(2)	33(1)
C(10)	6418(4)	2735(4)	827(2)	45(1)
C(11)	6929(5)	6959(5)	122(2)	60(1)
C(12)	4819(4)	5854(4)	1942(2)	42(1)
C(13)	5010(3)	2008(3)	2982(1)	26(1)
C(14)	6310(3)	2837(4)	3327(2)	36(1)
C(15)	3976(3)	488(3)	3608(2)	29(1)
C(16)	4084(4)	-713(4)	3586(2)	36(1)
C(17)	3899(4)	-1298(4)	4072(2)	39(1)
C(18)	3594(4)	-731(4)	4558(2)	42(1)
C(19)	3473(4)	449(4)	4572(2)	40(1)
C(20)	3656(3)	1072(4)	4099(2)	35(1)
C(21)	4350(5)	-1373(4)	3052(2)	56(1)

	C(22)	3487(4)	2342(4)	4114(2)	45(1)
	C(23)	8925(3)	6629(3)	2810(2)	28(1)
	C(24)	10795(3)	8673(3)	2982(2)	33(1)
	C(25)	10380(3)	8326(3)	3480(2)	35(1)
	C(26)	8584(3)	6350(3)	3804(2)	29(1)
	C(27)	9132(3)	5601(3)	4023(2)	32(1)
	C(28)	8505(4)	4913(4)	4461(2)	35(1)
	C(29)	7382(4)	4974(4)	4670(2)	34(1)
	C(30)	6863(4)	5722(4)	4437(2)	36(1)
	C(31)	7450(3)	6431(3)	4006(2)	32(1)
	C(32)	10333(4)	5503(4)	3794(2)	44(1)
	C(33)	6707(4)	4193(4)	5135(2)	47(1)
	C(34)	6855(4)	7234(4)	3749(2)	48(1)
	C(35)	10077(3)	7634(3)	1986(2)	28(1)
	C(36)	9073(3)	6463(4)	1589(2)	35(1)
	C(37)	11404(3)	8765(4)	1298(2)	34(1)
	C(38)	10868(4)	9408(4)	987(2)	41(1)
	C(39)	11377(4)	9718(4)	472(2)	50(1)
	C(40)	12360(5)	9382(5)	270(2)	54(1)
	C(41)	12850(4)	8731(5)	582(2)	51(1)
	C(42)	12370(4)	8396(4)	1094(2)	42(1)
	C(43)	12900(5)	7671(5)	1430(2)	59(1)
	C(44)	9798(5)	9756(5)	1209(2)	54(1)
	Cl(7)	10210(2)	4402(2)	525(1)	87(1)
	Cl(6)	11554(2)	3367(2)	1214(1)	84(1)
	Cl(2)	11043(1)	1978(1)	2855(1)	82(1)
	Cl(3)	13120(1)	4694(1)	3261(1)	63(1)
	C(1S)	11903(4)	3603(5)	2717(2)	56(1)
	Cl(4)	6468(2)	39(1)	1709(1)	107(1)
	Cl(5)	7759(1)	-964(1)	2442(1)	59(1)
	C(2S)	7647(5)	445(5)	2259(3)	66(1)
	C(3S)	10009(5)	3224(5)	957(2)	62(1)

Table 13. Bond lengths [Å] and angles [°] for k09221.

	Cu(1)-C(23)	1.933(3)
	Cu(1)-C(1)	1.937(3)
	Cu(1)-Cl(1)	2.4313(10)
	N(1)-C(1)	1.350(4)
	N(1)-C(3)	1.399(4)
	N(1)-C(4)	1.441(4)
	N(2)-C(1)	1.379(4)
	N(2)-C(2)	1.401(4)
	N(2)-C(13)	1.431(4)
	N(3)-C(13)	1.266(4)
	N(3)-C(15)	1.420(4)
	N(4)-C(23)	1.355(5)
	N(4)-C(25)	1.394(4)
	N(4)-C(26)	1.435(4)
	N(5)-C(23)	1.385(4)
	N(5)-C(24)	1.398(4)
	N(5)-C(35)	1.427(4)
	N(6)-C(35)	1.259(4)
	N(6)-C(37)	1.429(5)
	C(2)-C(3)	1.328(5)
	C(4)-C(5)	1.398(5)
	C(4)-C(9)	1.399(5)
	C(5)-C(6)	1.388(5)
	C(5)-C(10)	1.516(5)
	C(6)-C(7)	1.393(6)
	C(7)-C(8)	1.381(6)
	C(7)-C(11)	1.527(5)
	C(8)-C(9)	1.408(5)
	C(9)-C(12)	1.494(5)
	C(13)-C(14)	1.493(5)
	C(15)-C(20)	1.399(5)
	C(15)-C(16)	1.401(5)
	C(16)-C(17)	1.398(5)

	C(16)-C(21)	1.492(6)
	C(17)-C(18)	1.371(6)
	C(18)-C(19)	1.388(6)
	C(19)-C(20)	1.391(5)
	C(20)-C(22)	1.516(6)
	C(24)-C(25)	1.339(5)
	C(26)-C(27)	1.393(5)
	C(26)-C(31)	1.398(5)
	C(27)-C(28)	1.405(5)
	C(27)-C(32)	1.500(5)
	C(28)-C(29)	1.384(5)
	C(29)-C(30)	1.384(5)
	C(29)-C(33)	1.521(5)
	C(30)-C(31)	1.391(5)
	C(31)-C(34)	1.523(5)
	C(35)-C(36)	1.491(5)
	C(37)-C(42)	1.389(6)
	C(37)-C(38)	1.403(6)
	C(38)-C(39)	1.397(6)
	C(38)-C(44)	1.496(6)
	C(39)-C(40)	1.383(7)
	C(40)-C(41)	1.379(7)
	C(41)-C(42)	1.386(6)
	C(42)-C(43)	1.509(6)
	Cl(7)-C(3S)	1.737(5)
	Cl(6)-C(3S)	1.760(5)
	Cl(2)-C(1S)	1.732(5)
	Cl(3)-C(1S)	1.761(5)
	Cl(4)-C(2S)	1.720(5)
	Cl(5)-C(2S)	1.757(5)

C(23)-Cu(1)-C(1)	155.34(14)
C(23)-Cu(1)-Cl(1)	99.29(10)
C(1)-Cu(1)-Cl(1)	105.35(10)
C(1)-N(1)-C(3)	112.6(3)
C(1)-N(1)-C(4)	126.0(3)

	C(3)-N(1)-C(4)	121.4(3)
	C(1)-N(2)-C(2)	111.1(3)
	C(1)-N(2)-C(13)	127.4(3)
	C(2)-N(2)-C(13)	121.5(3)
	C(13)-N(3)-C(15)	122.6(3)
	C(23)-N(4)-C(25)	112.3(3)
	C(23)-N(4)-C(26)	124.6(3)
	C(25)-N(4)-C(26)	122.9(3)
	C(23)-N(5)-C(24)	111.6(3)
	C(23)-N(5)-C(35)	126.5(3)
	C(24)-N(5)-C(35)	121.9(3)
	C(35)-N(6)-C(37)	122.5(3)
	N(1)-C(1)-N(2)	102.9(3)
	N(1)-C(1)-Cu(1)	123.7(2)
	N(2)-C(1)-Cu(1)	132.9(3)
	C(3)-C(2)-N(2)	107.0(3)
	C(2)-C(3)-N(1)	106.4(3)
	C(5)-C(4)-C(9)	123.1(3)
	C(5)-C(4)-N(1)	118.3(3)
	C(9)-C(4)-N(1)	118.6(3)
	C(6)-C(5)-C(4)	117.7(3)
	C(6)-C(5)-C(10)	121.5(4)
	C(4)-C(5)-C(10)	120.8(3)
	C(5)-C(6)-C(7)	121.6(4)
	C(8)-C(7)-C(6)	118.8(3)
	C(8)-C(7)-C(11)	120.7(4)
	C(6)-C(7)-C(11)	120.4(4)
	C(7)-C(8)-C(9)	122.5(4)
	C(4)-C(9)-C(8)	116.2(3)
	C(4)-C(9)-C(12)	122.4(3)
	C(8)-C(9)-C(12)	121.4(3)
	N(3)-C(13)-N(2)	115.3(3)
	N(3)-C(13)-C(14)	128.1(3)
	N(2)-C(13)-C(14)	116.6(3)
	C(20)-C(15)-C(16)	121.0(3)
	C(20)-C(15)-N(3)	120.2(3)

	C(16)-C(15)-N(3)	118.2(3)
	C(17)-C(16)-C(15)	118.3(4)
	C(17)-C(16)-C(21)	120.8(4)
	C(15)-C(16)-C(21)	120.8(3)
5	C(18)-C(17)-C(16)	121.3(4)
	C(17)-C(18)-C(19)	119.8(4)
	C(18)-C(19)-C(20)	121.0(4)
	C(19)-C(20)-C(15)	118.6(4)
	C(19)-C(20)-C(22)	120.6(4)
10	C(15)-C(20)-C(22)	120.8(3)
	N(4)-C(23)-N(5)	102.8(3)
	N(4)-C(23)-Cu(1)	124.2(2)
	N(5)-C(23)-Cu(1)	132.5(3)
	C(25)-C(24)-N(5)	106.3(3)
15	C(24)-C(25)-N(4)	107.1(3)
	C(27)-C(26)-C(31)	122.1(3)
	C(27)-C(26)-N(4)	118.0(3)
	C(31)-C(26)-N(4)	119.9(3)
	C(26)-C(27)-C(28)	117.7(3)
20	C(26)-C(27)-C(32)	121.4(3)
	C(28)-C(27)-C(32)	120.9(3)
	C(29)-C(28)-C(27)	121.6(4)
	C(28)-C(29)-C(30)	118.9(3)
	C(28)-C(29)-C(33)	120.3(4)
25	C(30)-C(29)-C(33)	120.7(3)
	C(29)-C(30)-C(31)	121.8(3)
	C(30)-C(31)-C(26)	117.9(3)
	C(30)-C(31)-C(34)	121.2(3)
	C(26)-C(31)-C(34)	120.9(3)
30	N(6)-C(35)-N(5)	115.7(3)
	N(6)-C(35)-C(36)	127.3(3)
	N(5)-C(35)-C(36)	117.0(3)
	C(42)-C(37)-C(38)	121.5(4)
	C(42)-C(37)-N(6)	118.7(3)
35	C(38)-C(37)-N(6)	119.4(4)
	C(39)-C(38)-C(37)	117.7(4)

	C(39)-C(38)-C(44)	121.9(4)
	C(37)-C(38)-C(44)	120.4(4)
	C(40)-C(39)-C(38)	121.3(4)
	C(41)-C(40)-C(39)	119.6(4)
	C(40)-C(41)-C(42)	121.2(4)
	C(41)-C(42)-C(37)	118.7(4)
	C(41)-C(42)-C(43)	121.0(4)
	C(37)-C(42)-C(43)	120.3(4)
	Cl(2)-C(1S)-Cl(3)	113.3(3)
	Cl(4)-C(2S)-Cl(5)	113.0(3)
	Cl(7)-C(3S)-Cl(6)	111.9(3)

Symmetry transformations used to generate equivalent atoms:

Table 14. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for k09221. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu(1)	24(1)	23(1)	30(1)	9(1)	-2(1)	2(1)
Cl(1)	40(1)	37(1)	58(1)	12(1)	3(1)	20(1)
N(1)	23(1)	25(1)	27(2)	8(1)	-1(1)	3(1)
N(2)	25(1)	24(1)	26(2)	7(1)	0(1)	5(1)
N(3)	33(2)	28(2)	25(2)	9(1)	0(1)	8(1)
N(4)	28(1)	27(2)	30(2)	10(1)	2(1)	5(1)
N(5)	26(1)	22(1)	27(2)	7(1)	-1(1)	4(1)
N(6)	31(2)	27(2)	33(2)	10(1)	0(1)	3(1)
C(1)	25(2)	21(2)	29(2)	8(1)	2(1)	6(1)
C(2)	26(2)	24(2)	31(2)	9(2)	-4(1)	-3(1)
C(3)	25(2)	29(2)	32(2)	8(2)	-5(2)	0(2)
C(4)	24(2)	29(2)	27(2)	12(2)	-3(1)	5(1)
C(5)	28(2)	31(2)	31(2)	6(2)	-2(2)	7(2)
C(6)	35(2)	43(2)	29(2)	8(2)	2(2)	6(2)
C(7)	34(2)	45(2)	33(2)	20(2)	-3(2)	6(2)
C(8)	34(2)	33(2)	49(3)	17(2)	-1(2)	10(2)
C(9)	28(2)	31(2)	36(2)	12(2)	0(2)	7(2)
C(10)	51(2)	41(2)	41(2)	5(2)	10(2)	20(2)
C(11)	58(3)	65(3)	52(3)	37(2)	9(2)	16(2)
C(12)	43(2)	35(2)	49(3)	11(2)	12(2)	17(2)
C(13)	28(2)	22(2)	24(2)	6(1)	0(1)	6(1)
C(14)	32(2)	30(2)	34(2)	12(2)	-5(2)	3(2)
C(15)	24(2)	28(2)	28(2)	10(2)	-2(1)	3(1)
C(16)	36(2)	31(2)	39(2)	14(2)	5(2)	11(2)
C(17)	43(2)	33(2)	43(2)	17(2)	3(2)	15(2)
C(18)	41(2)	43(2)	37(2)	21(2)	-1(2)	10(2)
C(19)	40(2)	45(2)	30(2)	9(2)	3(2)	13(2)
C(20)	32(2)	34(2)	32(2)	9(2)	-3(2)	8(2)
C(21)	79(3)	45(2)	51(3)	19(2)	21(2)	33(2)
C(22)	53(2)	43(2)	40(2)	6(2)	3(2)	21(2)

	C(23)	24(2)	28(2)	31(2)	10(2)	1(1)	10(1)
	C(24)	27(2)	23(2)	36(2)	6(2)	-1(2)	-1(1)
	C(25)	32(2)	25(2)	31(2)	3(2)	-5(2)	-2(2)
	C(26)	31(2)	24(2)	27(2)	8(1)	-1(1)	5(1)
5	C(27)	28(2)	30(2)	33(2)	9(2)	0(2)	7(2)
	C(28)	36(2)	34(2)	32(2)	8(2)	-6(2)	12(2)
	C(29)	38(2)	33(2)	25(2)	5(2)	2(2)	9(2)
	C(30)	35(2)	35(2)	36(2)	7(2)	8(2)	12(2)
	C(31)	34(2)	27(2)	30(2)	4(2)	1(2)	10(2)
10	C(32)	37(2)	52(2)	48(3)	20(2)	6(2)	22(2)
	C(33)	50(2)	51(2)	36(2)	22(2)	4(2)	14(2)
	C(34)	53(2)	46(2)	56(3)	16(2)	8(2)	29(2)
	C(35)	26(2)	26(2)	32(2)	7(2)	0(1)	10(2)
	C(36)	33(2)	30(2)	30(2)	8(2)	-2(2)	2(2)
15	C(37)	32(2)	29(2)	26(2)	7(2)	-3(2)	-1(2)
	C(38)	41(2)	32(2)	36(2)	9(2)	-4(2)	2(2)
	C(39)	56(3)	44(2)	37(2)	18(2)	-6(2)	8(2)
	C(40)	55(3)	56(3)	29(2)	10(2)	2(2)	4(2)
	C(41)	44(2)	63(3)	36(2)	6(2)	5(2)	15(2)
20	C(42)	36(2)	45(2)	32(2)	5(2)	-1(2)	8(2)
	C(43)	59(3)	84(4)	45(3)	15(2)	3(2)	41(3)
	C(44)	60(3)	61(3)	48(3)	20(2)	1(2)	29(2)
	Cl(7)	90(1)	96(1)	90(1)	41(1)	12(1)	49(1)
	Cl(6)	77(1)	128(1)	64(1)	8(1)	-5(1)	65(1)
25	Cl(2)	67(1)	53(1)	111(1)	17(1)	-28(1)	15(1)
	Cl(3)	71(1)	52(1)	54(1)	10(1)	-8(1)	18(1)
	C(1S)	49(2)	61(3)	57(3)	16(2)	-3(2)	21(2)
	Cl(4)	93(1)	52(1)	162(2)	16(1)	-58(1)	22(1)
	Cl(5)	56(1)	45(1)	78(1)	19(1)	15(1)	23(1)
30	C(2S)	65(3)	40(2)	88(4)	9(3)	-6(3)	21(2)
	C(3S)	60(3)	66(3)	62(3)	11(3)	-2(2)	29(2)

Table 15. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for k09221.

	x	y	z	U(eq)
H(2A)	2996	809	2126	38
H(3A)	3292	1966	1306	40
H(6A)	7022	4641	177	47
H(8A)	5807	7149	1077	48
H(10A)	6815	2689	1183	67
H(10B)	7017	2761	530	67
H(10C)	5554	1941	726	67
H(11A)	7383	6627	-160	90
H(11B)	7551	7866	308	90
H(11C)	6158	6986	-63	90
H(12A)	5214	5731	2282	63
H(12B)	3854	5269	1901	63
H(12C)	4983	6793	1974	63
H(14A)	6341	2415	3653	53
H(14B)	6395	3740	3458	53
H(14C)	7047	2900	3098	53
H(17A)	3986	-2103	4066	47
H(18A)	3466	-1146	4884	51
H(19A)	3261	838	4909	48
H(21A)	4281	-2251	3102	83
H(21B)	5251	-807	2953	83
H(21C)	3691	-1495	2749	83
H(22A)	3035	2468	4447	68
H(22B)	2949	2264	3775	68
H(22C)	4367	3115	4130	68
H(24A)	11544	9468	2920	40
H(25A)	10784	8827	3840	42
H(28A)	8860	4394	4617	42
H(30A)	6084	5754	4576	44

	H(32A)	11100	6396	3857	66
	H(32B)	10147	5155	3390	66
	H(32C)	10538	4894	3986	66
	H(33A)	6379	4721	5391	71
5	H(33B)	7353	4017	5344	71
	H(33C)	5955	3338	4970	71
	H(34A)	7570	8119	3714	73
	H(34B)	6203	7345	3992	73
	H(34C)	6411	6755	3376	73
10	H(36A)	9308	6564	1202	52
	H(36B)	8185	6421	1629	52
	H(36C)	9066	5633	1674	52
	H(39A)	11042	10167	256	59
	H(40A)	12695	9599	-82	65
15	H(41A)	13530	8507	443	61
	H(43A)	13551	7468	1221	88
	H(43B)	12159	6832	1498	88
	H(43C)	13334	8242	1791	88
	H(44A)	9023	8936	1271	81
20	H(44B)	9530	10181	936	81
	H(44C)	10141	10380	1566	81
	H(1SA)	11255	3963	2658	67
	H(1SB)	12344	3581	2365	67
	H(2SA)	7422	911	2591	79
25	H(2SB)	8530	1076	2155	79
	H(3SA)	9476	2310	742	75
	H(3SB)	9508	3349	1278	75

References

1 R. T. Boere; V. Klassen; G. Wolmershauser. *J. Chem. Soc., Dalton Trans.*, **1998**, 4147-4154.

2 B. E. Ketz; A. P. Cole; R. M. Waymouth. *Organometallics*, **2004**, *23*, 2835-2837.

3 Otwinowski; Z.; Minor; W. *Processing of x-ray diffraction data collected in oscillation mode*.; Academic Press: London, 1997; **276 (Macromolecular Crystallography, Part A)**; pp 307-326.

4 R. H. Blessing. *Acta Crystallogr., Sect. A: Found. Crystallogr.*, **1995**, *A51*, 33-38.

5 G. M. Sheldrick. *Acta Crystallogr., Sect. A: Found. Crystallogr.*, **2008**, *A64*, 112-122.