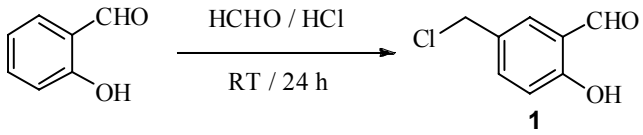
Supplementary Material (ESI) for Dalton Transactions

Electronic Supplementary Information

Preparation of 5-Chloromethyl-2-hydroxybenzaldehyde from salicylaldehyde



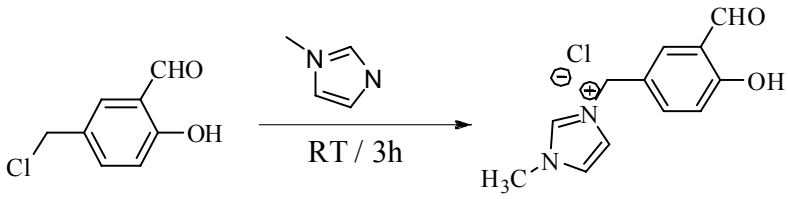
1

To a well stirred mixture of conc. hydrochloric acid (150 mL) and formaldehyde 37 wt % in H_2O (10.8 mL) was added salicylaldehyde (15 mL, 141.39 mmol) and the reaction was stirred at room temperature for 24 h. The solid that separated out was filtered dissolved in diethyl ether and evaporated. Recrystallization from n-hexane afforded the product, 5-chloromethyl-2-hydroxybenzaldehyde (12.46 g) in 51.5% yield.

Characterization data of compound 1:

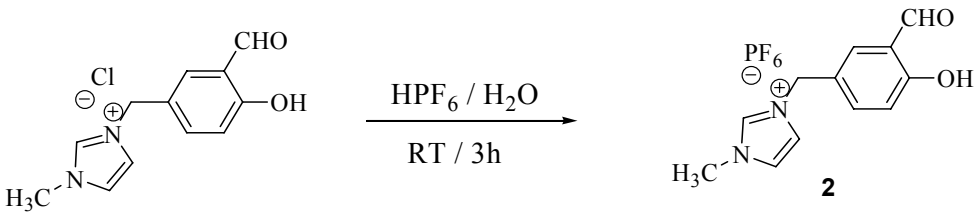
Yield: 51.5%. IR (KBr): 3242, 3196, 2875, 2361, 1656, 1578, 1482, 1437, 1379, 1318, 1282, 1246, 1189, 1147, 1111, 948, 908, 848 cm^{-1}. ^1H NMR (250 MHz, $CDCl_3$): δ 4.6 (s, 2H, -C*H*$_2$-), 6.98-7.02 (d, J = 8.25 Hz, 1H, 1 x C*H* arom.), 7.54-7.60 (m, 2H, 2 x C*H* arom.), 9.90 (s, 1H, D_2O exchangeable, Ph-O*H*), 11.08 (s, 1H, Ph-C*H*O) ppm. ^{13}C NMR (63 MHz, $CDCl_3$): δ 45.16, 118.19, 120.22, 129.10, 133.56, 137.24, 161.48, 196.11 ppm.

Preparation of 3-(3-formyl-4-hydroxybenzyl)-3-methylimidazolium chloride



To the solution of 1-methylimidazole (7 mL, 70.17 mmol) in toluene (15 mL) at room temperature was added 5-chloromethyl-2-hydroxybenzaldehyde (10 g, 58.48 mmol) under nitrogen atmosphere. The resulting solution was stirred at room temperature for 3 h with constant stirring. The solid separated out was washed with ether (3 x 10 mL) and dried to give pale yellow solid product (14.5 g) in 97% yield.

Preparation of 3-(3-formyl-4-hydroxybenzyl)-3-methylimidazolium hexafluorophosphate, 2.

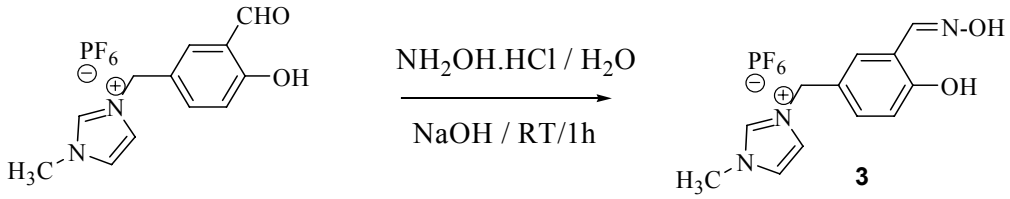


To a solution of 3-(3-formyl-4-hydroxybenzyl)-3-methylimidazolium chloride (14.8 g, 58.73 mmol) in water (100 mL) was added aqueous solution of HPF_6 (60 w % solution, 12.8 mL, 88.09 mmol) while cooling in ice bath over 1 h. After the addition was completed, the reaction was stirred at room temperature for 3 h. The solid product was filtered, washed with water and dried. The yield of the product was 22.04g, (99%).

Characterization data of compound 2:

m.p. 133 - 135 ^{o}C. IR (KBr): 3164, 2884, 1662, 1573, 1489, 1458, 1285, 1249, 1208, 1152, 825, 759, 717, 683, 660, 623, 558 cm^{-1}. ^{1}H NMR (250 MHz, DMSO-d^{6}): δ 3.85 (s, 3H, N-C*H3*-), 5.36 (s, 2H, -CH_2-), 7.04-7.08 (d, J = 8.5 Hz, 1H, 1 x C*H* arom.), 7.59-7.63 (m, 2H, 2 x C*H* arom.), 7.69 (m, 1H, 1 x C*H* arom.), 7.78 (m, 1H, 1 x C*H* arom.), 9.16 (s, 1H, 1 x CH arom.), 10.30 (s, 1H, D_2O exchangeable, Ph-O*H*), 10.98 (s, 1H, Ph-C*H*O) ppm. ^{13}C NMR (63 MHz, DMSO-d^{6}): δ 35.84, 51.09, 118.03, 122.14, 122.47, 123.98, 125.71, 128.93, 136.47, 136.60, 161.09, 190.39 ppm. ^{31}P NMR (101 MHz, DMSO-d^{6}): -159.43 to -117.33 ppm (septet). ^{19}F NMR (235 MHz, DMSO-d^{6}): -67.82 to -64.81 ppm (doublet). ESI MS: In positive mode peaks at m/z 217.1 (100%, $[C_{12}H_{13}N_2O_2]^{+}$) a.m.u. and in negative mode peak at m/z 145.0 (100%, $[PF_6]^{-}$) a.m.u. HRMS $[C_{12}H_{13}N_2O_2]^{+}$ Calcd.: 217.0977 Found: 217.0972.

Preparation of 3-(3-oxime-4-hydroxybenzyl)-3-methylimidazolium hexafluorophosphate, 3.

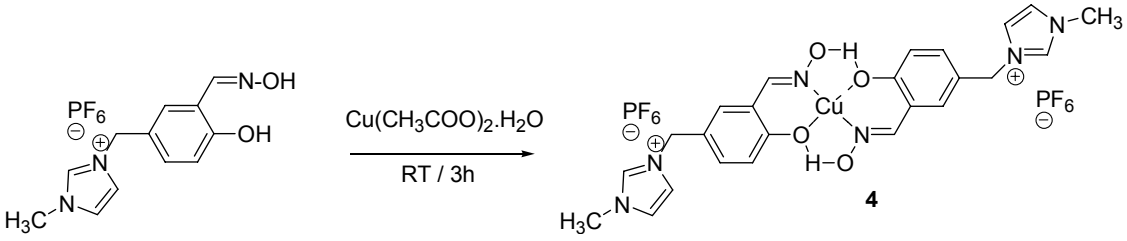


To a solution of 3-(3-oxime-4-hydroxybenzyl)-3-methylimidazolium hexafluorophosphate, 2, (10 g, 27.62 mmol) in 10 mL of ethanol was added NaOH (2.76 g, 69.05 mmol) in 25 mL of water with constant stirring at 25-30 ^{o}C. To this was added drop wise hydroxylamine hydrochloride (2.28 g, 33.14 mmol) in 25 mL water. The resultant solution was stirred for 1 h. The solution was neutralized by addition of dilute HCl and the precipitate thus formed was filtered. The crude product was recrystallized by hot water and dried. The yield of the product was 5.36 g (52%).

Characterization data of compound 3:

m.p. 135 - 137 ^{o}C. IR (KBr): 3365, 1627, 1569, 1507, 1399, 1359, 1313, 1271, 1168, 1130, 1018, 833, 674, 623, 557 cm^{-1}. ^{1}H NMR (250 MHz, DMSO-d^{6}): δ 3.85 (s, 3H, N-C*H3*-), 5.32 (s, 2H, -C*H*$_2$-), 6.92-6.96 (d, *J* = 8.25 Hz, 1H, 1 x C*H* arom.), 7.30-7.34 (dd, *J* = 10.5 Hz, 2H, 2 x C*H* arom.), 7.61-7.62 (m, 1H, 1 x CH arom.), 7.70 (m, 1H, 1 x C*H* arom.), 7.76-7.77 (m, 1H, 1 x C*H* arom.), 8.31 (s, 1H, -C*H*-N-OH), 9.14 (s, 1H, 1 x C*H* arom.), 10.30 (bs, 1H, D_2O exchangeable, Ph-*OH*), 11.37 (bs, 1H, D_2O exchangeable, -N-*OH*) ppm. ^{13}C NMR (63 MHz, DMSO-d^{6}): δ 35.83, 51.41, 116.59, 118.88, 122.19, 123.93, 125.53, 127.61, 130.88, 136.39, 145.96, 156.15 ppm. ^{31}P NMR (101 MHz, DMSO-d^{6}): -159.43 to -117.35 ppm (septet). ^{19}F NMR (235 MHz, DMSO-d^{6}): -67.83 to -64.81 ppm (doublet). ESI MS: In positive mode peaks at m/z 232.1 (100%, $[C_{12}H_{14}N_3O_2]^+$) a.m.u. and in negative mode peak at m/z 144.6 (100%, $[PF_6]^-$) a.m.u. HRMS $[C_{12}H_{14}N_3O_2]^+$ Calcd.: 232.1086 Found: 232.1086

***Preparation of* IL-bis(oxime)-Cu^{II} , 4.**



To a well stirred solution of 3-(3-oxime-4-hydroxybenzyl)-3-methylimidazolium hexafluorophosphate, 3, (0.1 g, 0.266 mmol) in 3 mL of methanol was added drop wise copper (II) acetate monohydrate (0.026 g, 0.133 mmol) dissolved in 3 mL of methanol, at room temperature. The reaction was stirred for 3h. The precipitate formed was filtered, washed with methanol and dried. The product was recrystallized by hot methanol-water to give dark brown crystals (0.098 g) in 70% yield.

Characterization data of compound 4:

IR (KBr): 3172, 3121, 1647, 1613, 1487, 1419, 1338, 1304, 1166, 1027, 825, 750, 670, 615, 553 cm^{-1}. HR-ESI-MS: In positive mode peaks at 670.0961 a.m.u. [$^{63}Cu(C_{24}H_{26}N_6O_4PF_6)$] and 672.0961 a.m.u. [$^{65}Cu(C_{24}H_{26}N_6O_4PF_6)$], and in negative mode peak at 145 a.m.u.([PF_6]$^-$)

***Preparation of* IL-salen-Cu^{II}, 5**:

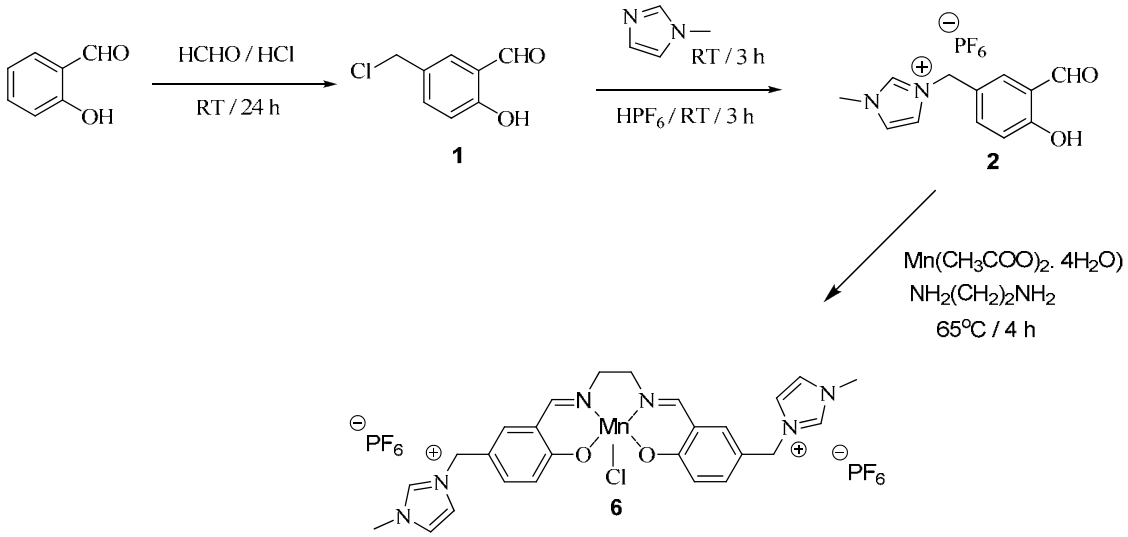
To a well stirred solution of $Cu(CH_3COO)_2$. H_2O (0.054 g, 0.276 mmol) in 100mL of dry methanol, under reflux, were added separately and simultaneously the solution of 3-(3-formyl-4-hydroxybenzyl)-3-methylimidazolium hexafluorophosphate, **2,** (0.100 g, 0.276 mmol) in 5 mL of methanol and ethylenediamine (0.016 g, 0.276 mmol) in 5 mL of methanol by a syringe pump over 30 minutes. The mixture was refluxed for 4 h. After cooling the reaction mixture was concentrated under reduced pressure to a volume about 10 mL and kept overnight at 0^oC. Under these conditions, the product precipitated was filtered from the mother liquor and dried. The yield of the product was 0.175 g, 78.47 %.

IR (KBr): 3168, 1635, 1571, 1536, 1477, 1392, 1310, 1220, 1163, 1087, 835, 751, 620, and 555 cm^{-1}. HR-ESI-MS: In positive mode peaks at 664.1185 a.m.u. [$^{63}Cu(C_{26}H_{28}N_6O_2PF_6)$] and in negative mode peak at 145 a.m.u.($[PF_6]^-$)

General procedure for epoxidation:

PhIO (5 mmol) was added in one portion to a stirred mixture of the respective alkene (1 mmol) and catalyst (0.1 mmol) in 2 mL of bmim[PF_6] ionic liquid. The reaction was stirred at room temperature for the time specified in table **1.** The progress of the reaction was monitored at different time intervals by GCMS by extraction using diethyl ether. Results are shown in **Table 1**.

Preparation of IL-Salen-Mn^{III} –Cl catalyst, 6.



To a well stirred solution of $Mn(CH_3COO)_2.\ 4H_2O$ (0.340 g, 1.38 mmol) in 100mL of dry methanol, under reflux, were added separately and simultaneously the solution of 3-(3-formyl-4-hydroxybenzyl)-3-methylimidazolium hexafluorophosphate **2** (0.500 g, 1.38 mmol) in 25 mL of methanol and ethylenediamine (0.091 g, 1.38 mmol) in 25 mL of methanol by a syringe pump over 30 minutes. The mixture was refluxed for 3 h. Then 2 mL of saturated NaCl was added and the solution was refluxed for additional 1h. After cooling, the reaction mixture was concentrated under reduced pressure to a volume about 10 mL and kept overnight at 0^{o}C. Under these conditions, the product precipitated and was filtered from the mother liquor and dried. The yield of the product was 1.067 g, 92.78 %.

IR (KBr): 2382, 2349, 1630, 1576, 1544, 1472, 1412, 1297, 1169, 1055, 1019, 842 cm^{-1}.

ESI-MS: In positive mode peaks at 690.9 and 693.9 a.m.u. [$Mn(C_{26}H_{28}N_6O_2Cl\ PF_6)$] and in negative mode peak at 145 a.m.u.([PF_6]$^{-}$). HRMS [$Mn(C_{26}H_{28}N_6O_2Cl\ PF_6]^{+}$ Calcd.: 691.0985 Found: 691.1010.

Supplementary Material (ESI) for Dalton Transactions

Crystallographic data for the structure IL-bis(oxime)-Cu^{II} , 4.

Table 1. Crystal data and structure refinement for IL-bis(oxime)-Cu^{II} , **4**.

Table 2. Atomic coordinates and equivalent isotropic displacement parameters for IL-bis(oxime)-Cu^{II} , **4**.

Table 3. Bond lengths and angles for the structure IL-bis(oxime)-Cu^{II} , **4**.

Table 4. Anisotropic displacement parameters for the structure IL-bis(oxime)-Cu^{II} , **4**.

Table 5. Hydrogen coordinates and isotropic displacement parameters for the structure IL-bis(oxime)-Cu^{II} , **4**.

Table 6. Torsion angles for the structure IL-bis(oxime)-Cu^{II} , **4**.

Table 1. Crystal data and structure refinement for IL-bis(oxime)-Cu^{II} , **4**.

Identification code	rs0101	
Empirical formula	C24 H26 Cu F12 N6 O4 P2	
Formula weight	815.99	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.115(4) Å	α= 70.115(8)°.
	b = 18.066(7) Å	β= 85.613(8)°.
	c = 18.153(6) Å	γ = 74.682(7)°.
Volume	3008.5(19) $Å^3$	
Z	4	
Density (calculated)	1.802 Mg/m^3	
Absorption coefficient	0.952 mm^{-1}	
F(000)	1644	
Crystal size	0.20 x 0.15 x 0.10 mm^3	
Theta range for data collection	1.19 to 28.31°.	
Index ranges	-13<=h<=13, -23<=k<=20, -20<=l<=23	
Reflections collected	17825	
Independent reflections	13069 [R(int) = 0.0544]	
Completeness to theta = 26.00°	97.1 %	
Absorption correction	Not measured	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13069 / 0 / 891	
Goodness-of-fit on F^2	0.965	
Final R indices [I>2sigma(I)]	R1 = 0.0802, wR2 = 0.1615	
R indices (all data)	R1 = 0.1575, wR2 = 0.2037	
Largest diff. peak and hole	0.906 and -0.735 $e.Å^{-3}$	

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

	x	y	z	U(eq)
Cu(1)	7695(1)	8683(1)	5029(1)	16(1)
Cu(2)	2992(1)	6148(1)	4852(1)	17(1)
N(11)	9283(5)	8954(3)	4438(3)	19(1)
N(12)	11321(5)	7068(3)	1903(3)	16(1)
N(13)	11337(5)	7981(3)	772(3)	21(1)
O(11)	7900(4)	7755(2)	4725(2)	17(1)
O(12)	9626(5)	9656(3)	4442(2)	23(1)
C(11)	10072(6)	8581(4)	4012(3)	18(1)
C(12)	9903(6)	7859(4)	3918(3)	18(1)
C(13)	8832(6)	7472(4)	4265(3)	16(1)
C(14)	8772(7)	6780(4)	4104(3)	19(1)
C(15)	9702(7)	6466(4)	3622(3)	20(2)
C(16)	10754(6)	6835(4)	3281(3)	16(1)
C(17)	10840(6)	7513(4)	3436(3)	16(1)
C(18)	11716(7)	6523(4)	2711(3)	21(2)
C(19)	12048(7)	7550(4)	1429(4)	22(2)
C(20)	10099(6)	7204(4)	1537(4)	22(2)
C(21)	10099(7)	7780(4)	830(4)	21(2)
C(22)	11794(7)	8586(4)	107(4)	33(2)
N(31)	6042(5)	8458(3)	5561(3)	17(1)
N(32)	3501(5)	10653(3)	7878(3)	17(1)
N(33)	4296(5)	9846(3)	9021(3)	21(1)
O(31)	7530(4)	9588(3)	5359(2)	20(1)
O(32)	5657(4)	7774(3)	5551(2)	20(1)
C(31)	5188(7)	8882(4)	5922(3)	20(1)
C(32)	5378(6)	9602(4)	6026(3)	17(1)
C(33)	6536(6)	9918(4)	5760(3)	18(1)
C(34)	6639(7)	10597(4)	5935(3)	21(2)
C(35)	5639(6)	10970(4)	6338(3)	20(1)
C(36)	4463(6)	10698(4)	6580(3)	18(1)

C(37)	4360(7)	10003(4)	6434(3)	20(2)
C(38)	3385(7)	11097(4)	7035(3)	27(2)
C(39)	4596(7)	10107(4)	8276(3)	19(1)
C(40)	2458(7)	10742(4)	8401(4)	25(2)
C(41)	2973(7)	10222(4)	9110(4)	28(2)
C(42)	5197(7)	9177(4)	9616(4)	30(2)
N(51)	1390(5)	5885(3)	5427(3)	18(1)
N(52)	-750(5)	7903(3)	7930(3)	17(1)
N(53)	-882(5)	7158(3)	9134(3)	17(1)
O(51)	2798(4)	7061(2)	5177(2)	20(1)
O(52)	1014(5)	5202(3)	5415(2)	26(1)
C(51)	581(6)	6279(4)	5828(3)	17(1)
C(52)	766(6)	6989(4)	5950(3)	15(1)
C(53)	1870(6)	7341(4)	5637(3)	17(1)
C(54)	1970(7)	8019(4)	5823(4)	22(2)
C(55)	1018(7)	8353(4)	6276(3)	20(2)
C(56)	-103(6)	8023(4)	6575(3)	18(1)
C(57)	-204(6)	7351(4)	6414(3)	20(1)
C(58)	-1116(7)	8378(4)	7098(3)	26(2)
C(59)	-1553(7)	7547(4)	8454(4)	20(1)
C(60)	503(7)	7742(4)	8281(4)	24(2)
C(61)	413(7)	7282(4)	9030(4)	24(2)
C(62)	-1425(7)	6652(4)	9842(3)	28(2)
N(71)	4627(6)	6410(3)	4310(3)	20(1)
N(72)	6497(6)	4706(3)	1607(3)	24(1)
N(73)	5148(5)	5560(3)	654(3)	21(1)
O(71)	3154(4)	5261(2)	4482(2)	20(1)
O(72)	5047(5)	7053(3)	4395(2)	22(1)
C(71)	5426(6)	6041(4)	3897(3)	18(1)
C(72)	5214(6)	5351(4)	3724(3)	18(1)
C(73)	4103(6)	4996(4)	4025(3)	17(1)
C(74)	4027(7)	4335(4)	3797(4)	22(2)
C(75)	4959(7)	4042(4)	3311(3)	21(2)
C(76)	6047(7)	4393(4)	3009(3)	20(1)
C(77)	6153(6)	5040(4)	3229(3)	19(1)
C(78)	6999(7)	4149(4)	2404(4)	27(2)

C(79)	5217(7)	5137(4)	1418(4)	22(2)
C(80)	7272(7)	4840(4)	936(4)	25(2)
C(81)	6411(7)	5391(4)	351(4)	27(2)
C(82)	3926(7)	6177(4)	248(4)	29(2)
P(101)	6050(2)	7313(1)	1561(1)	20(1)
F(101)	5149(4)	8171(2)	1576(2)	45(1)
F(102)	6944(4)	7230(3)	2280(2)	44(1)
F(103)	6940(5)	6460(2)	1531(2)	45(1)
F(104)	5132(4)	7405(3)	836(2)	40(1)
F(105)	5011(4)	6873(2)	2154(2)	34(1)
F(106)	7061(4)	7757(2)	959(2)	30(1)
P(201)	1195(2)	4724(1)	1731(1)	25(1)
F(201)	-178(5)	5316(3)	1876(3)	74(2)
F(202)	2027(4)	5377(3)	1703(2)	44(1)
F(203)	2550(4)	4159(2)	1538(2)	45(1)
F(204)	357(4)	4074(3)	1761(3)	47(1)
F(205)	1504(5)	4313(3)	2633(2)	61(2)
F(206)	903(5)	5141(3)	809(3)	65(2)
P(301)	1350(2)	9974(1)	1577(1)	27(1)
F(301)	2678(4)	9613(2)	1146(2)	35(1)
F(302)	2236(4)	10374(3)	1942(3)	56(1)
F(303)	29(5)	10348(3)	1990(3)	62(2)
F(304)	478(5)	9601(4)	1193(4)	104(3)
F(305)	1699(7)	9183(3)	2299(3)	101(2)
F(306)	1066(5)	10783(3)	846(3)	79(2)
P(401)	5550(2)	2247(1)	1798(1)	20(1)
F(401)	4481(4)	2702(2)	1076(2)	36(1)
F(402)	6703(5)	2122(4)	1195(2)	78(2)
F(403)	6617(4)	1793(3)	2511(2)	45(1)
F(404)	4369(5)	2384(3)	2394(2)	68(2)
F(405)	5220(7)	1430(3)	1881(3)	97(2)
F(406)	5847(6)	3079(3)	1716(3)	79(2)

Table 3. Bond lengths [Å] and angles [°] for IL-bis(oxime)-Cu^{II} , **4**.

Cu(1)-O(31)	1.890(4)
Cu(1)-O(11)	1.893(4)
Cu(1)-N(31)	1.933(5)
Cu(1)-N(11)	1.941(5)
Cu(2)-O(51)	1.892(4)
Cu(2)-O(71)	1.903(4)
Cu(2)-N(51)	1.937(5)
Cu(2)-N(71)	1.943(5)
N(11)-C(11)	1.291(7)
N(11)-O(12)	1.402(6)
N(12)-C(19)	1.332(7)
N(12)-C(20)	1.372(7)
N(12)-C(18)	1.478(7)
N(13)-C(19)	1.323(7)
N(13)-C(21)	1.381(8)
N(13)-C(22)	1.466(8)
O(11)-C(13)	1.327(7)
O(12)-H(12)	0.8400
C(11)-C(12)	1.426(8)
C(11)-H(11)	0.9500
C(12)-C(17)	1.409(8)
C(12)-C(13)	1.433(8)
C(13)-C(14)	1.395(8)
C(14)-C(15)	1.380(8)
C(14)-H(14)	0.9500
C(15)-C(16)	1.397(8)
C(15)-H(15)	0.9500
C(16)-C(17)	1.373(8)
C(16)-C(18)	1.512(8)
C(17)-H(17)	0.9500
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-H(19)	0.9500
C(20)-C(21)	1.349(8)

C(20)-H(20)	0.9500
C(21)-H(21)	0.9500
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
N(31)-C(31)	1.292(7)
N(31)-O(32)	1.396(5)
N(32)-C(39)	1.335(8)
N(32)-C(40)	1.379(8)
N(32)-C(38)	1.463(7)
N(33)-C(39)	1.314(7)
N(33)-C(41)	1.356(8)
N(33)-C(42)	1.463(8)
O(31)-C(33)	1.328(7)
O(32)-H(32)	0.8400
C(31)-C(32)	1.439(8)
C(31)-H(31)	0.9500
C(32)-C(37)	1.409(8)
C(32)-C(33)	1.417(8)
C(33)-C(34)	1.398(8)
C(34)-C(35)	1.369(8)
C(34)-H(34)	0.9500
C(35)-C(36)	1.390(8)
C(35)-H(35)	0.9500
C(36)-C(37)	1.399(8)
C(36)-C(38)	1.499(9)
C(37)-H(37)	0.9500
C(38)-H(38A)	0.9900
C(38)-H(38B)	0.9900
C(39)-H(39)	0.9500
C(40)-C(41)	1.354(9)
C(40)-H(40)	0.9500
C(41)-H(41)	0.9500
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800

N(51)-C(51)	1.289(7)
N(51)-O(52)	1.391(6)
N(52)-C(59)	1.311(7)
N(52)-C(60)	1.379(8)
N(52)-C(58)	1.480(7)
N(53)-C(59)	1.329(7)
N(53)-C(61)	1.375(8)
N(53)-C(62)	1.465(7)
O(51)-C(53)	1.324(7)
O(52)-H(52)	0.8400
C(51)-C(52)	1.435(8)
C(51)-H(51)	0.9500
C(52)-C(53)	1.417(8)
C(52)-C(57)	1.417(8)
C(53)-C(54)	1.405(8)
C(54)-C(55)	1.370(8)
C(54)-H(54)	0.9500
C(55)-C(56)	1.406(8)
C(55)-H(55)	0.9500
C(56)-C(57)	1.373(8)
C(56)-C(58)	1.510(8)
C(57)-H(57)	0.9500
C(58)-H(58A)	0.9900
C(58)-H(58B)	0.9900
C(59)-H(59)	0.9500
C(60)-C(61)	1.342(8)
C(60)-H(60)	0.9500
C(61)-H(61)	0.9500
C(62)-H(62A)	0.9800
C(62)-H(62B)	0.9800
C(62)-H(62C)	0.9800
N(71)-C(71)	1.274(7)
N(71)-O(72)	1.394(6)
N(72)-C(79)	1.324(8)
N(72)-C(80)	1.382(8)
N(72)-C(78)	1.490(8)

N(73)-C(79)	1.334(7)
N(73)-C(81)	1.352(8)
N(73)-C(82)	1.472(8)
O(71)-C(73)	1.320(7)
O(72)-H(72)	0.8400
C(71)-C(72)	1.456(8)
C(71)-H(71)	0.9500
C(72)-C(77)	1.398(8)
C(72)-C(73)	1.421(8)
C(73)-C(74)	1.413(8)
C(74)-C(75)	1.369(9)
C(74)-H(74)	0.9500
C(75)-C(76)	1.398(9)
C(75)-H(75)	0.9500
C(76)-C(77)	1.389(8)
C(76)-C(78)	1.506(8)
C(77)-H(77)	0.9500
C(78)-H(78A)	0.9900
C(78)-H(78B)	0.9900
C(79)-H(79)	0.9500
C(80)-C(81)	1.357(9)
C(80)-H(80)	0.9500
C(81)-H(81)	0.9500
C(82)-H(82A)	0.9800
C(82)-H(82B)	0.9800
C(82)-H(82C)	0.9800
P(101)-F(103)	1.584(4)
P(101)-F(101)	1.586(4)
P(101)-F(102)	1.587(4)
P(101)-F(106)	1.598(4)
P(101)-F(104)	1.606(4)
P(101)-F(105)	1.606(4)
P(201)-F(205)	1.569(4)
P(201)-F(203)	1.573(4)
P(201)-F(201)	1.578(5)
P(201)-F(206)	1.598(5)

P(201)-F(204)	1.604(4)
P(201)-F(202)	1.606(4)
P(301)-F(305)	1.554(5)
P(301)-F(304)	1.564(5)
P(301)-F(306)	1.580(5)
P(301)-F(303)	1.588(5)
P(301)-F(302)	1.588(4)
P(301)-F(301)	1.601(4)
P(401)-F(405)	1.552(5)
P(401)-F(402)	1.561(5)
P(401)-F(406)	1.567(5)
P(401)-F(404)	1.578(5)
P(401)-F(403)	1.593(4)
P(401)-F(401)	1.605(4)

O(31)-Cu(1)-O(11)	178.19(18)
O(31)-Cu(1)-N(31)	92.29(19)
O(11)-Cu(1)-N(31)	87.97(19)
O(31)-Cu(1)-N(11)	87.59(19)
O(11)-Cu(1)-N(11)	92.26(19)
N(31)-Cu(1)-N(11)	176.4(2)
O(51)-Cu(2)-O(71)	177.55(17)
O(51)-Cu(2)-N(51)	92.01(19)
O(71)-Cu(2)-N(51)	88.51(19)
O(51)-Cu(2)-N(71)	86.80(19)
O(71)-Cu(2)-N(71)	92.8(2)
N(51)-Cu(2)-N(71)	177.9(2)
C(11)-N(11)-O(12)	113.9(5)
C(11)-N(11)-Cu(1)	128.4(4)
O(12)-N(11)-Cu(1)	117.7(4)
C(19)-N(12)-C(20)	108.7(5)
C(19)-N(12)-C(18)	125.6(5)
C(20)-N(12)-C(18)	125.5(5)
C(19)-N(13)-C(21)	108.8(5)
C(19)-N(13)-C(22)	124.8(5)
C(21)-N(13)-C(22)	126.5(5)

C(13)-O(11)-Cu(1)	129.1(4)
N(11)-O(12)-H(12)	109.5
N(11)-C(11)-C(12)	123.4(6)
N(11)-C(11)-H(11)	118.3
C(12)-C(11)-H(11)	118.3
C(17)-C(12)-C(11)	117.5(6)
C(17)-C(12)-C(13)	117.9(5)
C(11)-C(12)-C(13)	124.6(6)
O(11)-C(13)-C(14)	119.5(5)
O(11)-C(13)-C(12)	122.2(5)
C(14)-C(13)-C(12)	118.3(6)
C(15)-C(14)-C(13)	121.9(6)
C(15)-C(14)-H(14)	119.0
C(13)-C(14)-H(14)	119.0
C(14)-C(15)-C(16)	120.4(6)
C(14)-C(15)-H(15)	119.8
C(16)-C(15)-H(15)	119.8
C(17)-C(16)-C(15)	118.6(6)
C(17)-C(16)-C(18)	120.9(5)
C(15)-C(16)-C(18)	120.3(5)
C(16)-C(17)-C(12)	122.8(6)
C(16)-C(17)-H(17)	118.6
C(12)-C(17)-H(17)	118.6
N(12)-C(18)-C(16)	109.5(5)
N(12)-C(18)-H(18A)	109.8
C(16)-C(18)-H(18A)	109.8
N(12)-C(18)-H(18B)	109.8
C(16)-C(18)-H(18B)	109.8
H(18A)-C(18)-H(18B)	108.2
N(13)-C(19)-N(12)	108.5(5)
N(13)-C(19)-H(19)	125.8
N(12)-C(19)-H(19)	125.8
C(21)-C(20)-N(12)	107.2(6)
C(21)-C(20)-H(20)	126.4
N(12)-C(20)-H(20)	126.4
C(20)-C(21)-N(13)	106.8(6)

C(20)-C(21)-H(21)	126.6
N(13)-C(21)-H(21)	126.6
N(13)-C(22)-H(22A)	109.5
N(13)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
N(13)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(31)-N(31)-O(32)	113.4(5)
C(31)-N(31)-Cu(1)	127.9(4)
O(32)-N(31)-Cu(1)	118.6(4)
C(39)-N(32)-C(40)	108.2(5)
C(39)-N(32)-C(38)	127.4(6)
C(40)-N(32)-C(38)	124.3(5)
C(39)-N(33)-C(41)	108.4(6)
C(39)-N(33)-C(42)	124.1(6)
C(41)-N(33)-C(42)	126.9(6)
C(33)-O(31)-Cu(1)	129.3(4)
N(31)-O(32)-H(32)	109.5
N(31)-C(31)-C(32)	123.7(6)
N(31)-C(31)-H(31)	118.1
C(32)-C(31)-H(31)	118.1
C(37)-C(32)-C(33)	118.5(5)
C(37)-C(32)-C(31)	117.5(6)
C(33)-C(32)-C(31)	124.0(6)
O(31)-C(33)-C(34)	118.8(6)
O(31)-C(33)-C(32)	122.5(5)
C(34)-C(33)-C(32)	118.6(6)
C(35)-C(34)-C(33)	121.6(6)
C(35)-C(34)-H(34)	119.2
C(33)-C(34)-H(34)	119.2
C(34)-C(35)-C(36)	121.4(6)
C(34)-C(35)-H(35)	119.3
C(36)-C(35)-H(35)	119.3
C(35)-C(36)-C(37)	117.9(6)
C(35)-C(36)-C(38)	121.2(6)

C(37)-C(36)-C(38)	120.8(6)
C(36)-C(37)-C(32)	121.9(6)
C(36)-C(37)-H(37)	119.0
C(32)-C(37)-H(37)	119.0
N(32)-C(38)-C(36)	112.6(5)
N(32)-C(38)-H(38A)	109.1
C(36)-C(38)-H(38A)	109.1
N(32)-C(38)-H(38B)	109.1
C(36)-C(38)-H(38B)	109.1
H(38A)-C(38)-H(38B)	107.8
N(33)-C(39)-N(32)	109.2(6)
N(33)-C(39)-H(39)	125.4
N(32)-C(39)-H(39)	125.4
C(41)-C(40)-N(32)	105.8(6)
C(41)-C(40)-H(40)	127.1
N(32)-C(40)-H(40)	127.1
C(40)-C(41)-N(33)	108.4(6)
C(40)-C(41)-H(41)	125.8
N(33)-C(41)-H(41)	125.8
N(33)-C(42)-H(42A)	109.5
N(33)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
N(33)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(51)-N(51)-O(52)	113.7(5)
C(51)-N(51)-Cu(2)	127.7(4)
O(52)-N(51)-Cu(2)	118.7(4)
C(59)-N(52)-C(60)	108.4(5)
C(59)-N(52)-C(58)	125.7(5)
C(60)-N(52)-C(58)	125.9(5)
C(59)-N(53)-C(61)	107.5(5)
C(59)-N(53)-C(62)	125.1(5)
C(61)-N(53)-C(62)	127.4(5)
C(53)-O(51)-Cu(2)	129.5(4)
N(51)-O(52)-H(52)	109.5

N(51)-C(51)-C(52)	124.5(6)
N(51)-C(51)-H(51)	117.7
C(52)-C(51)-H(51)	117.7
C(53)-C(52)-C(57)	118.6(5)
C(53)-C(52)-C(51)	123.5(6)
C(57)-C(52)-C(51)	117.9(5)
O(51)-C(53)-C(54)	119.1(6)
O(51)-C(53)-C(52)	122.7(5)
C(54)-C(53)-C(52)	118.1(6)
C(55)-C(54)-C(53)	121.8(6)
C(55)-C(54)-H(54)	119.1
C(53)-C(54)-H(54)	119.1
C(54)-C(55)-C(56)	120.7(6)
C(54)-C(55)-H(55)	119.6
C(56)-C(55)-H(55)	119.6
C(57)-C(56)-C(55)	118.4(6)
C(57)-C(56)-C(58)	121.4(6)
C(55)-C(56)-C(58)	120.2(6)
C(56)-C(57)-C(52)	122.3(6)
C(56)-C(57)-H(57)	118.9
C(52)-C(57)-H(57)	118.9
N(52)-C(58)-C(56)	109.9(5)
N(52)-C(58)-H(58A)	109.7
C(56)-C(58)-H(58A)	109.7
N(52)-C(58)-H(58B)	109.7
C(56)-C(58)-H(58B)	109.7
H(58A)-C(58)-H(58B)	108.2
N(52)-C(59)-N(53)	109.7(6)
N(52)-C(59)-H(59)	125.2
N(53)-C(59)-H(59)	125.2
C(61)-C(60)-N(52)	106.8(6)
C(61)-C(60)-H(60)	126.6
N(52)-C(60)-H(60)	126.6
C(60)-C(61)-N(53)	107.7(6)
C(60)-C(61)-H(61)	126.1
N(53)-C(61)-H(61)	126.1

N(53)-C(62)-H(62A)	109.5
N(53)-C(62)-H(62B)	109.5
H(62A)-C(62)-H(62B)	109.5
N(53)-C(62)-H(62C)	109.5
H(62A)-C(62)-H(62C)	109.5
H(62B)-C(62)-H(62C)	109.5
C(71)-N(71)-O(72)	113.9(5)
C(71)-N(71)-Cu(2)	127.7(4)
O(72)-N(71)-Cu(2)	118.4(4)
C(79)-N(72)-C(80)	108.5(6)
C(79)-N(72)-C(78)	125.5(6)
C(80)-N(72)-C(78)	126.0(6)
C(79)-N(73)-C(81)	108.5(6)
C(79)-N(73)-C(82)	124.3(6)
C(81)-N(73)-C(82)	126.8(6)
C(73)-O(71)-Cu(2)	128.2(4)
N(71)-O(72)-H(72)	109.5
N(71)-C(71)-C(72)	124.4(6)
N(71)-C(71)-H(71)	117.8
C(72)-C(71)-H(71)	117.8
C(77)-C(72)-C(73)	119.7(6)
C(77)-C(72)-C(71)	117.2(6)
C(73)-C(72)-C(71)	123.0(6)
O(71)-C(73)-C(74)	119.8(6)
O(71)-C(73)-C(72)	123.8(5)
C(74)-C(73)-C(72)	116.4(6)
C(75)-C(74)-C(73)	122.8(6)
C(75)-C(74)-H(74)	118.6
C(73)-C(74)-H(74)	118.6
C(74)-C(75)-C(76)	120.9(6)
C(74)-C(75)-H(75)	119.5
C(76)-C(75)-H(75)	119.5
C(77)-C(76)-C(75)	117.5(6)
C(77)-C(76)-C(78)	119.8(6)
C(75)-C(76)-C(78)	122.4(6)
C(76)-C(77)-C(72)	122.6(6)

C(76)-C(77)-H(77)	118.7
C(72)-C(77)-H(77)	118.7
N(72)-C(78)-C(76)	109.5(5)
N(72)-C(78)-H(78A)	109.8
C(76)-C(78)-H(78A)	109.8
N(72)-C(78)-H(78B)	109.8
C(76)-C(78)-H(78B)	109.8
H(78A)-C(78)-H(78B)	108.2
N(72)-C(79)-N(73)	108.7(6)
N(72)-C(79)-H(79)	125.6
N(73)-C(79)-H(79)	125.6
C(81)-C(80)-N(72)	106.1(6)
C(81)-C(80)-H(80)	126.9
N(72)-C(80)-H(80)	126.9
N(73)-C(81)-C(80)	108.1(6)
N(73)-C(81)-H(81)	126.0
C(80)-C(81)-H(81)	126.0
N(73)-C(82)-H(82A)	109.5
N(73)-C(82)-H(82B)	109.5
H(82A)-C(82)-H(82B)	109.5
N(73)-C(82)-H(82C)	109.5
H(82A)-C(82)-H(82C)	109.5
H(82B)-C(82)-H(82C)	109.5
F(103)-P(101)-F(101)	179.0(2)
F(103)-P(101)-F(102)	90.5(2)
F(101)-P(101)-F(102)	90.4(2)
F(103)-P(101)-F(106)	90.1(2)
F(101)-P(101)-F(106)	89.6(2)
F(102)-P(101)-F(106)	90.7(2)
F(103)-P(101)-F(104)	90.1(2)
F(101)-P(101)-F(104)	89.0(2)
F(102)-P(101)-F(104)	179.4(3)
F(106)-P(101)-F(104)	89.5(2)
F(103)-P(101)-F(105)	90.3(2)
F(101)-P(101)-F(105)	90.0(2)
F(102)-P(101)-F(105)	90.3(2)

F(106)-P(101)-F(105)	178.9(2)
F(104)-P(101)-F(105)	89.5(2)
F(205)-P(201)-F(203)	91.3(3)
F(205)-P(201)-F(201)	91.7(3)
F(203)-P(201)-F(201)	177.0(3)
F(205)-P(201)-F(206)	179.2(3)
F(203)-P(201)-F(206)	88.0(3)
F(201)-P(201)-F(206)	89.0(3)
F(205)-P(201)-F(204)	90.2(2)
F(203)-P(201)-F(204)	90.7(2)
F(201)-P(201)-F(204)	89.6(3)
F(206)-P(201)-F(204)	90.3(2)
F(205)-P(201)-F(202)	89.7(2)
F(203)-P(201)-F(202)	89.6(2)
F(201)-P(201)-F(202)	90.2(2)
F(206)-P(201)-F(202)	89.8(3)
F(204)-P(201)-F(202)	179.7(3)
F(305)-P(301)-F(304)	91.5(4)
F(305)-P(301)-F(306)	177.3(4)
F(304)-P(301)-F(306)	90.8(4)
F(305)-P(301)-F(303)	91.4(3)
F(304)-P(301)-F(303)	90.7(3)
F(306)-P(301)-F(303)	90.1(3)
F(305)-P(301)-F(302)	90.2(3)
F(304)-P(301)-F(302)	178.2(4)
F(306)-P(301)-F(302)	87.5(3)
F(303)-P(301)-F(302)	89.7(2)
F(305)-P(301)-F(301)	89.7(3)
F(304)-P(301)-F(301)	89.4(2)
F(306)-P(301)-F(301)	88.8(3)
F(303)-P(301)-F(301)	178.9(3)
F(302)-P(301)-F(301)	90.2(2)
F(405)-P(401)-F(402)	91.9(4)
F(405)-P(401)-F(406)	178.7(4)
F(402)-P(401)-F(406)	89.2(3)
F(405)-P(401)-F(404)	88.4(3)

F(402)-P(401)-F(404)	179.0(3)
F(406)-P(401)-F(404)	90.5(3)
F(405)-P(401)-F(403)	90.4(3)
F(402)-P(401)-F(403)	91.4(2)
F(406)-P(401)-F(403)	90.4(3)
F(404)-P(401)-F(403)	89.6(2)
F(405)-P(401)-F(401)	89.6(2)
F(402)-P(401)-F(401)	88.3(2)
F(406)-P(401)-F(401)	89.7(2)
F(404)-P(401)-F(401)	90.7(2)
F(403)-P(401)-F(401)	179.7(3)

Symmetry transformations used to generate equivalent atoms:

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu(1)	18(1)	13(1)	18(1)	-7(1)	0(1)	-6(1)
Cu(2)	20(1)	14(1)	17(1)	-5(1)	-1(1)	-6(1)
N(11)	26(3)	11(3)	22(3)	-1(2)	-4(2)	-12(2)
N(12)	18(3)	17(3)	14(3)	-8(2)	-2(2)	-1(2)
N(13)	18(3)	22(3)	21(3)	-7(2)	0(2)	-4(3)
O(11)	20(2)	16(2)	18(2)	-5(2)	0(2)	-9(2)
O(12)	26(3)	19(2)	32(3)	-13(2)	3(2)	-13(2)
C(11)	21(4)	19(3)	14(3)	-3(3)	-2(3)	-10(3)
C(12)	20(4)	22(4)	15(3)	-10(3)	-1(3)	-6(3)
C(13)	17(4)	17(3)	18(3)	-9(3)	0(3)	-6(3)
C(14)	22(4)	12(3)	25(4)	-5(3)	-6(3)	-8(3)
C(15)	27(4)	15(3)	18(3)	-3(3)	-10(3)	-3(3)
C(16)	15(3)	14(3)	18(3)	-5(3)	-3(3)	-1(3)
C(17)	10(3)	18(3)	19(3)	-4(3)	0(3)	-5(3)
C(18)	23(4)	18(3)	25(4)	-9(3)	1(3)	-7(3)
C(19)	20(4)	26(4)	22(4)	-9(3)	5(3)	-11(3)
C(20)	14(4)	27(4)	26(4)	-10(3)	-4(3)	-6(3)
C(21)	20(4)	20(4)	23(4)	-8(3)	-6(3)	-2(3)
C(22)	39(5)	36(4)	25(4)	-4(3)	5(3)	-23(4)
N(31)	21(3)	11(3)	23(3)	-9(2)	-6(2)	-6(2)
N(32)	22(3)	12(3)	18(3)	-5(2)	-2(2)	-6(2)
N(33)	19(3)	23(3)	23(3)	-11(2)	0(2)	-7(3)
O(31)	23(3)	23(2)	20(2)	-11(2)	2(2)	-9(2)
O(32)	23(3)	20(2)	25(3)	-12(2)	4(2)	-12(2)
C(31)	20(4)	16(3)	24(4)	-8(3)	-3(3)	-2(3)
C(32)	20(4)	15(3)	16(3)	-3(3)	-1(3)	-7(3)
C(33)	18(4)	11(3)	20(3)	-6(3)	-7(3)	4(3)
C(34)	25(4)	19(3)	19(3)	-3(3)	-4(3)	-9(3)
C(35)	23(4)	11(3)	21(3)	-1(3)	-3(3)	-2(3)
C(36)	21(4)	12(3)	13(3)	0(3)	-5(3)	4(3)

C(37)	24(4)	16(3)	18(3)	-1(3)	-8(3)	-4(3)
C(38)	39(4)	14(3)	22(4)	-3(3)	-7(3)	1(3)
C(39)	22(4)	22(4)	15(3)	-9(3)	3(3)	-9(3)
C(40)	24(4)	20(4)	32(4)	-6(3)	4(3)	-12(3)
C(41)	38(5)	25(4)	27(4)	-13(3)	12(3)	-17(4)
C(42)	29(4)	29(4)	27(4)	-1(3)	-1(3)	-8(3)
N(51)	24(3)	12(3)	20(3)	-5(2)	-3(2)	-11(2)
N(52)	19(3)	12(3)	23(3)	-7(2)	3(2)	-6(2)
N(53)	19(3)	14(3)	20(3)	-8(2)	-1(2)	-2(2)
O(51)	22(3)	20(2)	19(2)	-10(2)	1(2)	-5(2)
O(52)	37(3)	19(2)	28(3)	-11(2)	3(2)	-13(2)
C(51)	9(3)	23(4)	19(3)	-9(3)	0(3)	-4(3)
C(52)	15(3)	13(3)	17(3)	-1(3)	-4(3)	-4(3)
C(53)	19(4)	17(3)	15(3)	-1(3)	-5(3)	-6(3)
C(54)	28(4)	16(3)	25(4)	-5(3)	1(3)	-11(3)
C(55)	31(4)	19(3)	17(3)	-9(3)	2(3)	-11(3)
C(56)	19(4)	15(3)	14(3)	0(3)	-1(3)	1(3)
C(57)	17(4)	14(3)	24(4)	-1(3)	-3(3)	-2(3)
C(58)	30(4)	27(4)	23(4)	-7(3)	-5(3)	-11(3)
C(59)	17(4)	11(3)	26(4)	-3(3)	-3(3)	5(3)
C(60)	19(4)	32(4)	26(4)	-14(3)	3(3)	-10(3)
C(61)	16(4)	32(4)	25(4)	-13(3)	-4(3)	-2(3)
C(62)	31(4)	34(4)	22(4)	-6(3)	4(3)	-15(4)
N(71)	29(3)	15(3)	16(3)	-4(2)	-6(2)	-8(3)
N(72)	30(4)	23(3)	22(3)	-10(3)	-2(3)	-7(3)
N(73)	24(3)	28(3)	15(3)	-8(2)	-1(2)	-12(3)
O(71)	24(3)	18(2)	21(2)	-9(2)	-4(2)	-5(2)
O(72)	32(3)	15(2)	24(3)	-10(2)	6(2)	-11(2)
C(71)	19(4)	15(3)	18(3)	-3(3)	-4(3)	-4(3)
C(72)	21(4)	11(3)	13(3)	-1(3)	-5(3)	5(3)
C(73)	17(4)	18(3)	15(3)	-8(3)	-4(3)	1(3)
C(74)	28(4)	11(3)	26(4)	-3(3)	-8(3)	-8(3)
C(75)	26(4)	16(3)	22(4)	-8(3)	-9(3)	-3(3)
C(76)	23(4)	13(3)	17(3)	-2(3)	-7(3)	5(3)
C(77)	20(4)	18(3)	15(3)	-2(3)	-3(3)	-5(3)
C(78)	26(4)	17(4)	31(4)	-4(3)	-8(3)	3(3)

C(79)	19(4)	25(4)	25(4)	-12(3)	-1(3)	-8(3)
C(80)	19(4)	31(4)	30(4)	-18(3)	12(3)	-9(3)
C(81)	37(5)	27(4)	27(4)	-15(3)	10(3)	-19(4)
C(82)	34(4)	20(4)	29(4)	1(3)	-9(3)	-10(3)
P(101)	18(1)	19(1)	23(1)	-6(1)	-3(1)	-5(1)
F(101)	47(3)	27(2)	52(3)	-14(2)	14(2)	0(2)
F(102)	36(3)	74(3)	31(2)	-17(2)	-7(2)	-25(3)
F(103)	54(3)	21(2)	49(3)	-5(2)	9(2)	-2(2)
F(104)	41(3)	53(3)	30(2)	-2(2)	-11(2)	-32(2)
F(105)	27(2)	41(3)	24(2)	7(2)	-5(2)	-12(2)
F(106)	21(2)	38(2)	33(2)	-7(2)	1(2)	-17(2)
P(201)	23(1)	24(1)	33(1)	-16(1)	1(1)	-3(1)
F(201)	36(3)	52(3)	152(5)	-65(4)	23(3)	-7(3)
F(202)	49(3)	40(3)	59(3)	-27(2)	14(2)	-29(2)
F(203)	36(3)	33(3)	62(3)	-19(2)	12(2)	0(2)
F(204)	40(3)	41(3)	73(3)	-29(2)	-3(2)	-17(2)
F(205)	80(4)	96(4)	26(3)	-16(3)	12(2)	-63(3)
F(206)	79(4)	53(3)	49(3)	2(2)	-32(3)	-7(3)
P(301)	26(1)	26(1)	32(1)	-12(1)	6(1)	-6(1)
F(301)	30(2)	40(3)	41(3)	-23(2)	6(2)	-7(2)
F(302)	31(3)	73(4)	82(4)	-57(3)	-6(2)	-1(3)
F(303)	40(3)	62(3)	104(4)	-54(3)	33(3)	-20(3)
F(304)	42(3)	165(7)	186(7)	-151(6)	40(4)	-51(4)
F(305)	140(6)	45(3)	70(4)	16(3)	52(4)	-3(4)
F(306)	69(4)	63(4)	62(4)	14(3)	-14(3)	12(3)
P(401)	21(1)	22(1)	19(1)	-7(1)	-2(1)	-7(1)
F(401)	25(2)	53(3)	20(2)	4(2)	-9(2)	-15(2)
F(402)	37(3)	135(5)	24(3)	-12(3)	0(2)	23(3)
F(403)	21(2)	78(3)	21(2)	0(2)	-7(2)	-7(2)
F(404)	40(3)	105(4)	28(3)	-2(3)	5(2)	6(3)
F(405)	203(7)	26(3)	70(4)	11(3)	-58(4)	-58(4)
F(406)	154(6)	47(3)	54(3)	-4(3)	-30(3)	-61(4)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for IL-bis(oxime)-Cu^{II} , **4**.

	x	y	z	U(eq)
H(12)	9160	9830	4780	34
H(11)	10804	8798	3748	21
H(14)	8071	6516	4334	23
H(15)	9627	5996	3521	24
H(17)	11561	7761	3209	19
H(18A)	12669	6503	2824	25
H(18B)	11670	5965	2770	25
H(19)	12930	7580	1544	26
H(20)	9386	6942	1743	26
H(21)	9384	8004	447	26
H(22A)	12691	8629	232	49
H(22B)	11129	9116	2	49
H(22C)	11869	8418	-357	49
H(32)	6179	7561	5255	31
H(31)	4387	8709	6130	24
H(34)	7422	10805	5770	25
H(35)	5752	11424	6455	24
H(37)	3581	9795	6614	24
H(38A)	3461	11657	6938	32
H(38B)	2469	11135	6846	32
H(39)	5455	9934	8054	22
H(40)	1564	11095	8287	30
H(41)	2489	10134	9589	33
H(42A)	5178	8658	9562	45
H(42B)	4882	9183	10139	45
H(42C)	6136	9241	9547	45
H(52)	1360	5077	5024	39
H(51)	-191	6085	6059	20
H(54)	2720	8252	5630	27
H(55)	1115	8812	6388	24

H(57)	-950	7119	6622	24
H(58A)	-1110	8952	6992	31
H(58B)	-2051	8366	6986	31
H(59)	-2474	7565	8361	24
H(60)	1281	7922	8040	29
H(61)	1118	7078	9419	28
H(62A)	-2428	6837	9832	42
H(62B)	-1062	6698	10306	42
H(62C)	-1149	6084	9861	42
H(72)	4503	7257	4688	33
H(71)	6212	6230	3687	21
H(74)	3299	4082	3989	26
H(75)	4864	3594	3176	25
H(77)	6894	5281	3036	22
H(78A)	7935	4177	2493	32
H(78B)	7036	3582	2451	32
H(79)	4471	5144	1769	26
H(80)	8216	4595	893	30
H(81)	6654	5618	-179	33
H(82A)	3100	6029	504	44
H(82B)	3922	6204	-300	44
H(82C)	3943	6709	270	44

Table 6. Torsion angles [°] for IL-bis(oxime)-Cu^{II} , **4**.

O(31)-Cu(1)-N(11)-C(11)	179.0(5)
O(11)-Cu(1)-N(11)-C(11)	0.8(5)
N(31)-Cu(1)-N(11)-C(11)	-93(3)
O(31)-Cu(1)-N(11)-O(12)	-3.0(4)
O(11)-Cu(1)-N(11)-O(12)	178.8(4)
N(31)-Cu(1)-N(11)-O(12)	85(3)
O(31)-Cu(1)-O(11)-C(13)	-86(6)
N(31)-Cu(1)-O(11)-C(13)	175.8(5)
N(11)-Cu(1)-O(11)-C(13)	-0.6(5)
O(12)-N(11)-C(11)-C(12)	-179.4(5)
Cu(1)-N(11)-C(11)-C(12)	-1.3(9)
N(11)-C(11)-C(12)-C(17)	-180.0(6)
N(11)-C(11)-C(12)-C(13)	1.4(9)
Cu(1)-O(11)-C(13)-C(14)	-178.6(4)
Cu(1)-O(11)-C(13)-C(12)	0.9(8)
C(17)-C(12)-C(13)-O(11)	-179.8(5)
C(11)-C(12)-C(13)-O(11)	-1.2(9)
C(17)-C(12)-C(13)-C(14)	-0.3(8)
C(11)-C(12)-C(13)-C(14)	178.3(6)
O(11)-C(13)-C(14)-C(15)	179.1(5)
C(12)-C(13)-C(14)-C(15)	-0.4(9)
C(13)-C(14)-C(15)-C(16)	0.6(9)
C(14)-C(15)-C(16)-C(17)	-0.1(9)
C(14)-C(15)-C(16)-C(18)	-176.0(5)
C(15)-C(16)-C(17)-C(12)	-0.7(9)
C(18)-C(16)-C(17)-C(12)	175.3(6)
C(11)-C(12)-C(17)-C(16)	-177.9(5)
C(13)-C(12)-C(17)-C(16)	0.8(9)
C(19)-N(12)-C(18)-C(16)	111.8(7)
C(20)-N(12)-C(18)-C(16)	-63.1(7)
C(17)-C(16)-C(18)-N(12)	-73.6(7)
C(15)-C(16)-C(18)-N(12)	102.3(6)
C(21)-N(13)-C(19)-N(12)	1.1(7)
C(22)-N(13)-C(19)-N(12)	179.6(6)

C(20)-N(12)-C(19)-N(13)	-0.7(7)
C(18)-N(12)-C(19)-N(13)	-176.4(5)
C(19)-N(12)-C(20)-C(21)	0.0(7)
C(18)-N(12)-C(20)-C(21)	175.7(5)
N(12)-C(20)-C(21)-N(13)	0.6(7)
C(19)-N(13)-C(21)-C(20)	-1.1(7)
C(22)-N(13)-C(21)-C(20)	-179.5(6)
O(31)-Cu(1)-N(31)-C(31)	5.4(5)
O(11)-Cu(1)-N(31)-C(31)	-176.4(5)
N(11)-Cu(1)-N(31)-C(31)	-83(3)
O(31)-Cu(1)-N(31)-O(32)	-176.8(4)
O(11)-Cu(1)-N(31)-O(32)	1.5(4)
N(11)-Cu(1)-N(31)-O(32)	95(3)
O(11)-Cu(1)-O(31)-C(33)	-102(6)
N(31)-Cu(1)-O(31)-C(33)	-4.0(5)
N(11)-Cu(1)-O(31)-C(33)	172.3(5)
O(32)-N(31)-C(31)-C(32)	178.4(5)
Cu(1)-N(31)-C(31)-C(32)	-3.6(9)
N(31)-C(31)-C(32)-C(37)	-179.9(6)
N(31)-C(31)-C(32)-C(33)	-1.4(9)
Cu(1)-O(31)-C(33)-C(34)	-179.7(4)
Cu(1)-O(31)-C(33)-C(32)	1.0(8)
C(37)-C(32)-C(33)-O(31)	-178.7(5)
C(31)-C(32)-C(33)-O(31)	2.8(9)
C(37)-C(32)-C(33)-C(34)	2.0(8)
C(31)-C(32)-C(33)-C(34)	-176.5(6)
O(31)-C(33)-C(34)-C(35)	179.2(5)
C(32)-C(33)-C(34)-C(35)	-1.5(9)
C(33)-C(34)-C(35)-C(36)	-1.2(9)
C(34)-C(35)-C(36)-C(37)	3.2(9)
C(34)-C(35)-C(36)-C(38)	178.7(5)
C(35)-C(36)-C(37)-C(32)	-2.6(8)
C(38)-C(36)-C(37)-C(32)	-178.2(5)
C(33)-C(32)-C(37)-C(36)	0.1(9)
C(31)-C(32)-C(37)-C(36)	178.7(5)
C(39)-N(32)-C(38)-C(36)	19.3(9)

C(40)-N(32)-C(38)-C(36)	-160.9(6)
C(35)-C(36)-C(38)-N(32)	-98.8(7)
C(37)-C(36)-C(38)-N(32)	76.6(7)
C(41)-N(33)-C(39)-N(32)	0.9(7)
C(42)-N(33)-C(39)-N(32)	172.7(5)
C(40)-N(32)-C(39)-N(33)	0.1(7)
C(38)-N(32)-C(39)-N(33)	179.9(5)
C(39)-N(32)-C(40)-C(41)	-1.0(7)
C(38)-N(32)-C(40)-C(41)	179.1(5)
N(32)-C(40)-C(41)-N(33)	1.6(7)
C(39)-N(33)-C(41)-C(40)	-1.6(7)
C(42)-N(33)-C(41)-C(40)	-173.0(6)
O(51)-Cu(2)-N(51)-C(51)	2.2(5)
O(71)-Cu(2)-N(51)-C(51)	-175.4(5)
N(71)-Cu(2)-N(51)-C(51)	58(6)
O(51)-Cu(2)-N(51)-O(52)	-178.7(4)
O(71)-Cu(2)-N(51)-O(52)	3.7(4)
N(71)-Cu(2)-N(51)-O(52)	-123(6)
O(71)-Cu(2)-O(51)-C(53)	103(4)
N(51)-Cu(2)-O(51)-C(53)	0.7(5)
N(71)-Cu(2)-O(51)-C(53)	-177.6(5)
O(52)-N(51)-C(51)-C(52)	178.1(5)
Cu(2)-N(51)-C(51)-C(52)	-2.8(9)
N(51)-C(51)-C(52)-C(53)	0.1(9)
N(51)-C(51)-C(52)-C(57)	-179.3(6)
Cu(2)-O(51)-C(53)-C(54)	177.4(4)
Cu(2)-O(51)-C(53)-C(52)	-3.0(8)
C(57)-C(52)-C(53)-O(51)	-177.8(5)
C(51)-C(52)-C(53)-O(51)	2.8(9)
C(57)-C(52)-C(53)-C(54)	1.9(8)
C(51)-C(52)-C(53)-C(54)	-177.6(5)
O(51)-C(53)-C(54)-C(55)	177.9(6)
C(52)-C(53)-C(54)-C(55)	-1.8(9)
C(53)-C(54)-C(55)-C(56)	0.2(10)
C(54)-C(55)-C(56)-C(57)	1.2(9)
C(54)-C(55)-C(56)-C(58)	177.7(6)

C(55)-C(56)-C(57)-C(52)	-1.0(9)
C(58)-C(56)-C(57)-C(52)	-177.5(5)
C(53)-C(52)-C(57)-C(56)	-0.5(9)
C(51)-C(52)-C(57)-C(56)	178.9(5)
C(59)-N(52)-C(58)-C(56)	-123.4(6)
C(60)-N(52)-C(58)-C(56)	54.8(8)
C(57)-C(56)-C(58)-N(52)	80.5(7)
C(55)-C(56)-C(58)-N(52)	-95.9(7)
C(60)-N(52)-C(59)-N(53)	0.0(7)
C(58)-N(52)-C(59)-N(53)	178.4(5)
C(61)-N(53)-C(59)-N(52)	0.3(7)
C(62)-N(53)-C(59)-N(52)	-176.2(5)
C(59)-N(52)-C(60)-C(61)	-0.2(7)
C(58)-N(52)-C(60)-C(61)	-178.7(5)
N(52)-C(60)-C(61)-N(53)	0.4(7)
C(59)-N(53)-C(61)-C(60)	-0.4(7)
C(62)-N(53)-C(61)-C(60)	175.9(6)
O(51)-Cu(2)-N(71)-C(71)	-179.1(5)
O(71)-Cu(2)-N(71)-C(71)	-1.6(5)
N(51)-Cu(2)-N(71)-C(71)	125(6)
O(51)-Cu(2)-N(71)-O(72)	3.8(4)
O(71)-Cu(2)-N(71)-O(72)	-178.7(4)
N(51)-Cu(2)-N(71)-O(72)	-52(6)
O(51)-Cu(2)-O(71)-C(73)	79(4)
N(51)-Cu(2)-O(71)-C(73)	-178.2(5)
N(71)-Cu(2)-O(71)-C(73)	0.1(5)
O(72)-N(71)-C(71)-C(72)	179.9(5)
Cu(2)-N(71)-C(71)-C(72)	2.7(9)
N(71)-C(71)-C(72)-C(77)	177.0(6)
N(71)-C(71)-C(72)-C(73)	-2.2(9)
Cu(2)-O(71)-C(73)-C(74)	-178.4(4)
Cu(2)-O(71)-C(73)-C(72)	0.1(8)
C(77)-C(72)-C(73)-O(71)	-178.5(5)
C(71)-C(72)-C(73)-O(71)	0.7(9)
C(77)-C(72)-C(73)-C(74)	0.1(8)
C(71)-C(72)-C(73)-C(74)	179.3(5)

O(71)-C(73)-C(74)-C(75)	178.5(6)
C(72)-C(73)-C(74)-C(75)	-0.2(9)
C(73)-C(74)-C(75)-C(76)	-0.2(9)
C(74)-C(75)-C(76)-C(77)	0.8(9)
C(74)-C(75)-C(76)-C(78)	-173.1(6)
C(75)-C(76)-C(77)-C(72)	-0.9(9)
C(78)-C(76)-C(77)-C(72)	173.1(5)
C(73)-C(72)-C(77)-C(76)	0.5(9)
C(71)-C(72)-C(77)-C(76)	-178.8(5)
C(79)-N(72)-C(78)-C(76)	-23.3(8)
C(80)-N(72)-C(78)-C(76)	159.1(6)
C(77)-C(76)-C(78)-N(72)	-80.0(7)
C(75)-C(76)-C(78)-N(72)	93.7(7)
C(80)-N(72)-C(79)-N(73)	-1.7(7)
C(78)-N(72)-C(79)-N(73)	-179.6(5)
C(81)-N(73)-C(79)-N(72)	0.3(7)
C(82)-N(73)-C(79)-N(72)	-173.0(5)
C(79)-N(72)-C(80)-C(81)	2.4(7)
C(78)-N(72)-C(80)-C(81)	-179.7(5)
C(79)-N(73)-C(81)-C(80)	1.2(7)
C(82)-N(73)-C(81)-C(80)	174.3(6)
N(72)-C(80)-C(81)-N(73)	-2.2(7)

Symmetry transformations used to generate equivalent atoms:

Supplementary Material (ESI) for Dalton Transactions

Crystallographic data for the structure IL-salen-Cu^{II}, 5.

Table 1. Crystal data and structure refinement for IL-salen-Cu^{II}, **5**.

Table 2. Atomic coordinates and equivalent isotropic displacement parameters for IL-salen-Cu^{II}, **5**.

Table 3. Bond lengths and angles for the structure IL-salen-Cu^{II}, **5**.

Table 4. Anisotropic displacement parameters for the structure IL-salen-Cu^{II}, **5**.

Table 5. Hydrogen coordinates and isotropic displacement parameters for the structure IL-salen-Cu^{II}, **5**.

Table 6. Torsion angles for the structure IL-salen-Cu^{II}, **5**.

Table 1. Crystal data and structure refinement for *of* IL-salen-Cu^{II}, 5.

Identification code	rs0213	
Empirical formula	C26 H28 Cu F12 N6 O4 P2	
Formula weight	842.02	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 8.492(4) Å	α= 90°.
	b = 10.988(5) Å	β= 91.442(12)°.
	c = 35.208(17) Å	γ = 90°.
Volume	3284(3) $Å^3$	
Z	4	
Density (calculated)	1.703 Mg/m^3	
Absorption coefficient	0.875 mm^{-1}	
F(000)	1700	
Crystal size	0.35 x 0.20 x 0.10 mm^3	
Theta range for data collection	1.16 to 25.23°.	
Index ranges	-7<=h<=10, -10<=k<=12, -42<=l<=36	
Reflections collected	12988	
Independent reflections	5754 [R(int) = 0.1029]	
Completeness to theta = 25.23°	96.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.480	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5754 / 0 / 462	
Goodness-of-fit on F^2	1.106	
Final R indices [I>2sigma(I)]	R1 = 0.1151, wR2 = 0.2477	
R indices (all data)	R1 = 0.2015, wR2 = 0.2935	
Largest diff. peak and hole	0.896 and -0.555 $e.Å^{-3}$	

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

	x	y	z	U(eq)
Cu(1)	7313(2)	5018(1)	5051(1)	37(1)
N(11)	8405(12)	5624(10)	4615(3)	42(3)
N(12)	11527(11)	678(11)	3630(3)	45(3)
N(13)	10578(11)	-871(10)	3350(3)	46(3)
N(14)	6330(11)	6589(9)	5051(2)	39(2)
N(15)	3167(11)	7282(9)	6890(3)	39(2)
N(16)	4678(12)	7786(10)	7358(3)	49(3)
O(11)	8076(9)	3390(7)	4988(2)	39(2)
O(12)	6473(9)	4552(7)	5528(2)	38(2)
C(11)	8175(16)	6958(12)	4547(3)	55(4)
C(12)	9352(14)	4990(13)	4402(3)	48(3)
C(13)	9688(14)	3709(12)	4440(3)	44(3)
C(14)	10694(14)	3209(15)	4180(3)	51(4)
C(15)	11084(13)	1967(14)	4187(3)	45(3)
C(16)	10371(14)	1254(13)	4456(3)	47(3)
C(17)	9338(15)	1727(13)	4710(3)	47(3)
C(18)	8994(13)	2961(12)	4720(3)	38(3)
C(19)	12254(15)	1453(14)	3932(3)	59(4)
C(20)	11290(15)	-475(14)	3669(4)	51(4)
C(21)	10977(14)	1069(12)	3273(3)	40(3)
C(22)	10401(14)	68(14)	3097(4)	50(3)
C(23)	10170(20)	-2159(13)	3257(5)	99(7)
C(24)	6591(14)	7266(11)	4696(3)	41(3)
C(25)	5457(14)	7030(11)	5309(3)	40(3)
C(26)	5024(12)	6405(10)	5656(3)	29(3)
C(27)	4071(12)	7047(11)	5905(3)	40(3)
C(28)	3564(13)	6531(12)	6237(3)	41(3)
C(29)	4064(14)	5312(11)	6314(3)	39(3)
C(30)	5024(14)	4680(10)	6078(3)	37(3)
C(31)	5531(13)	5239(11)	5738(3)	36(3)

C(32)	2515(12)	7170(12)	6497(3)	39(3)
C(33)	4353(15)	7965(12)	6993(4)	52(4)
C(34)	2678(16)	6625(14)	7202(4)	61(4)
C(35)	3643(17)	6975(15)	7491(4)	63(4)
C(36)	5965(18)	8366(15)	7588(4)	85(6)
P(41)	8081(4)	9662(3)	2044(1)	39(1)
F(41)	9286(12)	9645(9)	1723(3)	108(4)
F(42)	9149(14)	10593(8)	2273(3)	117(4)
F(43)	6879(14)	9647(9)	2370(3)	120(4)
F(44)	7090(12)	8699(7)	1816(3)	104(4)
F(45)	7185(9)	10767(6)	1840(2)	59(2)
F(46)	8976(9)	8567(7)	2256(2)	64(2)
P(51)	5924(4)	9007(3)	3590(1)	46(1)
F(51)	7339(14)	8999(19)	3836(3)	203(9)
F(52)	5404(12)	10298(7)	3708(3)	111(4)
F(53)	4445(12)	9012(16)	3325(3)	179(7)
F(54)	6371(16)	7711(9)	3459(5)	188(8)
F(55)	6891(11)	9475(8)	3261(3)	92(3)
F(56)	4843(16)	8502(11)	3891(4)	191(8)
O(1S)	7645(12)	1971(11)	5601(3)	91(4)
O(2S)	4210(40)	9942(18)	4640(6)	265(13)

Table 3. Bond lengths [Å] and angles [°] for **IL-salen-Cu^{II}, 5**.

Cu(1)-O(12)	1.911(7)
Cu(1)-O(11)	1.917(8)
Cu(1)-N(14)	1.918(11)
Cu(1)-N(11)	1.931(10)
N(11)-C(12)	1.312(16)
N(11)-C(11)	1.497(16)
N(12)-C(20)	1.291(16)
N(12)-C(21)	1.396(13)
N(12)-C(19)	1.485(14)
N(13)-C(20)	1.336(16)
N(13)-C(22)	1.369(16)
N(13)-C(23)	1.490(17)
N(14)-C(25)	1.283(14)
N(14)-C(24)	1.475(13)
N(15)-C(33)	1.300(15)
N(15)-C(34)	1.388(15)
N(15)-C(32)	1.482(13)
N(16)-C(33)	1.322(15)
N(16)-C(35)	1.344(17)
N(16)-C(36)	1.488(16)
O(11)-C(18)	1.325(13)
O(12)-C(31)	1.339(13)
C(11)-C(24)	1.495(17)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(13)	1.442(18)
C(12)-H(12)	0.9500
C(13)-C(14)	1.381(17)
C(13)-C(18)	1.423(16)
C(14)-C(15)	1.404(18)
C(14)-H(14)	0.9500
C(15)-C(16)	1.382(17)
C(15)-C(19)	1.468(16)
C(16)-C(17)	1.371(16)

C(16)-H(16)	0.9500
C(17)-C(18)	1.388(17)
C(17)-H(17)	0.9500
C(19)-H(19A)	0.9900
C(19)-H(19B)	0.9900
C(20)-H(20)	0.9500
C(21)-C(22)	1.350(17)
C(21)-H(21)	0.9500
C(22)-H(22)	0.9500
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(25)-C(26)	1.456(15)
C(25)-H(25)	0.9500
C(26)-C(31)	1.381(15)
C(26)-C(27)	1.400(15)
C(27)-C(28)	1.377(15)
C(27)-H(27)	0.9500
C(28)-C(29)	1.429(17)
C(28)-C(32)	1.471(15)
C(29)-C(30)	1.369(16)
C(29)-H(29)	0.9500
C(30)-C(31)	1.420(15)
C(30)-H(30)	0.9500
C(32)-H(32A)	0.9900
C(32)-H(32B)	0.9900
C(33)-H(33)	0.9500
C(34)-C(35)	1.346(18)
C(34)-H(34)	0.9500
C(35)-H(35)	0.9500
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
P(41)-F(41)	1.543(9)

P(41)-F(43)	1.556(9)
P(41)-F(44)	1.562(8)
P(41)-F(42)	1.577(8)
P(41)-F(45)	1.594(7)
P(41)-F(46)	1.599(7)
P(51)-F(51)	1.462(11)
P(51)-F(56)	1.524(9)
P(51)-F(55)	1.527(8)
P(51)-F(52)	1.546(9)
P(51)-F(53)	1.547(11)
P(51)-F(54)	1.548(11)

O(12)-Cu(1)-O(11)	89.2(3)
O(12)-Cu(1)-N(14)	94.0(4)
O(11)-Cu(1)-N(14)	171.3(3)
O(12)-Cu(1)-N(11)	171.1(3)
O(11)-Cu(1)-N(11)	93.4(4)
N(14)-Cu(1)-N(11)	84.7(4)
C(12)-N(11)-C(11)	120.5(11)
C(12)-N(11)-Cu(1)	125.7(9)
C(11)-N(11)-Cu(1)	113.6(9)
C(20)-N(12)-C(21)	110.3(11)
C(20)-N(12)-C(19)	123.4(12)
C(21)-N(12)-C(19)	126.3(12)
C(20)-N(13)-C(22)	110.0(11)
C(20)-N(13)-C(23)	126.2(14)
C(22)-N(13)-C(23)	123.5(13)
C(25)-N(14)-C(24)	120.8(11)
C(25)-N(14)-Cu(1)	126.8(8)
C(24)-N(14)-Cu(1)	112.3(8)
C(33)-N(15)-C(34)	108.9(11)
C(33)-N(15)-C(32)	125.3(11)
C(34)-N(15)-C(32)	125.7(11)
C(33)-N(16)-C(35)	108.4(11)
C(33)-N(16)-C(36)	126.8(13)
C(35)-N(16)-C(36)	124.9(13)

C(18)-O(11)-Cu(1)	128.4(7)
C(31)-O(12)-Cu(1)	125.3(7)
C(24)-C(11)-N(11)	106.3(10)
C(24)-C(11)-H(11A)	110.5
N(11)-C(11)-H(11A)	110.5
C(24)-C(11)-H(11B)	110.5
N(11)-C(11)-H(11B)	110.5
H(11A)-C(11)-H(11B)	108.7
N(11)-C(12)-C(13)	126.0(11)
N(11)-C(12)-H(12)	117.0
C(13)-C(12)-H(12)	117.0
C(14)-C(13)-C(18)	120.2(13)
C(14)-C(13)-C(12)	116.9(12)
C(18)-C(13)-C(12)	122.9(12)
C(13)-C(14)-C(15)	121.7(12)
C(13)-C(14)-H(14)	119.1
C(15)-C(14)-H(14)	119.1
C(16)-C(15)-C(14)	117.1(12)
C(16)-C(15)-C(19)	121.0(14)
C(14)-C(15)-C(19)	121.9(13)
C(17)-C(16)-C(15)	122.1(14)
C(17)-C(16)-H(16)	118.9
C(15)-C(16)-H(16)	118.9
C(16)-C(17)-C(18)	121.7(12)
C(16)-C(17)-H(17)	119.2
C(18)-C(17)-H(17)	119.2
O(11)-C(18)-C(17)	119.6(11)
O(11)-C(18)-C(13)	123.2(12)
C(17)-C(18)-C(13)	117.1(12)
C(15)-C(19)-N(12)	112.5(10)
C(15)-C(19)-H(19A)	109.1
N(12)-C(19)-H(19A)	109.1
C(15)-C(19)-H(19B)	109.1
N(12)-C(19)-H(19B)	109.1
H(19A)-C(19)-H(19B)	107.8
N(12)-C(20)-N(13)	107.4(13)

N(12)-C(20)-H(20)	126.3
N(13)-C(20)-H(20)	126.3
C(22)-C(21)-N(12)	105.9(11)
C(22)-C(21)-H(21)	127.1
N(12)-C(21)-H(21)	127.1
C(21)-C(22)-N(13)	106.3(11)
C(21)-C(22)-H(22)	126.8
N(13)-C(22)-H(22)	126.8
N(13)-C(23)-H(23A)	109.5
N(13)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
N(13)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
N(14)-C(24)-C(11)	109.8(10)
N(14)-C(24)-H(24A)	109.7
C(11)-C(24)-H(24A)	109.7
N(14)-C(24)-H(24B)	109.7
C(11)-C(24)-H(24B)	109.7
H(24A)-C(24)-H(24B)	108.2
N(14)-C(25)-C(26)	125.4(11)
N(14)-C(25)-H(25)	117.3
C(26)-C(25)-H(25)	117.3
C(31)-C(26)-C(27)	121.2(10)
C(31)-C(26)-C(25)	122.0(11)
C(27)-C(26)-C(25)	116.8(11)
C(28)-C(27)-C(26)	121.5(11)
C(28)-C(27)-H(27)	119.3
C(26)-C(27)-H(27)	119.3
C(27)-C(28)-C(29)	116.7(11)
C(27)-C(28)-C(32)	122.5(12)
C(29)-C(28)-C(32)	120.7(11)
C(30)-C(29)-C(28)	122.6(10)
C(30)-C(29)-H(29)	118.7
C(28)-C(29)-H(29)	118.7
C(29)-C(30)-C(31)	119.3(11)

C(29)-C(30)-H(30)	120.3
C(31)-C(30)-H(30)	120.3
O(12)-C(31)-C(26)	126.5(10)
O(12)-C(31)-C(30)	114.9(11)
C(26)-C(31)-C(30)	118.7(11)
C(28)-C(32)-N(15)	113.7(9)
C(28)-C(32)-H(32A)	108.8
N(15)-C(32)-H(32A)	108.8
C(28)-C(32)-H(32B)	108.8
N(15)-C(32)-H(32B)	108.8
H(32A)-C(32)-H(32B)	107.7
N(15)-C(33)-N(16)	109.1(13)
N(15)-C(33)-H(33)	125.5
N(16)-C(33)-H(33)	125.5
C(35)-C(34)-N(15)	105.1(13)
C(35)-C(34)-H(34)	127.4
N(15)-C(34)-H(34)	127.4
N(16)-C(35)-C(34)	108.5(13)
N(16)-C(35)-H(35)	125.8
C(34)-C(35)-H(35)	125.8
N(16)-C(36)-H(36A)	109.5
N(16)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
N(16)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
F(41)-P(41)-F(43)	178.6(5)
F(41)-P(41)-F(44)	88.5(6)
F(43)-P(41)-F(44)	91.0(7)
F(41)-P(41)-F(42)	89.9(7)
F(43)-P(41)-F(42)	90.5(7)
F(44)-P(41)-F(42)	177.3(6)
F(41)-P(41)-F(45)	89.9(5)
F(43)-P(41)-F(45)	91.5(5)
F(44)-P(41)-F(45)	92.3(4)
F(42)-P(41)-F(45)	89.9(4)

F(41)-P(41)-F(46)	91.0(5)
F(43)-P(41)-F(46)	87.7(5)
F(44)-P(41)-F(46)	88.6(4)
F(42)-P(41)-F(46)	89.3(4)
F(45)-P(41)-F(46)	178.8(4)
F(51)-P(51)-F(56)	95.0(9)
F(51)-P(51)-F(55)	90.1(7)
F(56)-P(51)-F(55)	174.6(9)
F(51)-P(51)-F(52)	94.7(9)
F(56)-P(51)-F(52)	88.0(6)
F(55)-P(51)-F(52)	93.3(5)
F(51)-P(51)-F(53)	179.1(7)
F(56)-P(51)-F(53)	85.8(9)
F(55)-P(51)-F(53)	89.1(7)
F(52)-P(51)-F(53)	85.7(7)
F(51)-P(51)-F(54)	88.1(10)
F(56)-P(51)-F(54)	91.7(6)
F(55)-P(51)-F(54)	86.7(5)
F(52)-P(51)-F(54)	177.1(9)
F(53)-P(51)-F(54)	91.4(9)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **IL-salen-Cu^{II}, 5**.. 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}
Cu(1)	41(1)	39(1)	29(1)	7(1)	-12(1)	-8(1)
N(11)	35(6)	55(7)	35(5)	15(5)	-26(5)	-22(5)
N(12)	31(6)	69(9)	35(6)	-2(6)	1(4)	2(6)
N(13)	30(6)	37(7)	70(8)	-9(6)	1(5)	1(5)
N(14)	35(6)	54(7)	25(5)	5(5)	-16(4)	-16(5)
N(15)	26(5)	34(6)	58(6)	-7(5)	3(5)	6(5)
N(16)	40(7)	44(7)	61(7)	-27(6)	-10(5)	19(6)
O(11)	41(5)	50(6)	25(4)	7(4)	-7(3)	4(4)
O(12)	47(5)	34(5)	33(4)	-1(3)	-2(4)	0(4)
C(11)	63(10)	61(10)	38(7)	26(7)	-24(6)	-15(8)
C(12)	34(7)	68(10)	42(7)	21(7)	-13(5)	-18(8)
C(13)	46(8)	60(10)	24(6)	3(6)	-18(5)	-10(7)
C(14)	37(7)	95(12)	22(6)	-9(7)	-5(5)	-15(8)
C(15)	28(7)	74(11)	33(7)	-8(7)	-9(5)	-2(7)
C(16)	43(8)	67(10)	32(7)	-6(6)	-10(6)	-3(7)
C(17)	52(8)	58(10)	30(7)	1(6)	-5(6)	0(7)
C(18)	37(7)	58(9)	19(6)	-2(6)	-15(5)	-7(6)
C(19)	40(8)	91(12)	46(8)	-30(7)	-12(6)	-4(8)
C(20)	37(8)	47(9)	70(10)	-4(8)	27(7)	10(7)
C(21)	45(8)	49(9)	27(6)	3(6)	4(5)	-2(7)
C(22)	36(7)	67(10)	48(7)	-9(8)	5(5)	10(8)
C(23)	97(14)	39(10)	164(17)	-43(11)	60(12)	0(9)
C(24)	52(8)	37(8)	33(6)	8(5)	-15(5)	-14(6)
C(25)	39(7)	35(8)	44(7)	6(6)	-22(6)	-13(6)
C(26)	27(6)	20(6)	40(6)	3(5)	-14(5)	-6(5)
C(27)	23(6)	41(8)	54(8)	7(6)	-26(5)	-3(6)
C(28)	32(7)	48(9)	44(7)	-4(6)	-15(5)	-11(6)
C(29)	50(7)	47(8)	21(5)	2(5)	-1(5)	-13(6)
C(30)	61(8)	23(7)	27(6)	2(5)	-16(5)	5(6)
C(31)	30(6)	47(8)	31(6)	2(6)	-8(5)	-19(6)

C(32)	17(6)	53(8)	47(7)	0(6)	-2(5)	2(6)
C(33)	46(8)	39(8)	71(9)	0(7)	-22(7)	11(7)
C(34)	42(8)	92(12)	48(8)	-7(8)	15(6)	2(8)
C(35)	55(9)	98(13)	37(7)	-26(8)	16(7)	-5(9)
C(36)	66(11)	79(12)	109(13)	-60(10)	-30(9)	12(9)
P(41)	39(2)	31(2)	47(2)	2(1)	-3(1)	-3(1)
F(41)	107(8)	105(8)	114(7)	39(6)	59(6)	48(6)
F(42)	178(11)	50(6)	117(7)	36(5)	-111(7)	-42(6)
F(43)	159(10)	75(7)	129(8)	37(6)	92(8)	39(7)
F(44)	120(9)	42(5)	145(9)	-14(5)	-81(7)	-2(5)
F(45)	59(5)	41(5)	76(5)	7(4)	-16(4)	4(4)
F(46)	58(5)	45(5)	88(6)	14(4)	-28(4)	2(4)
P(51)	45(2)	46(2)	48(2)	13(2)	17(2)	13(2)
F(51)	95(9)	420(30)	88(8)	-20(11)	-38(7)	107(13)
F(52)	115(8)	40(5)	183(10)	0(6)	83(8)	4(5)
F(53)	60(7)	340(20)	142(10)	-155(12)	-4(6)	-9(9)
F(54)	177(13)	57(7)	339(19)	12(9)	204(14)	17(7)
F(55)	87(7)	93(7)	100(6)	47(5)	56(5)	38(5)
F(56)	207(14)	139(11)	238(14)	120(10)	192(12)	115(10)
O(1S)	73(8)	108(9)	94(8)	51(7)	31(6)	23(7)
O(2S)	400(40)	150(19)	240(20)	22(16)	-120(20)	-90(20)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **IL-salen-Cu^{II}, 5**.

	x	y	z	U(eq)
H(11A)	9007	7431	4683	65
H(11B)	8216	7144	4273	65
H(12)	9863	5415	4205	58
H(14)	11135	3718	3993	62
H(16)	10605	409	4465	57
H(17)	8845	1196	4884	56
H(19A)	13019	960	4083	71
H(19B)	12840	2124	3813	71
H(20)	11571	-954	3885	61
H(21)	11002	1874	3175	48
H(22)	9960	23	2846	60
H(23A)	10831	-2705	3413	149
H(23B)	10360	-2312	2988	149
H(23C)	9061	-2305	3309	149
H(24A)	6528	8151	4745	49
H(24B)	5764	7051	4505	49
H(25)	5061	7831	5271	48
H(27)	3767	7858	5845	48
H(29)	3716	4925	6538	47
H(30)	5348	3875	6140	45
H(32A)	1500	6728	6504	47
H(32B)	2297	7995	6395	47
H(33)	4899	8506	6832	63
H(34)	1843	6051	7210	73
H(35)	3600	6696	7746	76
H(36A)	5717	8319	7858	128
H(36B)	6068	9221	7513	128
H(36C)	6958	7939	7544	128

Table 6. Torsion angles [°] for **IL-salen-Cu^{II}, 5**.

O(12)-Cu(1)-N(11)-C(12)	104(3)
O(11)-Cu(1)-N(11)-C(12)	-3.1(9)
N(14)-Cu(1)-N(11)-C(12)	-174.5(9)
O(12)-Cu(1)-N(11)-C(11)	-72(3)
O(11)-Cu(1)-N(11)-C(11)	-178.9(7)
N(14)-Cu(1)-N(11)-C(11)	9.6(7)
O(12)-Cu(1)-N(14)-C(25)	0.6(9)
O(11)-Cu(1)-N(14)-C(25)	112(2)
N(11)-Cu(1)-N(14)-C(25)	-170.6(9)
O(12)-Cu(1)-N(14)-C(24)	-175.6(7)
O(11)-Cu(1)-N(14)-C(24)	-64(3)
N(11)-Cu(1)-N(14)-C(24)	13.3(7)
O(12)-Cu(1)-O(11)-C(18)	-172.9(8)
N(14)-Cu(1)-O(11)-C(18)	76(3)
N(11)-Cu(1)-O(11)-C(18)	-1.4(9)
O(11)-Cu(1)-O(12)-C(31)	-171.4(8)
N(14)-Cu(1)-O(12)-C(31)	0.5(8)
N(11)-Cu(1)-O(12)-C(31)	81(3)
C(12)-N(11)-C(11)-C(24)	154.7(10)
Cu(1)-N(11)-C(11)-C(24)	-29.2(10)
C(11)-N(11)-C(12)-C(13)	179.3(10)
Cu(1)-N(11)-C(12)-C(13)	3.7(16)
N(11)-C(12)-C(13)-C(14)	178.5(10)
N(11)-C(12)-C(13)-C(18)	0.6(18)
C(18)-C(13)-C(14)-C(15)	-1.0(17)
C(12)-C(13)-C(14)-C(15)	-179.0(10)
C(13)-C(14)-C(15)-C(16)	2.3(17)
C(13)-C(14)-C(15)-C(19)	-174.8(10)
C(14)-C(15)-C(16)-C(17)	-0.6(17)
C(19)-C(15)-C(16)-C(17)	176.5(11)
C(15)-C(16)-C(17)-C(18)	-2.4(18)
Cu(1)-O(11)-C(18)-C(17)	-175.9(8)
Cu(1)-O(11)-C(18)-C(13)	5.4(14)
C(16)-C(17)-C(18)-O(11)	-175.2(10)

C(16)-C(17)-C(18)-C(13)	3.6(17)
C(14)-C(13)-C(18)-O(11)	176.8(10)
C(12)-C(13)-C(18)-O(11)	-5.4(16)
C(14)-C(13)-C(18)-C(17)	-1.9(16)
C(12)-C(13)-C(18)-C(17)	175.9(10)
C(16)-C(15)-C(19)-N(12)	74.5(15)
C(14)-C(15)-C(19)-N(12)	-108.6(14)
C(20)-N(12)-C(19)-C(15)	-89.5(15)
C(21)-N(12)-C(19)-C(15)	89.1(15)
C(21)-N(12)-C(20)-N(13)	-0.7(13)
C(19)-N(12)-C(20)-N(13)	178.1(10)
C(22)-N(13)-C(20)-N(12)	1.7(14)
C(23)-N(13)-C(20)-N(12)	175.7(11)
C(20)-N(12)-C(21)-C(22)	-0.5(13)
C(19)-N(12)-C(21)-C(22)	-179.3(10)
N(12)-C(21)-C(22)-N(13)	1.5(12)
C(20)-N(13)-C(22)-C(21)	-2.0(13)
C(23)-N(13)-C(22)-C(21)	-176.3(11)
C(25)-N(14)-C(24)-C(11)	150.3(10)
Cu(1)-N(14)-C(24)-C(11)	-33.3(11)
N(11)-C(11)-C(24)-N(14)	39.0(12)
C(24)-N(14)-C(25)-C(26)	175.1(9)
Cu(1)-N(14)-C(25)-C(26)	-0.7(16)
N(14)-C(25)-C(26)-C(31)	-0.2(16)
N(14)-C(25)-C(26)-C(27)	179.3(10)
C(31)-C(26)-C(27)-C(28)	-1.9(16)
C(25)-C(26)-C(27)-C(28)	178.5(9)
C(26)-C(27)-C(28)-C(29)	0.2(15)
C(26)-C(27)-C(28)-C(32)	-177.6(10)
C(27)-C(28)-C(29)-C(30)	1.3(16)
C(32)-C(28)-C(29)-C(30)	179.2(10)
C(28)-C(29)-C(30)-C(31)	-1.1(17)
Cu(1)-O(12)-C(31)-C(26)	-1.4(14)
Cu(1)-O(12)-C(31)-C(30)	178.4(7)
C(27)-C(26)-C(31)-O(12)	-178.1(9)
C(25)-C(26)-C(31)-O(12)	1.4(16)

C(27)-C(26)-C(31)-C(30)	2.1(15)
C(25)-C(26)-C(31)-C(30)	-178.4(9)
C(29)-C(30)-C(31)-O(12)	179.6(9)
C(29)-C(30)-C(31)-C(26)	-0.6(16)
C(27)-C(28)-C(32)-N(15)	-123.3(11)
C(29)-C(28)-C(32)-N(15)	58.9(14)
C(33)-N(15)-C(32)-C(28)	69.6(15)
C(34)-N(15)-C(32)-C(28)	-106.2(13)
C(34)-N(15)-C(33)-N(16)	0.3(14)
C(32)-N(15)-C(33)-N(16)	-176.1(10)
C(35)-N(16)-C(33)-N(15)	-1.0(14)
C(36)-N(16)-C(33)-N(15)	178.7(11)
C(33)-N(15)-C(34)-C(35)	0.4(15)
C(32)-N(15)-C(34)-C(35)	176.8(11)
C(33)-N(16)-C(35)-C(34)	1.2(15)
C(36)-N(16)-C(35)-C(34)	-178.4(12)
N(15)-C(34)-C(35)-N(16)	-1.0(15)

Symmetry transformations used to generate equivalent atoms: