Supporting information

Interaction of 2-(2'-Pyridyl)benzimidazolyl Derivative Ligands with Group 12 Metal Ions: Coordination, Structures and Luminescence

Louise de la Durantaye, Theresa M^{c}Cormick, Xiang-Yang Liu, Su-ning Wang*

Department of Chemistry, Queen's University, Kingston, Ontario, K7L 3N6 Canada

Figure S1: TGA diagram of **1**

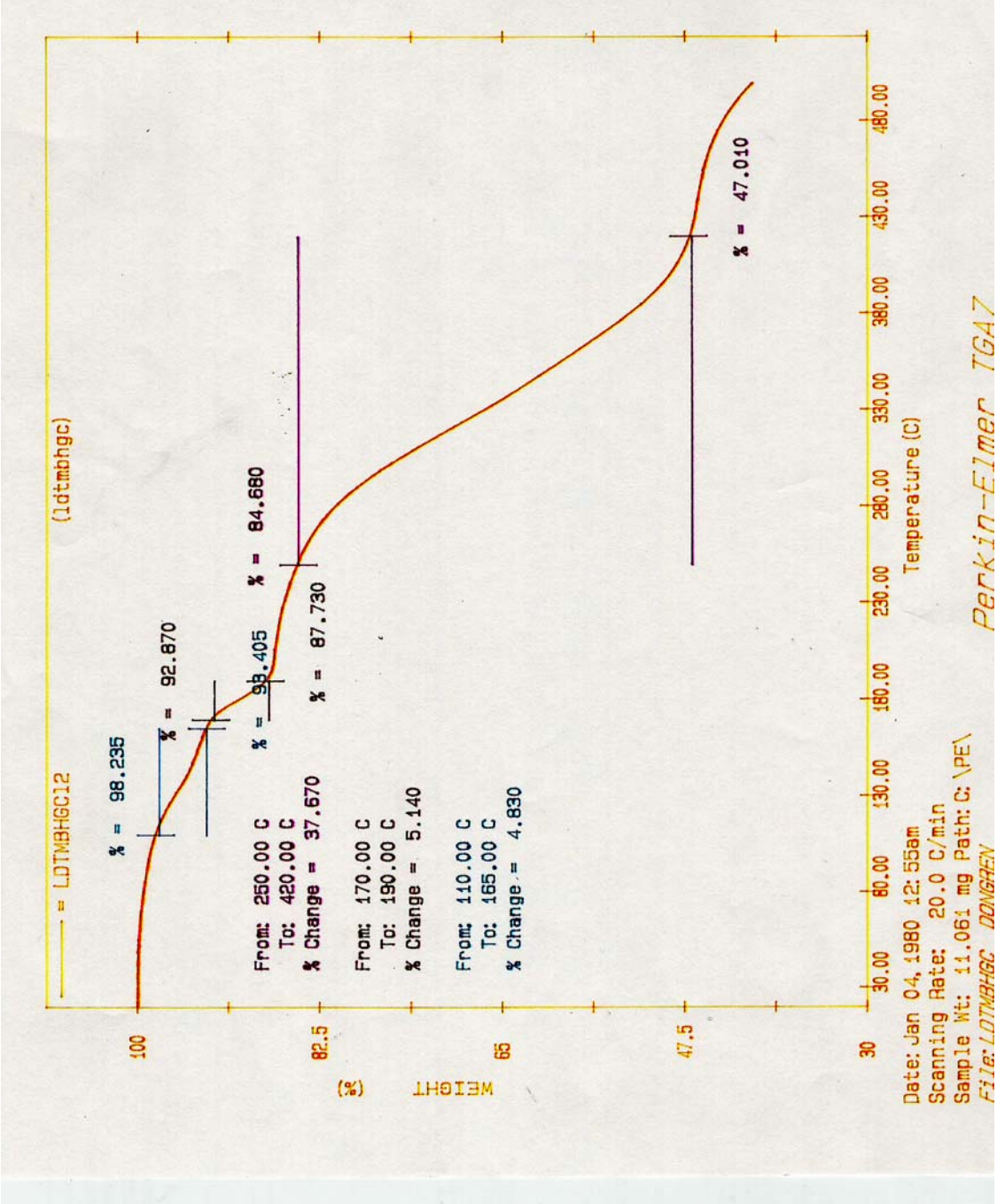


Figure S2. Titration diagram of mb (0.01 mM in THF) by $Cd(ClO_4)_2$.

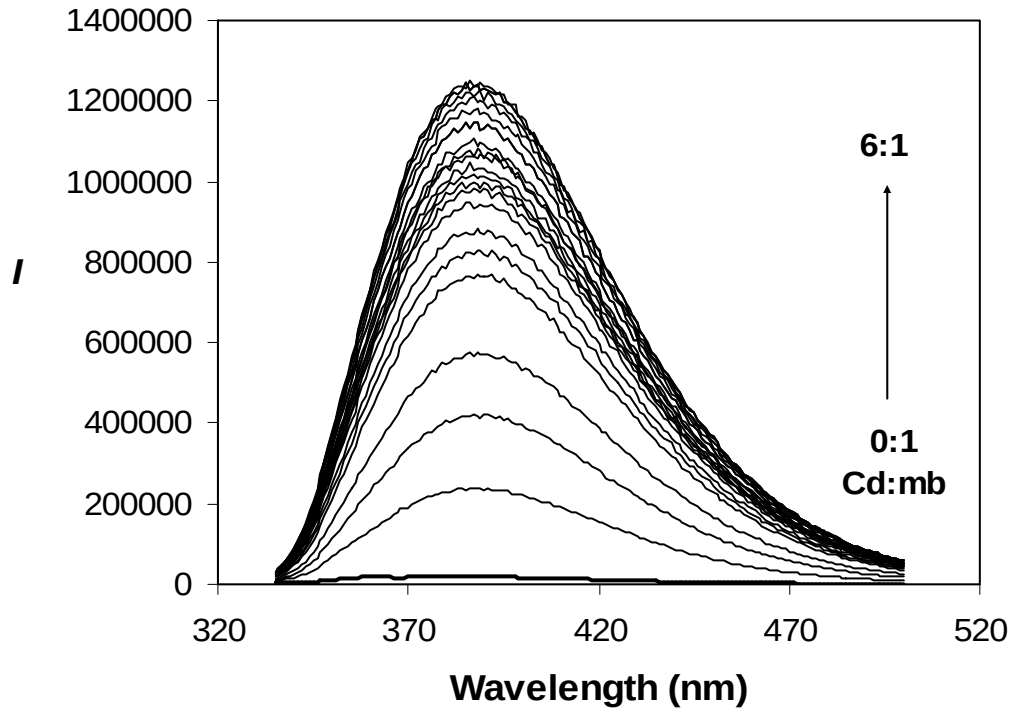


Figure S3. Titration diagram of tmb (0.01 mM in THF) by $Cd(ClO_4)_2$

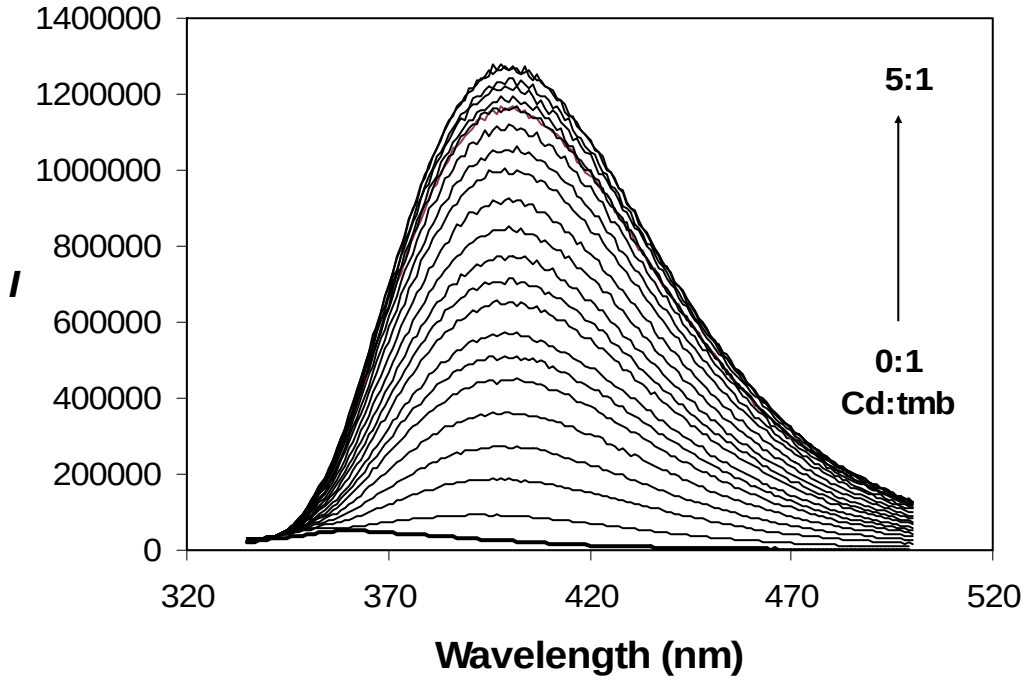


Figure S4. Titration diagram of tmb (0.01 mM in THF) by $Cd(OAc)_2$

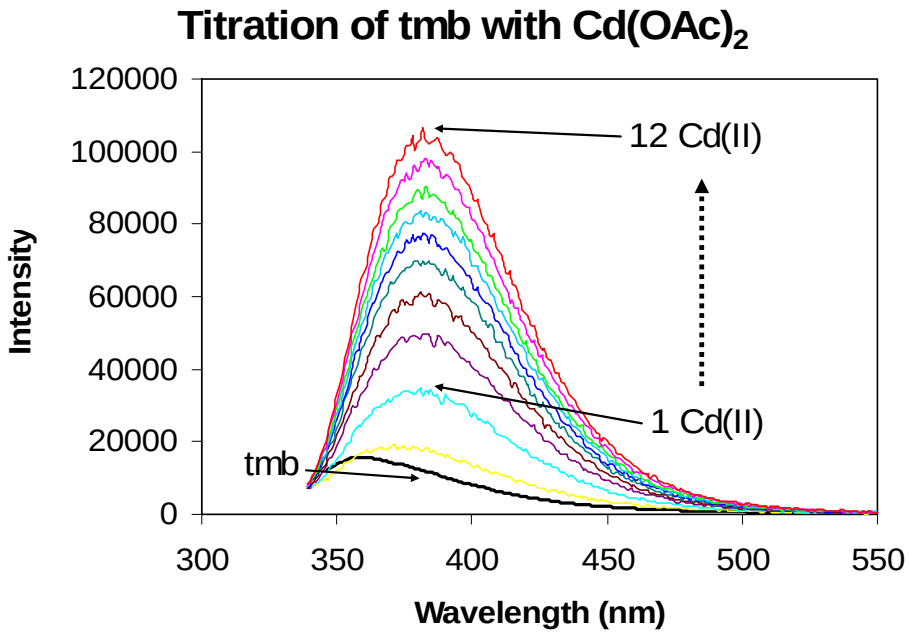


Figure S5. Titration diagram of tmb (0.01 mM in THF) by $Hg(ClO_4)_2$

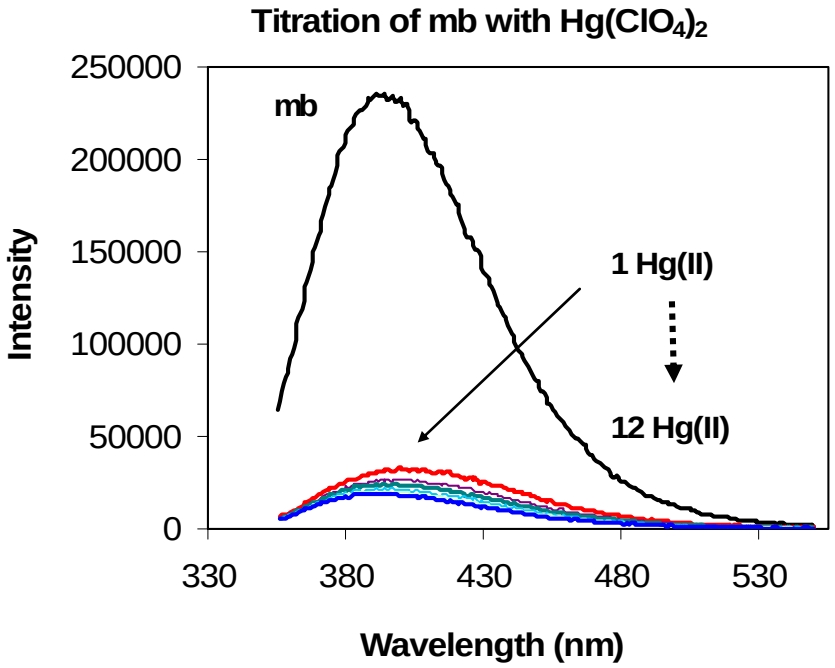


Figure S6. Titration diagram of tmb (0.01 mM in THF) by $HgCl_2$.

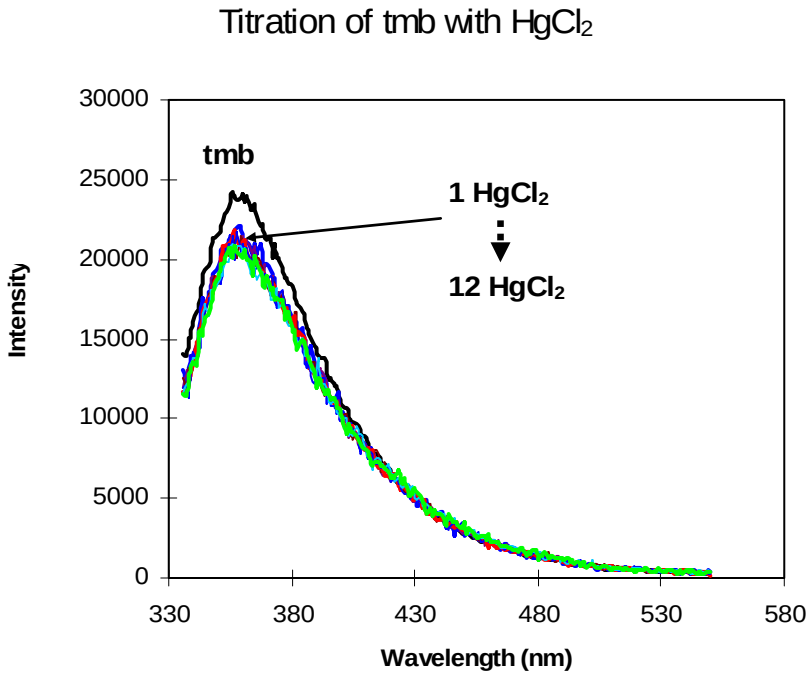


Figure S7. Stern-Volmer plots of titration of tmb (0.01 mM in THF) by $M(ClO_4)_2$

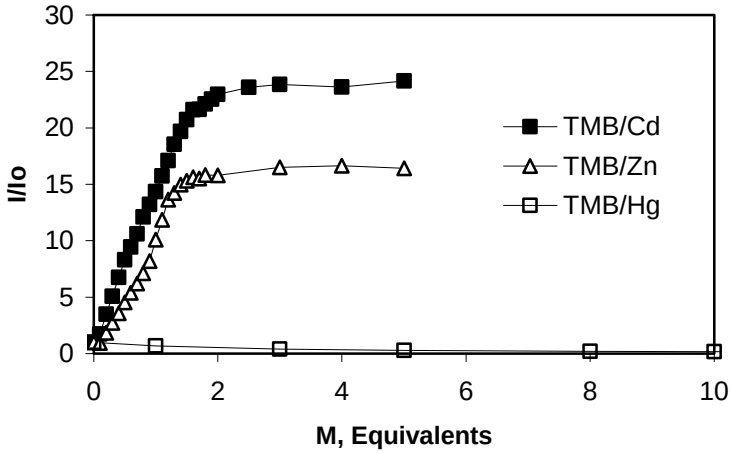


Figure S8. Stern-Volmer plots of titration of mb (0.01 mM in THF) by $M(ClO_4)_2$

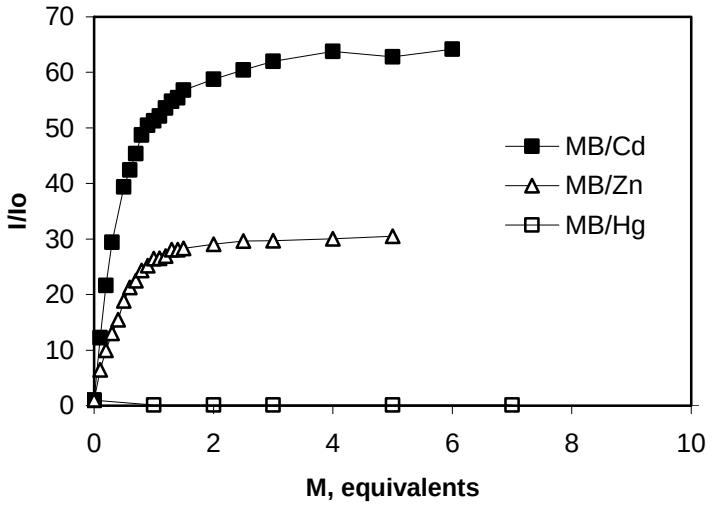


Fig. S9. The fluorescent intensity change of tmb and mb after the addition of 4 equivalents of metal perchlorates in THF (0.01 mM)

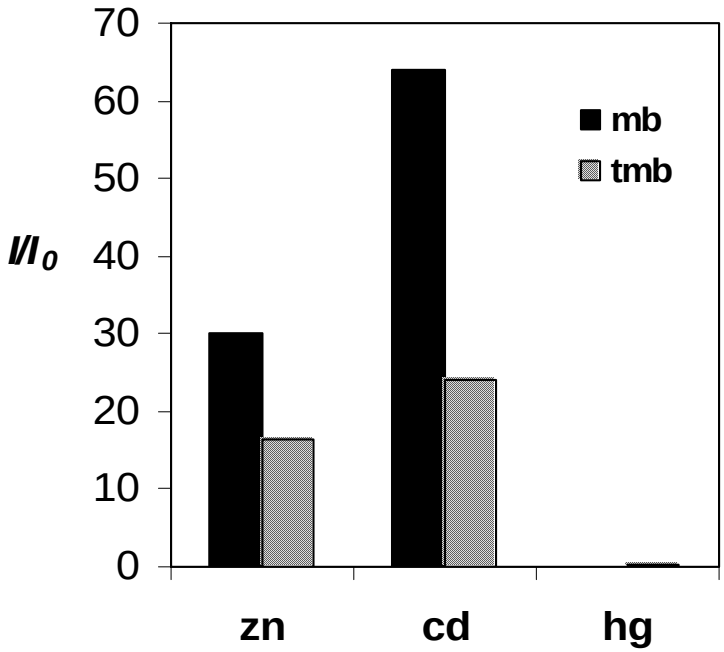


Figure S10. The ^{1}H NMR spectra of the reaction of tmb with $Zn(O_2CCF_3)_2$ in CD_2Cl_2

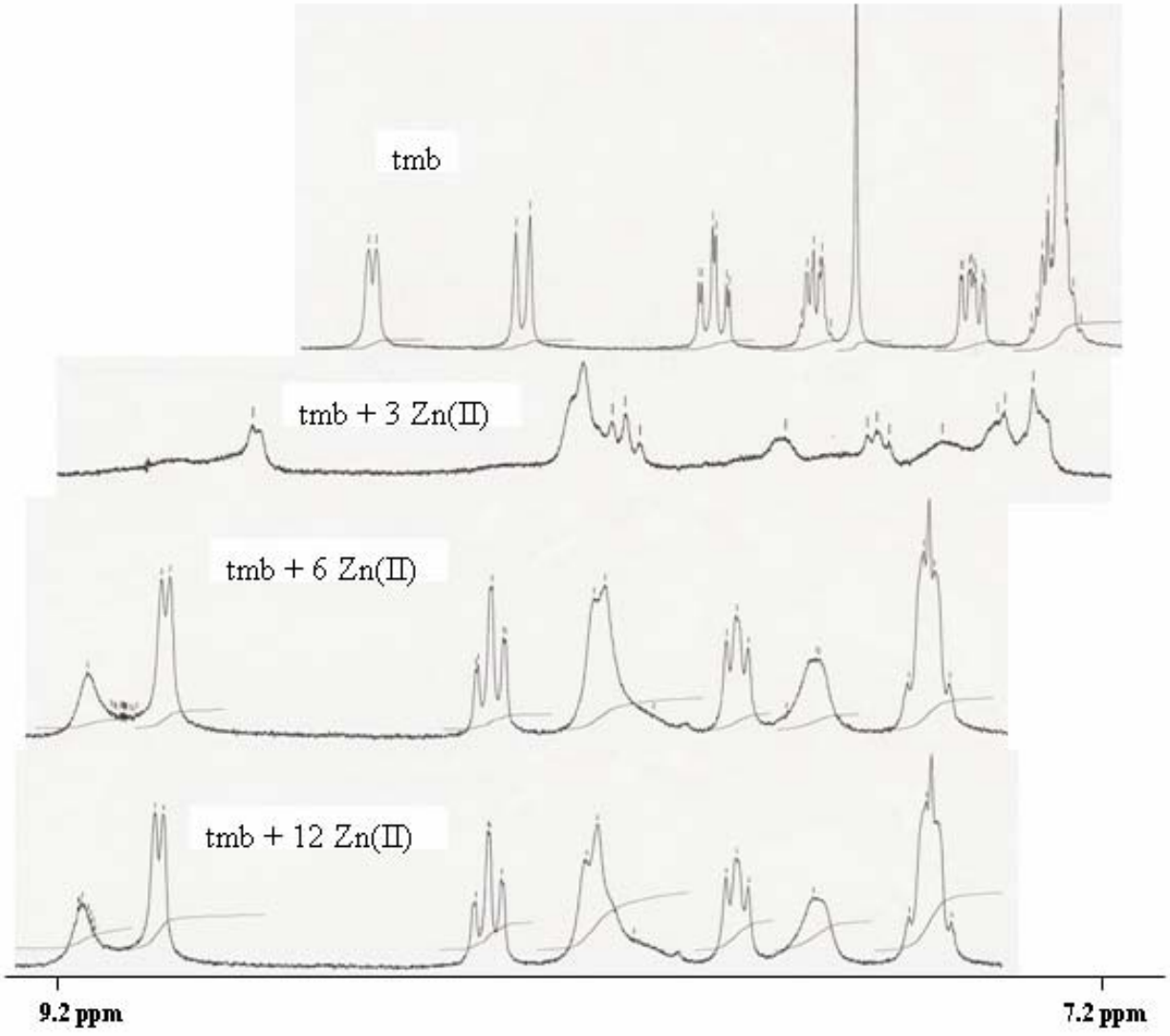
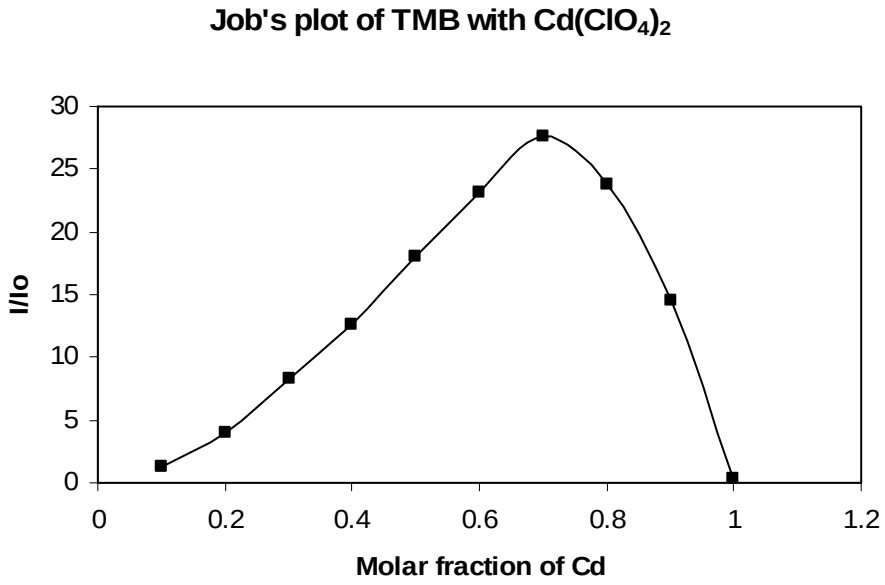


Figure S11. The Job's diagrams for MB and TMB with $Cd(ClO_4)_2$, respectively (recorded in THF).



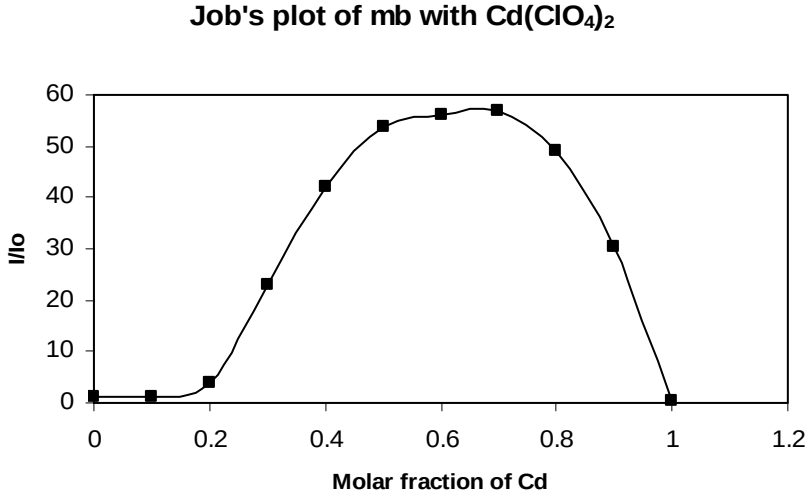
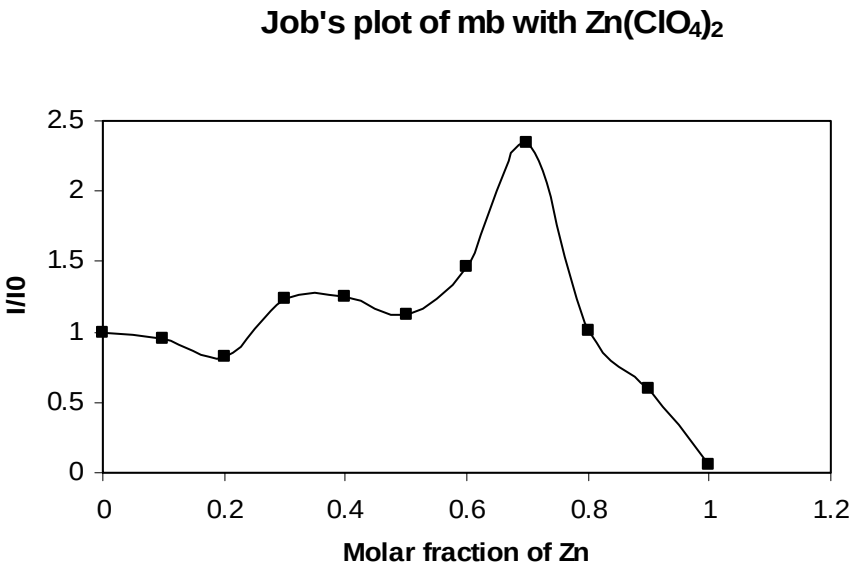


Figure S12. The Job's diagrams for MB and TMB with $Zn(ClO_4)_2$, respectively (recorded in THF).



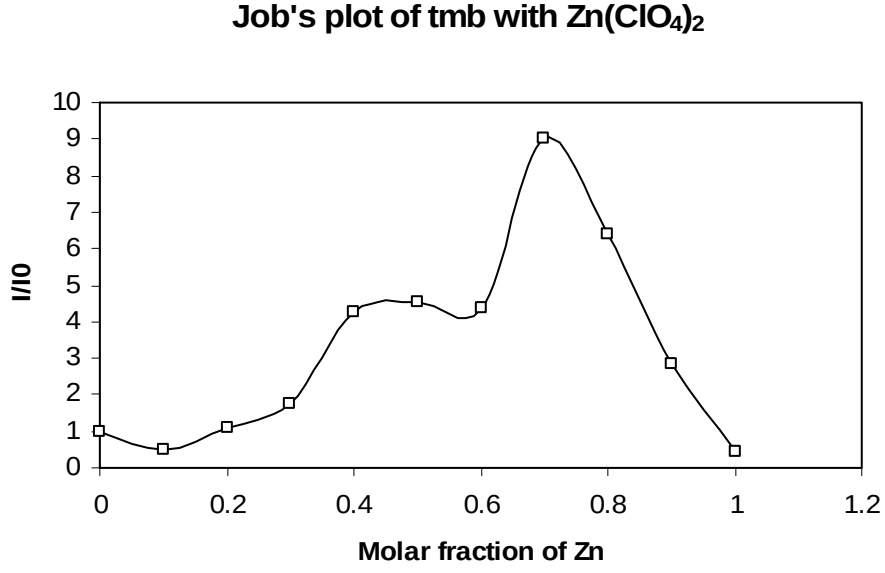


Table 1. Crystal data and structure refinement for 1

Identification code	1	
Empirical formula	C56 H43 Cl4 Hg2 N9	
Formula weight	1384.97	
Temperature	295(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 13.492(6) Å	α= 102.163(7)°.
	b = 14.686(5) Å	β= 113.679(6)°.
	c = 15.880(6) Å	γ = 103.799(8)°.
Volume	2627.1(18) $Å^3$	
Z	2	
Density (calculated)	1.751 Mg/m^3	
Absorption coefficient	6.087 mm^{-1}	
F(000)	1340	
Crystal size	0.40 x 0.20 x 0.10 mm^3	
Theta range for data collection	2.35 to 25.00°.	
Index ranges	-16<=h<=15, -17<=k<=16, -18<=l<=18	
Reflections collected	12062	
Independent reflections	8301 [R(int) = 0.0486]	
Completeness to theta = 25.00°	89.9 %	
Absorption correction	Empirical (Bruker SADABS)	
Max. and min. transmission	1.0000 and 0.6570	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8301 / 0 / 479	
Goodness-of-fit on F^2	0.779	
Final R indices [I>2sigma(I)]	R1 = 0.0671, wR2 = 0.1096	
R indices (all data)	R1 = 0.1474, wR2 = 0.1151	
Largest diff. peak and hole	1.258 and -0.728 $e.Å^{-3}$	

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

	x	y	z	U(eq)
Hg(1)	839(1)	1961(1)	2928(1)	77(1)
Hg(2)	2555(1)	-5655(1)	2680(1)	69(1)
Cl(1)	3034(3)	-6562(3)	1615(3)	87(1)
Cl(2)	2489(4)	-5718(3)	4121(3)	89(1)
Cl(3)	-49(4)	2572(3)	1681(3)	94(1)
Cl(4)	846(3)	1820(3)	4354(3)	98(2)
N(1)	4190(11)	-4148(7)	3147(8)	65(4)
N(4)	2312(10)	1496(8)	2732(7)	51(3)
N(5)	2938(10)	378(8)	2167(7)	48(3)
N(6)	74(13)	217(8)	1742(9)	68(4)
N(7)	4401(12)	-1510(9)	398(9)	49(3)
N(8)	5784(11)	-1159(10)	20(12)	67(4)
C(1)	5293(16)	-4006(13)	3669(11)	86(6)
C(2)	6200(15)	-3141(14)	3908(11)	90(6)
C(3)	5953(13)	-2383(13)	3686(12)	119(8)
C(4)	4797(14)	-2513(11)	3144(10)	70(5)
C(5)	3907(12)	-3416(11)	2831(9)	50(4)
C(6)	2682(7)	-3625(6)	2268(6)	60(4)
N(3)	1884(8)	-4430(6)	2206(6)	39(3)
C(7)	821(8)	-4425(6)	1653(7)	53(4)
C(12)	962(8)	-3617(7)	1374(7)	60(5)
N(2)	2112(9)	-3122(5)	1754(6)	47(3)
C(8)	-254(13)	-5064(10)	1354(11)	72(5)
C(9)	-1178(13)	-4849(11)	805(10)	83(5)
C(10)	-1053(14)	-4030(13)	467(11)	97(6)
C(11)	58(16)	-3376(12)	802(11)	95(6)
C(13)	-1038(14)	-343(12)	1162(12)	73(5)
C(14)	-1473(15)	-1074(12)	361(13)	77(6)
C(15)	-729(18)	-1309(11)	58(10)	75(6)
C(16)	446(13)	-741(10)	624(11)	44(4)
C(17)	760(12)	-65(10)	1460(11)	41(4)

C(18)	1981(15)	585(10)	2107(10)	50(4)
C(19)	3560(12)	1932(11)	3283(11)	59(5)
C(20)	4261(16)	2813(11)	3928(11)	70(5)
C(21)	5423(16)	3010(11)	4279(10)	76(5)
C(22)	5771(13)	2288(13)	3925(11)	77(5)
C(23)	5108(13)	1385(11)	3237(10)	64(4)
C(24)	3902(13)	1186(11)	2850(10)	51(4)
N(9)	6281(9)	-439(7)	2402(11)	72(4)
C(25)	7040(12)	197(11)	3328(9)	110(7)
C(26)	7791(9)	1088(10)	3479(7)	87(6)
C(27)	7782(8)	1345(6)	2705(11)	79(5)
C(28)	7022(9)	709(8)	1780(9)	62(4)
C(29)	6272(7)	-183(7)	1628(8)	54(4)
C(30)	5490(15)	-904(11)	691(14)	60(5)
C(31)	2900(13)	-2973(13)	-1142(14)	70(5)
C(32)	2754(17)	-3515(14)	-2027(15)	94(6)
C(33)	3660(20)	-3292(15)	-2257(13)	91(6)
C(34)	4711(19)	-2553(15)	-1640(15)	80(5)
C(35)	4837(16)	-1987(13)	-770(14)	57(4)
C(36)	3942(16)	-2224(11)	-527(12)	54(4)
C(37)	2637(7)	-2254(6)	1593(6)	47(4)
C(38)	2502(7)	-1364(7)	1937(6)	54(4)
C(39)	2983(7)	-523(6)	1760(6)	46(4)
C(40)	3599(7)	-573(6)	1240(6)	50(4)
C(41)	3734(7)	-1463(7)	896(6)	51(4)
C(42)	3253(7)	-2304(6)	1073(6)	37(3)

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

Hg(1)-Cl(4)	2.312(4)	N(2)-C(37)	1.430(9)
Hg(1)-Cl(3)	2.350(4)	C(8)-C(9)	1.358(16)
Hg(1)-N(4)	2.360(11)	C(9)-C(10)	1.418(17)
Hg(1)-N(6)	2.514(11)	C(10)-C(11)	1.382(18)
Hg(2)-Cl(1)	2.323(4)	C(13)-C(14)	1.281(17)
Hg(2)-N(3)	2.328(7)	C(14)-C(15)	1.357(19)
Hg(2)-Cl(2)	2.345(4)	C(15)-C(16)	1.387(18)
Hg(2)-N(1)	2.445(11)	C(16)-C(17)	1.311(15)
N(1)-C(1)	1.317(16)	C(17)-C(18)	1.469(18)
N(1)-C(5)	1.351(14)	C(19)-C(20)	1.303(17)
N(4)-C(18)	1.332(14)	C(19)-C(24)	1.436(18)
N(4)-C(19)	1.441(14)	C(20)-C(21)	1.367(18)
N(5)-C(24)	1.365(14)	C(21)-C(22)	1.363(19)
N(5)-C(18)	1.368(15)	C(22)-C(23)	1.339(17)
N(5)-C(39)	1.372(11)	C(23)-C(24)	1.416(17)
N(6)-C(17)	1.290(15)	N(9)-C(29)	1.355(5)
N(6)-C(13)	1.326(16)	N(9)-C(25)	1.355(5)
N(7)-C(30)	1.348(16)	C(25)-C(26)	1.356(5)
N(7)-C(36)	1.397(15)	C(26)-C(27)	1.355(5)
N(7)-C(41)	1.421(12)	C(27)-C(28)	1.355(5)
N(8)-C(30)	1.295(16)	C(28)-C(29)	1.355(5)
N(8)-C(35)	1.419(18)	C(29)-C(30)	1.411(18)
C(1)-C(2)	1.391(18)	C(31)-C(36)	1.360(18)
C(2)-C(3)	1.313(18)	C(31)-C(32)	1.371(19)
C(3)-C(4)	1.386(17)	C(32)-C(33)	1.40(2)
C(4)-C(5)	1.389(16)	C(33)-C(34)	1.36(2)
C(5)-C(6)	1.442(14)	C(34)-C(35)	1.373(19)
C(6)-N(2)	1.350(5)	C(35)-C(36)	1.400(18)
C(6)-N(3)	1.350(5)	C(37)-C(38)	1.390(5)
N(3)-C(7)	1.350(5)	C(37)-C(42)	1.391(5)
C(7)-C(8)	1.350(14)	C(38)-C(39)	1.391(5)
C(7)-C(12)	1.350(5)	C(39)-C(40)	1.391(5)
C(12)-N(2)	1.350(5)	C(40)-C(41)	1.391(5)
C(12)-C(11)	1.374(16)	C(41)-C(42)	1.391(5)

		N(2)-C(6)-N(3)	108.0
Cl(4)-Hg(1)-Cl(3)	139.98(16)	N(2)-C(6)-C(5)	131.0(9)
Cl(4)-Hg(1)-N(4)	110.8(2)	N(3)-C(6)-C(5)	121.0(9)
Cl(3)-Hg(1)-N(4)	108.8(2)	C(7)-N(3)-C(6)	108.0
Cl(4)-Hg(1)-N(6)	107.1(3)	C(7)-N(3)-Hg(2)	133.7(5)
Cl(3)-Hg(1)-N(6)	92.7(3)	C(6)-N(3)-Hg(2)	116.1(5)
N(4)-Hg(1)-N(6)	67.5(4)	C(8)-C(7)-C(12)	120.2(9)
Cl(1)-Hg(2)-N(3)	114.7(2)	C(8)-C(7)-N(3)	131.7(9)
Cl(1)-Hg(2)-Cl(2)	135.16(14)	C(12)-C(7)-N(3)	108.0
N(3)-Hg(2)-Cl(2)	110.0(2)	C(7)-C(12)-N(2)	108.0
Cl(1)-Hg(2)-N(1)	91.2(3)	C(7)-C(12)-C(11)	123.8(10)
N(3)-Hg(2)-N(1)	69.8(4)	N(2)-C(12)-C(11)	128.2(10)
Cl(2)-Hg(2)-N(1)	106.8(3)	C(6)-N(2)-C(12)	108.0
C(1)-N(1)-C(5)	118.9(12)	C(6)-N(2)-C(37)	125.7(8)
C(1)-N(1)-Hg(2)	125.5(10)	C(12)-N(2)-C(37)	126.2(8)
C(5)-N(1)-Hg(2)	115.6(10)	C(7)-C(8)-C(9)	118.3(12)
C(18)-N(4)-C(19)	110.2(13)	C(8)-C(9)-C(10)	122.3(15)
C(18)-N(4)-Hg(1)	116.5(10)	C(11)-C(10)-C(9)	117.9(14)
C(19)-N(4)-Hg(1)	132.3(10)	C(12)-C(11)-C(10)	117.1(13)
C(24)-N(5)-C(18)	108.2(12)	C(14)-C(13)-N(6)	127.1(17)
C(24)-N(5)-C(39)	123.1(12)	C(13)-C(14)-C(15)	117.4(17)
C(18)-N(5)-C(39)	127.8(12)	C(14)-C(15)-C(16)	118.4(15)
C(17)-N(6)-C(13)	113.7(13)	C(17)-C(16)-C(15)	116.6(14)
C(17)-N(6)-Hg(1)	118.0(11)	N(6)-C(17)-C(16)	126.1(13)
C(13)-N(6)-Hg(1)	125.4(12)	N(6)-C(17)-C(18)	112.1(15)
C(30)-N(7)-C(36)	110.7(14)	C(16)-C(17)-C(18)	120.9(16)
C(30)-N(7)-C(41)	127.9(14)	N(4)-C(18)-N(5)	109.6(14)
C(36)-N(7)-C(41)	121.3(14)	N(4)-C(18)-C(17)	123.4(14)
C(30)-N(8)-C(35)	108.0(15)	N(5)-C(18)-C(17)	127.1(14)
N(1)-C(1)-C(2)	123.8(14)	C(20)-C(19)-C(24)	125.5(15)
C(3)-C(2)-C(1)	118.7(16)	C(20)-C(19)-N(4)	131.7(17)
C(2)-C(3)-C(4)	118.2(15)	C(24)-C(19)-N(4)	102.3(12)
C(3)-C(4)-C(5)	122.0(13)	C(19)-C(20)-C(21)	116.9(15)
N(1)-C(5)-C(4)	117.8(12)	C(22)-C(21)-C(20)	118.5(14)
N(1)-C(5)-C(6)	115.7(12)	C(23)-C(22)-C(21)	128.1(16)
C(4)-C(5)-C(6)	126.2(12)	C(22)-C(23)-C(24)	113.7(14)

N(5)-C(24)-C(23)	133.4(15)	C(34)-C(35)-C(36)	120.3(18)
N(5)-C(24)-C(19)	109.6(13)	C(34)-C(35)-N(8)	131.5(19)
C(23)-C(24)-C(19)	116.9(13)	C(36)-C(35)-N(8)	108.2(16)
C(29)-N(9)-C(25)	120.0	C(31)-C(36)-N(7)	134(2)
N(9)-C(25)-C(26)	120.0	C(31)-C(36)-C(35)	122.9(17)
C(27)-C(26)-C(25)	120.0	N(7)-C(36)-C(35)	103.2(16)
C(28)-C(27)-C(26)	120.0	C(38)-C(37)-C(42)	120.0
C(27)-C(28)-C(29)	120.0	C(38)-C(37)-N(2)	119.6(7)
N(9)-C(29)-C(28)	120.0	C(42)-C(37)-N(2)	120.3(7)
N(9)-C(29)-C(30)	116.4(11)	C(37)-C(38)-C(39)	120.0
C(28)-C(29)-C(30)	123.5(12)	N(5)-C(39)-C(38)	120.3(8)
N(8)-C(30)-N(7)	109.8(16)	N(5)-C(39)-C(40)	119.5(9)
N(8)-C(30)-C(29)	123.2(17)	C(38)-C(39)-C(40)	120.0
N(7)-C(30)-C(29)	126.5(17)	C(41)-C(40)-C(39)	120.0
C(36)-C(31)-C(32)	117.0(16)	C(42)-C(41)-C(40)	120.0
C(31)-C(32)-C(33)	120.0(18)	C(42)-C(41)-N(7)	119.6(8)
C(34)-C(33)-C(32)	123.4(19)	C(40)-C(41)-N(7)	120.4(8)
C(33)-C(34)-C(35)	116.4(18)	C(37)-C(42)-C(41)	120.0

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 1. 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}
Hg(1)	88(1)	68(1)	82(1)	24(1)	42(1)	38(1)
Hg(2)	65(1)	55(1)	79(1)	28(1)	26(1)	19(1)
Cl(1)	70(3)	93(3)	75(3)	13(2)	21(2)	34(2)
Cl(2)	110(4)	77(3)	77(3)	30(2)	42(3)	30(3)
Cl(3)	103(4)	93(3)	111(3)	45(3)	55(3)	59(3)
Cl(4)	63(3)	117(4)	81(3)	27(3)	24(3)	4(3)
N(1)	59(10)	50(7)	83(9)	42(7)	25(8)	13(7)
N(4)	75(10)	37(7)	35(7)	16(6)	18(7)	24(7)
N(5)	49(9)	34(7)	55(8)	8(6)	20(7)	18(7)
N(6)	52(10)	53(8)	75(10)	-1(7)	20(9)	18(8)

N(7)	47(10)	63(8)	61(9)	24(7)	45(8)	25(8)
N(8)	54(10)	73(10)	93(11)	39(9)	46(10)	24(9)
C(1)	55(12)	91(13)	101(14)	46(11)	14(11)	38(11)
C(2)	65(14)	98(14)	87(13)	42(12)	12(10)	31(13)
C(3)	35(12)	87(14)	124(16)	29(12)	-37(11)	-19(10)
C(4)	56(12)	63(11)	87(12)	41(9)	16(10)	33(10)
C(5)	42(11)	63(10)	53(10)	30(8)	26(8)	15(9)
C(6)	48(12)	69(11)	90(12)	43(9)	48(10)	23(10)
N(3)	14(6)	41(6)	56(7)	13(5)	13(6)	10(5)
C(7)	61(12)	37(8)	80(11)	47(8)	37(10)	21(8)
C(12)	6(9)	56(9)	81(11)	28(9)	-7(8)	-8(8)
N(2)	57(9)	26(6)	69(8)	27(6)	32(7)	21(6)
C(8)	47(11)	68(10)	118(14)	57(10)	44(10)	19(9)
C(9)	48(12)	74(12)	86(13)	29(10)	6(10)	-1(9)
C(10)	48(12)	99(14)	114(14)	62(12)	10(11)	7(11)
C(11)	90(15)	82(12)	119(15)	64(11)	42(12)	28(12)
C(13)	50(12)	55(10)	80(13)	3(10)	8(10)	20(9)
C(14)	67(14)	39(10)	112(16)	-5(10)	49(12)	13(10)
C(15)	118(18)	65(12)	31(10)	11(9)	20(12)	48(13)
C(16)	33(11)	47(9)	53(11)	17(8)	19(9)	17(8)
C(17)	22(10)	31(8)	41(10)	-4(8)	2(8)	3(8)
C(18)	94(14)	51(10)	62(11)	44(9)	60(11)	58(11)
C(19)	17(10)	43(9)	96(13)	38(9)	14(10)	-11(8)
C(20)	75(14)	46(10)	75(12)	1(9)	35(11)	15(10)
C(21)	77(15)	47(11)	50(11)	-14(8)	10(11)	-3(10)
C(22)	50(12)	77(12)	46(11)	7(10)	-5(9)	-9(11)
C(23)	39(11)	83(12)	43(10)	4(9)	5(8)	21(9)
C(24)	44(12)	43(9)	60(11)	16(8)	22(9)	14(9)
N(9)	67(10)	106(11)	77(10)	58(9)	51(9)	30(9)
C(25)	48(13)	150(18)	95(17)	67(14)	12(12)	-9(12)
C(26)	55(13)	139(18)	75(13)	52(12)	33(10)	31(13)
C(27)	37(11)	48(10)	105(14)	-4(11)	20(11)	-9(8)
C(28)	28(9)	57(9)	114(14)	42(10)	36(10)	20(8)
C(29)	9(9)	49(10)	83(13)	-1(10)	14(9)	12(8)
C(30)	34(12)	51(10)	137(18)	52(12)	67(13)	20(9)
C(31)	36(12)	72(12)	91(14)	34(11)	32(12)	-4(10)

C(32)	68(15)	109(16)	94(17)	21(13)	46(14)	11(12)
C(33)	99(18)	102(16)	85(15)	42(13)	45(15)	47(15)
C(34)	104(19)	96(14)	89(15)	38(12)	83(14)	46(14)
C(35)	58(14)	80(13)	83(15)	60(12)	59(13)	32(11)
C(36)	75(14)	48(10)	59(13)	33(10)	39(12)	29(10)
C(37)	32(9)	60(10)	53(9)	23(8)	17(7)	25(8)
C(39)	20(9)	55(9)	42(9)	20(8)	-1(7)	1(7)
C(40)	47(11)	66(11)	54(10)	49(8)	20(8)	28(8)
C(41)	24(9)	41(9)	71(11)	29(8)	12(8)	-4(7)
C(42)	31(9)	40(8)	49(9)	16(7)	26(7)	16(7)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 1.

	x	y	z	U(eq)
H(1A)	5476	-4512	3890	103
H(2A)	6966	-3101	4220	108
H(3A)	6539	-1775	3886	143
H(4A)	4611	-1980	2986	84
H(8A)	-360	-5638	1520	87
H(9A)	-1919	-5254	644	100
H(10A)	-1697	-3936	35	117
H(11A)	189	-2798	647	114
H(13A)	-1558	-189	1359	88
H(14A)	-2269	-1430	0	92
H(15A)	-1000	-1838	-515	90
H(16A)	982	-835	420	53
H(20A)	3983	3286	4141	84
H(21A)	5965	3622	4750	91
H(22A)	6568	2443	4195	92
H(23A)	5411	930	3032	76
H(25A)	7046	21	3859	132
H(26A)	8312	1524	4114	104
H(27A)	8297	1956	2809	94
H(28A)	7016	885	1249	75
H(31A)	2312	-3111	-970	84
H(32A)	2053	-4032	-2474	113
H(33A)	3537	-3668	-2864	109
H(34A)	5312	-2438	-1798	96
H(38A)	2090	-1330	2284	65
H(40A)	3921	-11	1122	61
H(42A)	3343	-2899	843	44

Table 1. Crystal data and structure refinement for 2.

Identification code	2	
Empirical formula	C36 H28 Cl2 N6 O9 Zn	
Formula weight	824.91	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pccn	
Unit cell dimensions	a = 27.83(5) Å	α= 90°.
	b = 9.917(16) Å	β= 90°.
	c = 13.27(2) Å	γ = 90°.
Volume	3664(10) $Å^3$	
Z	4	
Density (calculated)	1.495 Mg/m^3	
Absorption coefficient	0.880 mm^{-1}	
F(000)	1688	
Crystal size	0.05 x .3 x .5 mm^3	
Theta range for data collection	1.46 to 28.25°.	
Index ranges	-36<=h<=36, -12<=k<=12, -16<=l<=17	
Reflections collected	20604	
Independent reflections	4347 [R(int) = 0.1988]	
Completeness to theta = 28.25°	95.9 %	
Absorption correction	SADABS	
Max. and min. transmission	1.000 and 0.809	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4347 / 0 / 246	
Goodness-of-fit on F^2	1.068	
Final R indices [I>2sigma(I)]	R1 = 0.1321, wR2 = 0.3340	
R indices (all data)	R1 = 0.2978, wR2 = 0.4184	
Largest diff. peak and hole	1.070 and -0.956 e.$Å^{-3}$	

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

	x	y	z	U(eq)
Cl(1)	6558(1)	265(4)	6125(3)	62(1)
Zn(1)	7500	2500	3997(2)	70(1)
N(1)	6848(4)	3365(13)	3969(8)	69(3)
N(2)	6069(4)	3103(11)	3727(8)	67(3)
N(3)	7083(4)	965(12)	3216(8)	69(3)
C(1)	6124(5)	4383(15)	4164(10)	72(4)
C(2)	5831(7)	5415(17)	4408(12)	99(6)
C(3)	6044(9)	6540(20)	4736(17)	132(8)
C(4)	6516(9)	6660(20)	4873(15)	123(7)
C(5)	6851(6)	5669(13)	4684(11)	79(4)
C(6)	6637(6)	4420(16)	4288(9)	75(4)
C(7)	6506(4)	2483(14)	3642(8)	56(3)
C(8)	6623(5)	1207(13)	3222(9)	59(3)
C(9)	6299(5)	283(15)	2861(12)	81(4)
C(10)	6464(6)	-940(18)	2489(12)	97(5)
C(11)	6958(6)	-1218(18)	2451(12)	96(5)
C(12)	7257(5)	-165(13)	2839(11)	71(4)
C(13)	5609(5)	2560(17)	3424(12)	86(4)
C(14)	5347(5)	1820(16)	4105(11)	79(4)
C(15)	4899(5)	1377(18)	3847(15)	106(6)
C(16)	4702(5)	1767(17)	2949(17)	96(6)
C(17)	4971(7)	2500(20)	2327(16)	123(7)
C(18)	5425(5)	2894(18)	2511(11)	94(6)
O(1)	6660(4)	1580(11)	6433(10)	129(5)
O(2)	6136(4)	172(15)	5572(11)	142(5)
O(3)	6488(5)	-553(14)	6945(9)	131(5)
O(4)	6933(4)	-137(11)	5532(11)	128(5)
O(5)	7500	2500	5547(10)	89(4)

Table 3. Bond lengths [Å] and angles [°] for 2.

Cl(1)-O(4)	1.366(10)	O(3)-Cl(1)-O(1)	110.4(8)
Cl(1)-O(3)	1.372(11)	O(4)-Cl(1)-O(2)	108.8(10)
Cl(1)-O(1)	1.396(11)	O(3)-Cl(1)-O(2)	105.0(8)
Cl(1)-O(2)	1.389(11)	O(1)-Cl(1)-O(2)	112.8(9)
Zn(1)-N(1)	2.007(11)	N(1)-Zn(1)-N(1)#1	177.9(6)
Zn(1)-O(5)	2.058(13)	N(1)-Zn(1)-O(5)	91.1(3)
Zn(1)-N(3)	2.177(11)	N(1)-Zn(1)-N(3)	78.9(5)
N(1)-C(6)	1.274(17)	N(1)#1-Zn(1)-N(3)	100.1(4)
N(1)-C(7)	1.364(15)	O(5)-Zn(1)-N(3)	118.4(3)
N(2)-C(7)	1.368(14)	N(3)-Zn(1)-N(3)#1	123.1(6)
N(2)-C(1)	1.404(16)	C(6)-N(1)-C(7)	108.0(12)
N(2)-C(13)	1.446(17)	C(6)-N(1)-Zn(1)	139.8(11)
N(3)-C(8)	1.303(15)	C(7)-N(1)-Zn(1)	111.3(9)
N(3)-C(12)	1.320(15)	C(7)-N(2)-C(1)	110.1(11)
C(1)-C(2)	1.349(19)	C(7)-N(2)-C(13)	126.7(11)
C(1)-C(6)	1.44(2)	C(1)-N(2)-C(13)	123.2(12)
C(2)-C(3)	1.34(2)	C(8)-N(3)-C(12)	121.3(12)
C(3)-C(4)	1.33(3)	C(8)-N(3)-Zn(1)	113.1(9)
C(4)-C(5)	1.38(2)	C(12)-N(3)-Zn(1)	125.4(9)
C(5)-C(6)	1.471(19)	C(2)-C(1)-N(2)	136.0(15)
C(7)-C(8)	1.420(17)	C(2)-C(1)-C(6)	123.6(15)
C(8)-C(9)	1.371(18)	N(2)-C(1)-C(6)	100.3(12)
C(9)-C(10)	1.39(2)	C(3)-C(2)-C(1)	116.2(18)
C(10)-C(11)	1.40(2)	C(4)-C(3)-C(2)	124(2)
C(11)-C(12)	1.43(2)	C(3)-C(4)-C(5)	125.3(18)
C(13)-C(18)	1.357(19)	C(4)-C(5)-C(6)	113.1(15)
C(13)-C(14)	1.375(18)	N(1)-C(6)-C(1)	113.6(14)
C(14)-C(15)	1.37(2)	N(1)-C(6)-C(5)	128.5(15)
C(15)-C(16)	1.37(2)	C(1)-C(6)-C(5)	117.7(13)
C(16)-C(17)	1.33(2)	N(2)-C(7)-N(1)	107.8(11)
C(17)-C(18)	1.34(2)	N(2)-C(7)-C(8)	129.5(11)
		N(1)-C(7)-C(8)	122.5(11)
O(4)-Cl(1)-O(3)	113.2(9)	N(3)-C(8)-C(9)	121.3(13)
O(4)-Cl(1)-O(1)	106.7(6)	N(3)-C(8)-C(7)	113.0(11)

C(9)-C(8)-C(7)	125.7(12)	C(14)-C(13)-N(2)	119.0(14)
C(8)-C(9)-C(10)	119.4(13)	C(13)-C(14)-C(15)	119.4(15)
C(11)-C(10)-C(9)	120.6(15)	C(16)-C(15)-C(14)	119.6(15)
C(10)-C(11)-C(12)	114.4(14)	C(17)-C(16)-C(15)	118.0(15)
N(3)-C(12)-C(11)	122.9(12)	C(18)-C(17)-C(16)	125.0(17)
C(18)-C(13)-C(14)	121.1(13)	C(17)-C(18)-C(13)	116.6(15)
C(18)-C(13)-N(2)	119.6(12)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+3/2,-y+1/2,z

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 2. 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}
Cl(1)	52(2)	65(2)	70(2)	-11(2)	8(2)	-14(2)
Zn(1)	34(1)	106(2)	71(1)	0	0	-10(1)
N(1)	50(6)	78(8)	79(7)	-13(7)	7(6)	2(6)
N(2)	53(7)	58(7)	89(8)	-11(6)	4(6)	10(6)
N(3)	54(7)	75(8)	79(7)	-15(6)	9(6)	9(6)
C(1)	69(9)	69(10)	79(10)	-20(7)	-5(7)	-1(8)
C(2)	107(13)	83(12)	107(12)	-14(10)	-8(10)	55(11)
C(3)	120(18)	95(15)	180(20)	-79(15)	-3(16)	-2(14)
C(4)	142(19)	93(15)	132(16)	-53(12)	-10(14)	-19(15)
C(5)	89(11)	40(8)	108(11)	-44(8)	-19(9)	3(8)
C(6)	93(12)	84(11)	48(7)	-3(7)	8(7)	17(9)
C(7)	42(6)	63(8)	63(7)	-16(6)	10(5)	4(8)
C(8)	53(8)	53(8)	71(8)	0(7)	1(6)	-23(7)
C(9)	47(8)	72(10)	123(12)	-24(9)	12(8)	3(8)
C(10)	89(12)	102(14)	101(12)	-17(11)	2(9)	-25(11)
C(11)	79(11)	94(13)	115(13)	-23(10)	21(10)	16(10)
C(12)	41(7)	54(9)	118(11)	-24(8)	4(7)	6(7)
C(13)	42(7)	114(12)	100(11)	31(11)	3(8)	-14(9)
C(14)	55(8)	94(11)	87(10)	24(9)	6(8)	-8(8)
C(15)	48(9)	110(14)	161(17)	53(13)	4(10)	-12(9)
C(16)	33(7)	77(11)	179(18)	5(12)	8(10)	-9(8)
C(17)	89(13)	132(16)	149(17)	44(14)	-55(12)	-1(13)
C(18)	52(8)	144(16)	85(10)	-3(10)	-1(8)	-41(9)
O(1)	138(11)	75(8)	173(11)	-37(7)	93(9)	-46(8)
O(2)	82(8)	165(13)	179(12)	23(10)	-64(8)	-16(8)
O(3)	144(11)	146(11)	102(8)	54(8)	0(7)	-52(9)
O(4)	86(8)	94(8)	204(12)	-69(8)	78(8)	-39(7)
O(5)	59(8)	132(12)	76(8)	0	0	-29(9)

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

	x	y	z	U(eq)
H(2A)	5498	5348	4352	119
H(3A)	5852	7282	4877	158
H(4A)	6629	7482	5115	147
H(5A)	7178	5777	4797	95
H(9A)	5972	473	2866	97
H(10A)	6245	-1580	2261	116
H(11A)	7081	-2021	2197	115
H(12A)	7588	-282	2824	85
H(14A)	5474	1624	4737	94
H(15A)	4729	812	4279	128
H(16A)	4389	1528	2779	116
H(17A)	4834	2761	1718	148
H(18A)	5603	3370	2037	112
H(5B)	7238	2847	5898	107
H(5C)	7762	2153	5898	107