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APPENDICES

APPENDIX A

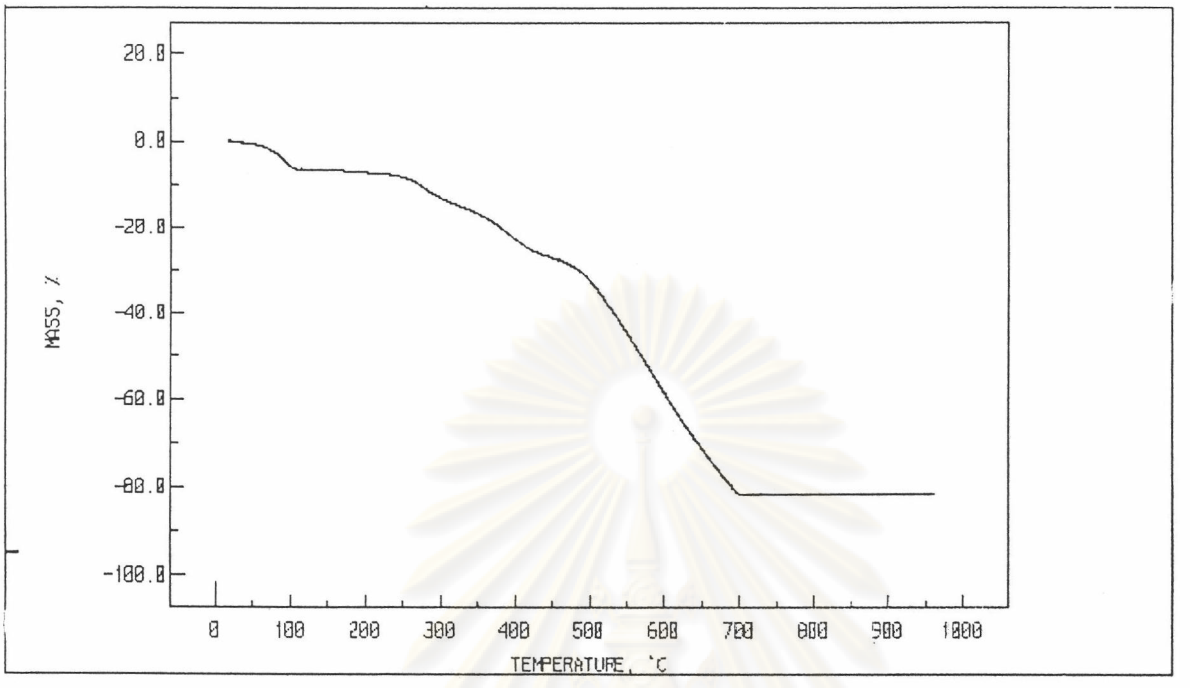

Figure A.1 TGA thermogram of ZnL_1

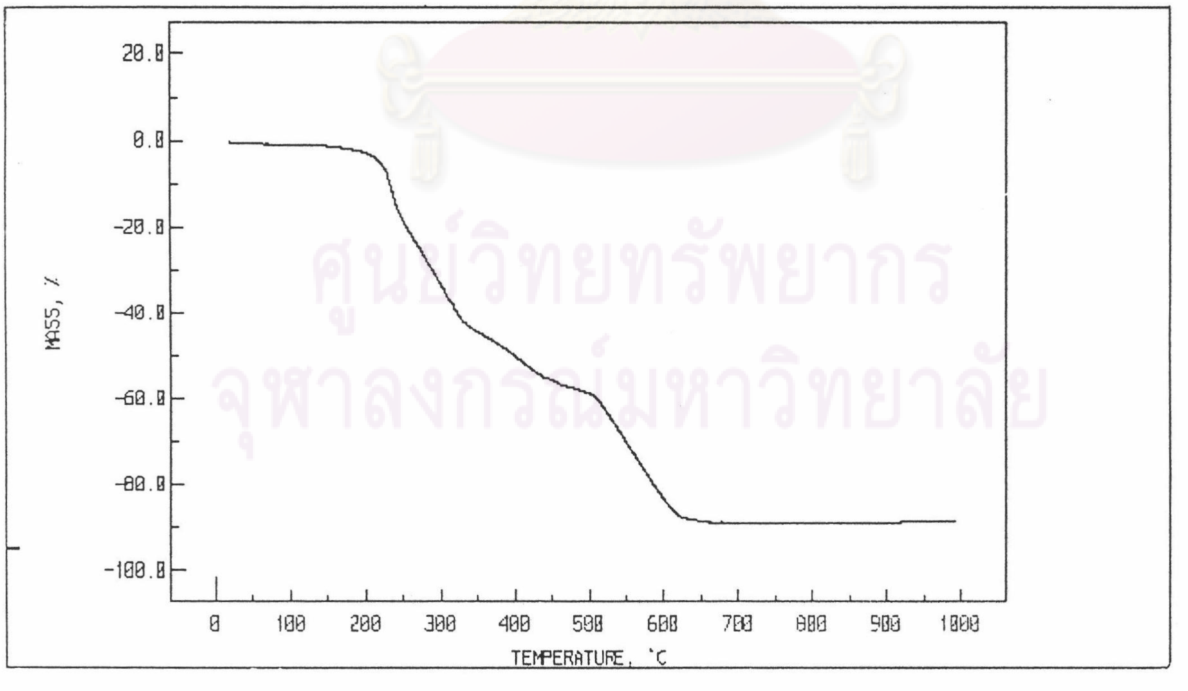

Figure A.2 TGA thermogram of ZnL_2

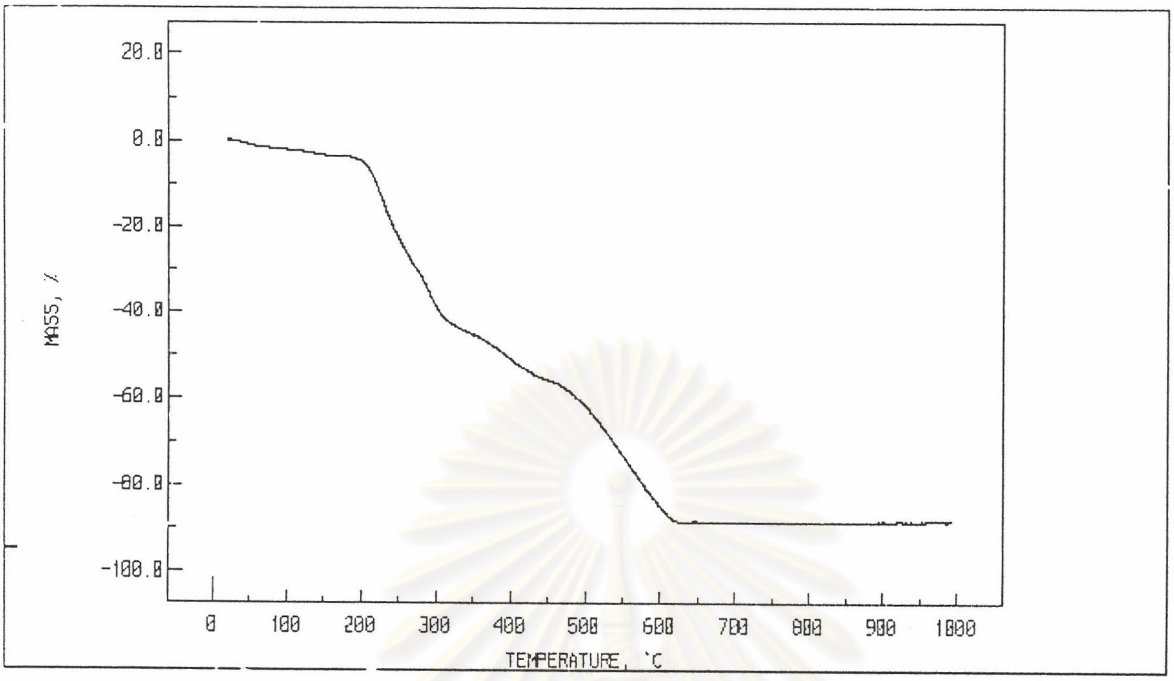

Figure A.3 TGA thermogram of ZnL_3

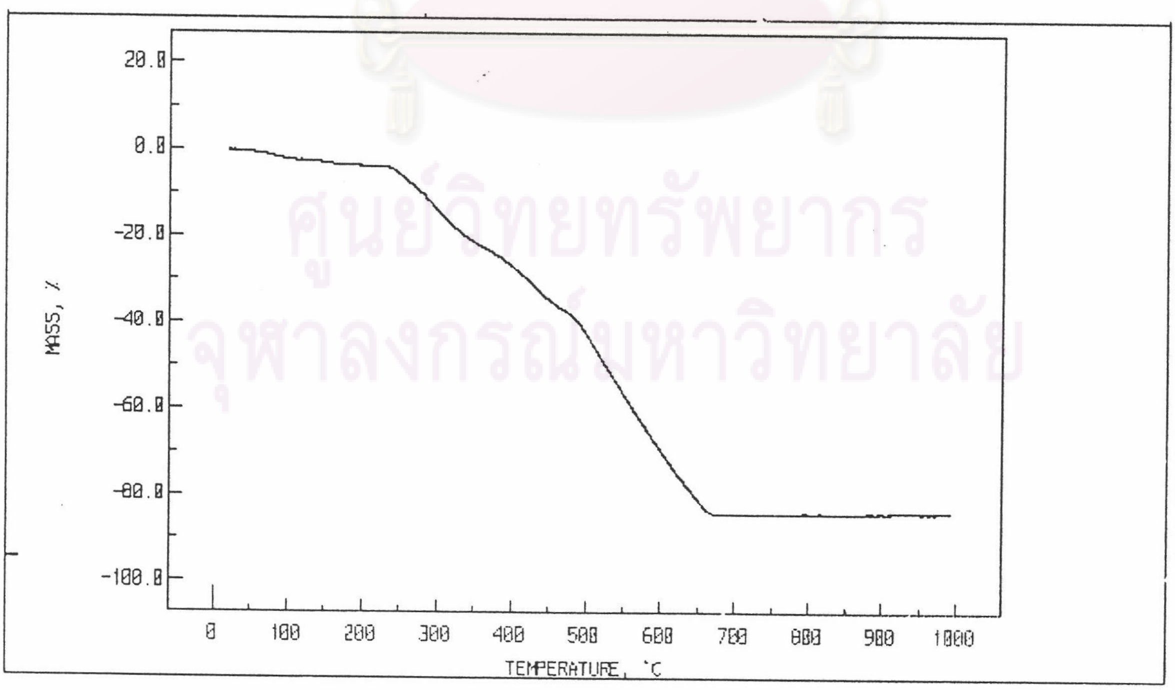

Figure A.4 TGA thermogram of PU_1ZnL_1

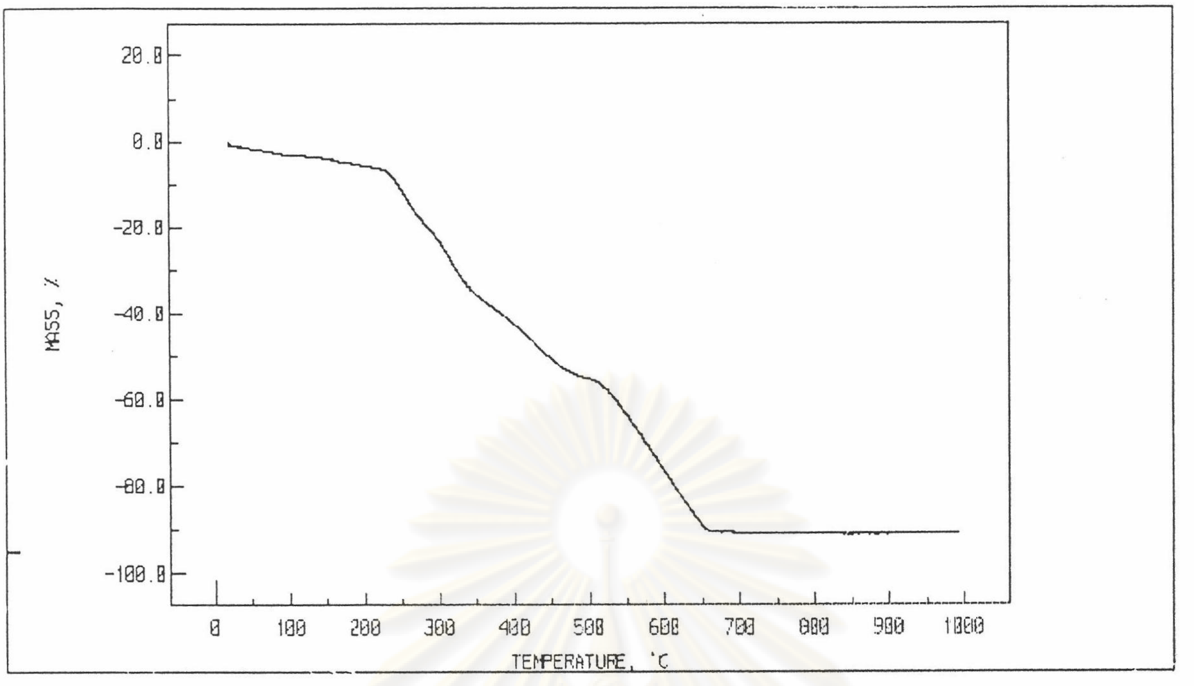

Figure A.5 TGA thermogram of PU_2ZnL_1

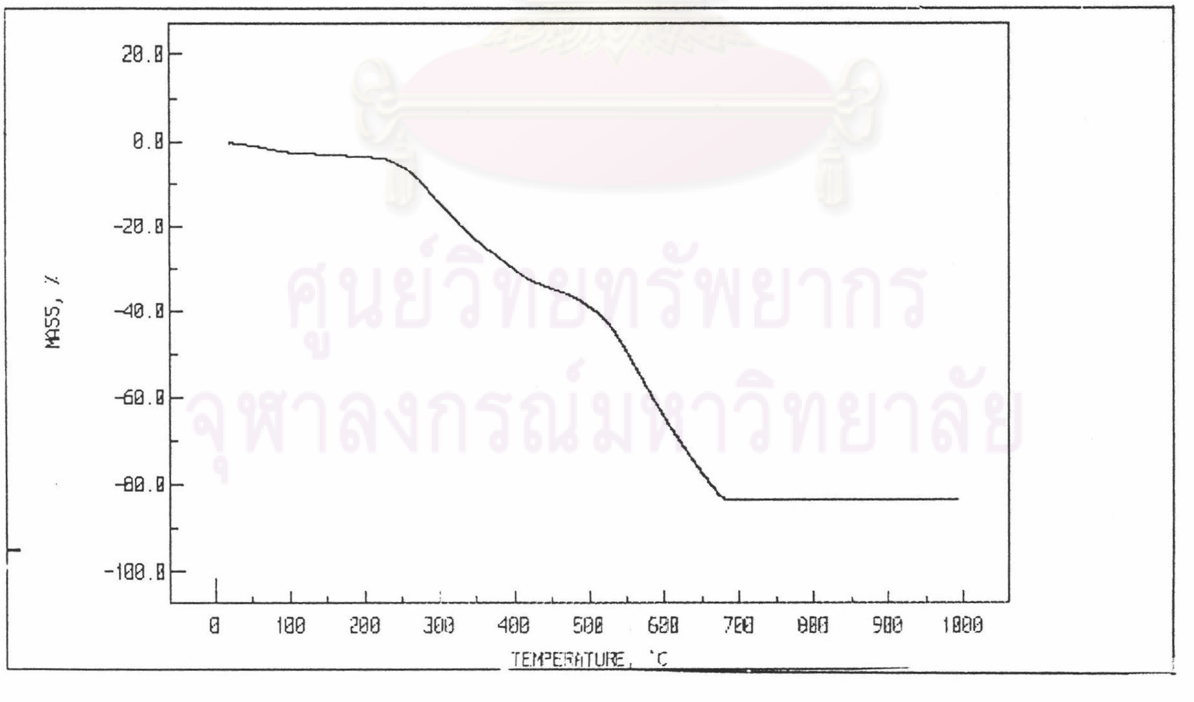

Figure A.6 TGA thermogram of PU_3ZnL_1

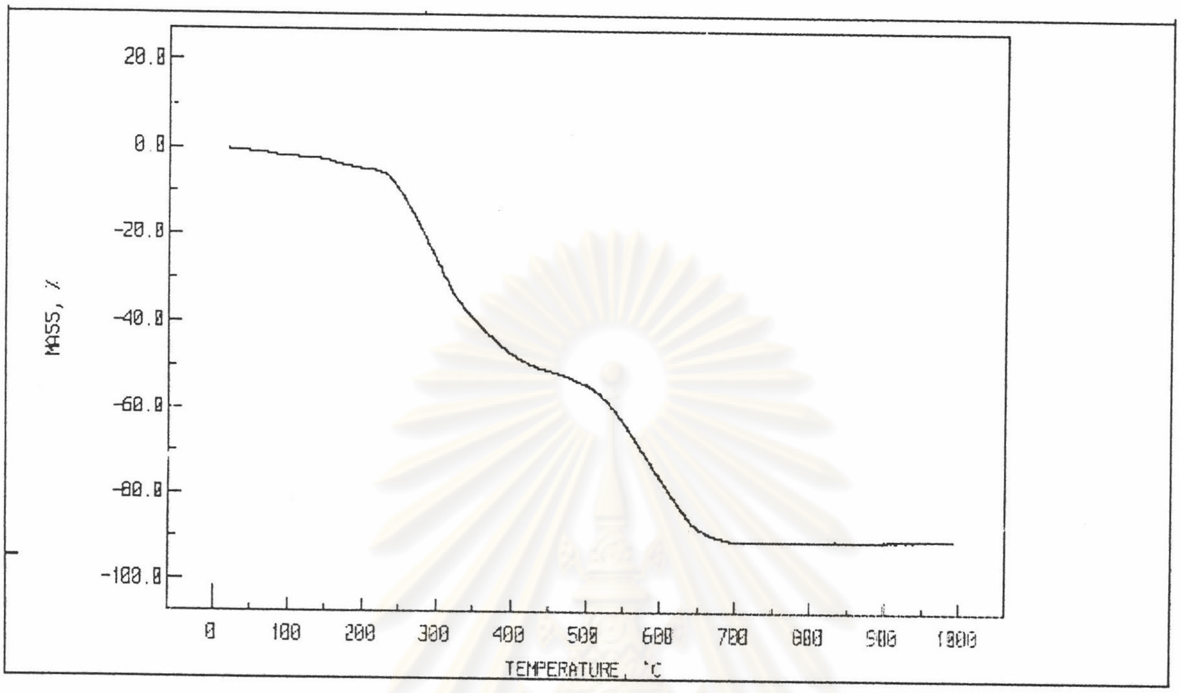

Figure A.7 TGA thermogram of PU_4ZnL_1

APPENDIX B

Table B.1 Crystal data and structure refinement for ZnL_1.

Identification code	ZnL_1
Empirical formula	C20 H28 N4 O5 Zn
Formula weight	469.83
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	monoclinic, Cc (No.6)
Unit cell dimensions	a = 15.6624(3) A alpha = 90 deg.
	b = 16.4014(3) A beta = 102.1670(10) deg.
	c = 17.3847(4) A gamma = 90 deg.
Volume	4365.56(15) A^3
Z, Calculated density	8, 1.430 Mg/m^3
Absorption coefficient	1.163 mm^ -1
F(000)	1968
Crystal size	? x ? x ? mm
Theta range for data collection	1.82 to 30.51 deg.
Limiting indices	-19<=h<=22, -23<=k<=23, -24<=l<=13
Reflections collected / unique	15967 / 7964 [R(int) = 0.0351]
Completeness to theta	= 30.51 94.3 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7964 / 2 / 586
Goodness-of-fit on F^2	1.081
Final R indices [I>2sigma(I)]	R1 = 0.0420, wR2 = 0.0803
R indices (all data)	R1 = 0.0808, wR2 = 0.0952
Absolute structure parameter	0.43(3)
Largest diff. peak and hole	0.277 and -0.314 e.A^-3

Table B.2 Atomic coordination (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for ZnL_1. U (eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(42)	1483(7)	3050(9)	736(7)	62(3)
C(40)	1542(9)	3081(11)	4581(8)	91(5)
C(43)	1243(8)	2240(10)	781(8)	93(5)
C(32)	-2688(7)	3419(10)	1618(9)	66(4)
C(36)	5675(9)	3479(10)	3623(9)	70(4)
C(41)	1866(7)	2154(8)	4487(5)	53(2)
C(39)	5435(9)	5035(9)	4117(9)	81(4)
C(35)	-2372(10)	4981(8)	1188(10)	88(5)
C(34)	-3078(11)	4888(11)	1360(11)	95(5)
C(38)	6219(11)	4768(11)	3802(12)	103(5)
C(33)	-3279(9)	4051(12)	1654(10)	107(6)
C(37)	6286(9)	4052(11)	3601(9)	89(5)
C(45)	1746(9)	4421(9)	4031(8)	68(4)
O(1W)	-2157(7)	1458(6)	1470(7)	78(3)
O(2W)	5160(9)	1453(7)	3801(9)	91(4)
O(3W)	12(7)	5599(5)	2344(6)	73(2)
O(4W)	2851(8)	5552(7)	2783(7)	119(4)
O(5W)	6038(7)	1562(6)	1545(8)	115(3)
O(6W)	1926(10)	6635(9)	3581(12)	209(7)

	x	y	z	U(eq)
Zn(1)	-19(1)	3175(1)	1540(1)	39(1)
O(4)	-1380(4)	3007(5)	1280(5)	41(2)
O(1)	16(6)	3827(5)	2562(5)	46(2)
C(2)	-458(7)	3588(7)	3081(7)	39(2)
C(10)	-48(8)	1401(7)	1105(8)	55(3)
N(1)	90(6)	2151(6)	2281(6)	46(2)
C(8)	-302(7)	2094(6)	2867(7)	55(3)
N(5)	-289(8)	4256(7)	881(6)	53(3)
C(7)	-597(7)	2784(7)	3234(7)	43(3)
N(6)	1288(7)	3547(8)	1378(6)	58(3)
C(20)	1264(8)	4422(10)	1234(7)	82(5)
C(23)	-1764(8)	4386(8)	1124(7)	56(3)
C(24)	-1916(7)	3606(6)	1347(7)	45(3)
C(3)	-818(8)	4226(7)	3527(7)	56(3)
C(22)	-979(10)	4686(7)	870(7)	52(3)
C(9)	306(9)	1361(6)	1940(7)	75(4)
C(4)	-1291(9)	3995(10)	4051(8)	65(4)
C(5)	-1400(11)	3220(10)	4250(9)	73(5)
C(6)	-1061(10)	2617(9)	3837(9)	66(4)
C(21)	422(9)	4625(8)	625(8)	68(4)
N(2)	236(7)	2181(8)	778(7)	59(3)

	x	y	z	U(eq)
Zn(2)	3040(1)	3176(1)	3712(1)	40(1)
O(2)	2989(6)	3849(5)	2662(5)	42(2)
O(3)	4379(5)	2990(5)	3970(5)	47(2)
C(12)	3446(8)	3651(7)	2156(7)	41(3)
N(3)	2940(6)	2120(6)	2926(6)	46(2)
N(9)	1713(7)	3539(8)	3886(6)	60(3)
C(30)	3043(8)	1428(9)	4227(8)	69(4)
C(18)	3343(7)	2111(6)	2368(5)	41(3)
C(17)	3616(7)	2804(7)	1948(7)	42(3)
N(10)	2753(7)	2168(7)	4501(6)	51(3)
N(8)	3338(7)	4279(6)	4378(6)	46(2)
C(25)	4908(7)	3596(7)	3902(6)	44(3)
C(31)	2768(7)	1366(7)	3285(7)	55(3)
C(26)	4783(8)	4438(6)	4111(7)	45(3)
C(13)	3797(8)	4214(7)	1747(7)	54(3)
C(28)	2557(9)	4688(9)	4589(8)	75(4)
C(27)	4012(10)	4687(8)	4341(7)	61(4)
C(16)	4095(10)	2635(8)	1390(9)	60(4)
C(15)	4427(11)	3229(9)	1009(10)	75(5)
C(14)	4254(10)	4052(10)	1165(9)	69(4)

Table B.3 Bond lengths [A] and angles [deg] for ZnL_1.

C(42)-C(43)	1.39(2)
C(42)-N(6)	1.465(16)
C(40)-N(9)	1.494(17)
C(40)-C(41)	1.62(2)
C(43)-N(2)	1.579(16)
C(32)-C(33)	1.400(19)
C(32)-C(24)	1.422(17)
C(36)-C(37)	1.349(19)
C(36)-C(25)	1.399(17)
C(41)-N(10)	1.386(15)
C(39)-C(26)	1.415(15)
C(39)-C(38)	1.51(2)
C(35)-C(34)	1.21(2)
C(35)-C(23)	1.384(17)
C(34)-C(33)	1.52(2)
C(38)-C(37)	1.24(2)
C(45)-N(9)	1.467(19)
C(45)-C(28)	1.492(19)
Zn(1)-O(1)	2.064(8)
Zn(1)-N(5)	2.105(11)
Zn(1)-O(4)	2.101(7)
Zn(1)-N(1)	2.101(11)
Zn(1)-N(2)	2.189(12)
Zn(1)-N(6)	2.211(10)
O(4)-C(24)	1.313(11)

O(1)-C(2)	1.342(14)
C(2)-C(7)	1.372(17)
C(2)-C(3)	1.482(14)
C(10)-C(9)	1.443(16)
C(10)-N(2)	1.505(19)
N(1)-C(8)	1.298(16)
N(1)-C(9)	1.493(12)
C(8)-C(7)	1.424(16)
N(5)-C(22)	1.289(17)
N(5)-C(21)	1.419(15)
C(7)-C(6)	1.422(18)
N(6)-C(20)	1.456(19)
C(20)-C(21)	1.543(17)
C(23)-C(24)	1.373(17)
C(23)-C(22)	1.476(18)
C(3)-C(4)	1.344(18)
C(4)-C(5)	1.338(19)
C(5)-C(6)	1.392(19)
Zn(2)-O(3)	2.072(8)
Zn(2)-O(2)	2.122(8)
Zn(2)-N(8)	2.145(10)
Zn(2)-N(3)	2.190(11)
Zn(2)-N(9)	2.243(11)
Zn(2)-N(10)	2.251(10)
O(2)-C(12)	1.287(15)
O(3)-C(25)	1.315(13)
C(12)-C(13)	1.351(16)
C(12)-C(17)	1.474(16)

N(3)-C(18)	1.264(15)
N(3)-C(31)	1.438(14)
C(30)-N(10)	1.41(2)
C(30)-C(31)	1.605(16)
C(18)-C(17)	1.464(16)
C(17)-C(16)	1.373(17)
N(8)-C(27)	1.263(16)
N(8)-C(28)	1.507(14)
C(25)-C(26)	1.453(16)
C(26)-C(27)	1.410(19)
C(13)-C(14)	1.383(18)
C(16)-C(15)	1.343(18)
C(15)-C(14)	1.414(19)
C(43)-C(42)-N(6)	112.8(11)
N(9)-C(40)-C(41)	106.1(11)
C(42)-C(43)-N(2)	109.9(11)
C(33)-C(32)-C(24)	118.1(14)
C(37)-C(36)-C(25)	125.5(16)
N(10)-C(41)-C(40)	108.4(9)
C(26)-C(39)-C(38)	115.9(14)
C(34)-C(35)-C(23)	127.5(16)
C(35)-C(34)-C(33)	117.3(14)
C(37)-C(38)-C(39)	120.2(14)
C(32)-C(33)-C(34)	118.0(13)
C(38)-C(37)-C(36)	123.4(17)
N(9)-C(45)-C(28)	113.3(11)
O(1)-Zn(1)-N(5)	89.9(4)
O(1)-Zn(1)-O(4)	95.5(3)

C(8)-C(7)-C(6)	116.3(12)
C(20)-N(6)-C(42)	114.8(11)
C(20)-N(6)-Zn(1)	107.6(8)
C(42)-N(6)-Zn(1)	106.9(8)
N(6)-C(20)-C(21)	108.6(10)
C(24)-C(23)-C(35)	118.2(13)
C(24)-C(23)-C(22)	126.9(11)
C(35)-C(23)-C(22)	114.8(14)
O(4)-C(24)-C(23)	121.4(11)
O(4)-C(24)-C(32)	118.2(11)
C(23)-C(24)-C(32)	120.3(10)
C(4)-C(3)-C(2)	118.6(12)
N(5)-C(22)-C(23)	124.2(11)
C(10)-C(9)-N(1)	106.8(10)
C(5)-C(4)-C(3)	124.3(13)
C(4)-C(5)-C(6)	117.3(14)
C(5)-C(6)-C(7)	123.6(14)
N(5)-C(21)-C(20)	107.8(10)
C(10)-N(2)-C(43)	115.2(11)
C(10)-N(2)-Zn(1)	107.4(8)
C(43)-N(2)-Zn(1)	105.2(8)
O(3)-Zn(2)-O(2)	96.6(3)
O(3)-Zn(2)-N(8)	85.0(4)
O(2)-Zn(2)-N(8)	89.4(4)
O(3)-Zn(2)-N(3)	87.4(4)
O(2)-Zn(2)-N(3)	83.6(3)
N(8)-Zn(2)-N(3)	169.0(4)
O(3)-Zn(2)-N(9)	159.1(4)

O(2)-Zn(2)-N(9)	96.3(4)
N(8)-Zn(2)-N(9)	78.8(4)
N(3)-Zn(2)-N(9)	110.4(4)
O(3)-Zn(2)-N(10)	94.8(4)
O(2)-Zn(2)-N(10)	158.4(3)
N(8)-Zn(2)-N(10)	109.8(4)
N(3)-Zn(2)-N(10)	78.6(4)
N(9)-Zn(2)-N(10)	78.7(5)
C(12)-O(2)-Zn(2)	122.1(7)
C(25)-O(3)-Zn(2)	119.9(7)
O(2)-C(12)-C(13)	122.2(11)
O(2)-C(12)-C(17)	124.2(10)
C(13)-C(12)-C(17)	113.6(11)
C(18)-N(3)-C(31)	119.5(10)
C(18)-N(3)-Zn(2)	120.5(7)
C(31)-N(3)-Zn(2)	113.8(8)
C(45)-N(9)-C(40)	111.3(11)
C(45)-N(9)-Zn(2)	106.6(8)
C(40)-N(9)-Zn(2)	107.7(9)
N(10)-C(30)-C(31)	111.2(11)
N(3)-C(18)-C(17)	128.2(9)
C(16)-C(17)-C(18)	117.1(11)
C(16)-C(17)-C(12)	121.2(11)
C(18)-C(17)-C(12)	121.5(10)
C(41)-N(10)-C(30)	111.8(10)
C(41)-N(10)-Zn(2)	109.3(8)
C(30)-N(10)-Zn(2)	107.8(8)
C(27)-N(8)-C(28)	120.4(11)

C(27)-N(8)-Zn(2)	120.6(9)
C(28)-N(8)-Zn(2)	114.3(8)
O(3)-C(25)-C(36)	122.1(12)
O(3)-C(25)-C(26)	125.0(10)
C(36)-C(25)-C(26)	112.9(11)
N(3)-C(31)-C(30)	110.7(9)
C(27)-C(26)-C(39)	117.2(12)
C(27)-C(26)-C(25)	121.1(10)
C(39)-C(26)-C(25)	121.7(13)
C(14)-C(13)-C(12)	125.7(12)
C(45)-C(28)-N(8)	109.5(10)
N(8)-C(27)-C(26)	129.5(12)
C(17)-C(16)-C(15)	121.9(12)
C(16)-C(15)-C(14)	119.1(14)
C(13)-C(14)-C(15)	118.3(13)

Table B.4 Anisotropic displacement parameters ($A^2 \times 10^3$) for ZnL_1.

The anisotropic displacement factor exponent takes the form:

$-2 pi^2 [h^2 a*^2 U11+... + 2 h k a* b* U12]$

	U11	U22	U33	U23	U13	U12
C(42)	34(5)	111(10)	35(5)	6(5)	-2(4)	3(5)
C(40)	57(7)	172(15)	52(7)	27(7)	27(6)	-23(8)
C(43)	36(5)	153(13)	92(9)	-38(9)	15(5)	31(7)
C(32)	30(5)	81(8)	90(10)	-15(7)	21(6)	5(5)
C(36)	62(8)	77(8)	70(9)	18(7)	10(7)	-8(7)
C(41)	46(5)	76(6)	30(4)	15(4)	-6(3)	-22(4)
C(39)	71(7)	79(7)	90(9)	16(6)	9(6)	-56(6)
C(35)	102(10)	43(5)	99(10)	-13(6)	-27(8)	17(6)
C(34)	73(8)	82(8)	122(11)	-24(7)	2(7)	45(6)
C(38)	69(7)	102(10)	138(12)	36(9)	24(7)	-44(7)
C(33)	41(7)	146(15)	141(13)	-74(11)	38(8)	-3(7)
C(37)	62(8)	120(12)	81(9)	7(8)	7(7)	-44(8)
C(45)	67(9)	88(10)	57(8)	10(7)	30(7)	26(8)
O(1W)	86(7)	69(6)	83(7)	15(6)	26(6)	-1(6)
O(2W)	121(9)	63(7)	81(8)	10(6)	4(7)	15(7)
O(3W)	89(4)	49(4)	74(5)	-9(3)	0(3)	-11(3)
O(4W)	201(10)	76(5)	85(6)	5(4)	41(6)	11(6)
O(5W)	94(6)	82(5)	168(8)	16(5)	22(5)	7(4)
O(6W)	127(10)	188(11)	340(20)	-38(12)	123(12)	34(7)
Zn(1)	34(1)	46(1)	35(1)	-4(1)	5(1)	6(1)
O(4)	27(3)	45(4)	46(5)	-6(4)	-1(3)	3(3)

	U11	U22	U33	U23	U13	U12
O(1)	57(5)	38(4)	42(5)	-8(3)	12(4)	-8(4)
C(2)	32(5)	54(6)	30(5)	-13(4)	5(4)	6(4)
C(10)	62(6)	44(6)	57(6)	-22(5)	9(5)	7(4)
N(1)	48(6)	48(5)	39(4)	-18(4)	1(4)	22(4)
C(8)	51(6)	38(5)	67(7)	-17(5)	-7(5)	13(5)
N(5)	60(6)	59(6)	40(6)	4(5)	10(5)	-3(5)
C(7)	44(6)	52(6)	30(4)	2(4)	3(4)	-12(4)
N(6)	47(6)	88(8)	43(6)	-12(6)	17(5)	-4(5)
C(20)	57(7)	128(12)	54(7)	12(7)	-1(5)	-38(8)
C(23)	52(7)	70(7)	42(6)	-13(5)	-2(5)	29(6)
C(24)	46(6)	38(5)	43(6)	-13(5)	-5(5)	23(4)
C(3)	67(7)	49(6)	50(7)	-19(5)	6(6)	20(5)
C(22)	76(9)	39(7)	37(6)	2(5)	6(6)	-5(6)
C(9)	106(9)	42(6)	68(8)	-29(5)	-5(6)	45(6)
C(4)	58(6)	87(9)	57(7)	-24(6)	28(6)	6(6)
C(5)	73(10)	111(14)	40(8)	-1(7)	22(7)	-4(8)
C(6)	64(8)	73(9)	58(8)	4(7)	7(7)	0(7)
C(21)	74(8)	63(6)	61(7)	19(5)	3(6)	-2(5)
N(2)	35(5)	92(8)	44(6)	-15(5)	-3(4)	15(5)
Zn(2)	37(1)	45(1)	35(1)	4(1)	2(1)	-8(1)
O(2)	51(5)	46(5)	31(4)	3(3)	9(4)	0(4)
O(3)	47(4)	34(4)	60(5)	-1(4)	11(4)	-18(3)
C(12)	43(6)	37(5)	38(6)	0(4)	-2(5)	4(4)
N(3)	47(5)	38(5)	46(5)	-6(4)	-8(4)	-9(4)

	U11	U22	U33	U23	U13	U12
N(9)	43(6)	100(9)	32(5)	-6(6)	-6(4)	10(6)
C(30)	72(8)	74(8)	49(6)	20(6)	-18(5)	-42(6)
C(18)	46(6)	50(6)	25(4)	-18(4)	3(4)	3(5)
C(17)	42(5)	44(6)	40(5)	3(4)	5(4)	-14(4)
N(10)	55(6)	55(5)	37(5)	7(4)	-3(4)	-28(5)
N(8)	54(6)	45(5)	36(5)	-1(4)	-1(5)	5(5)
C(25)	29(5)	66(7)	35(6)	6(5)	1(4)	2(5)
C(31)	54(5)	57(6)	50(6)	-13(5)	0(4)	-18(4)
C(26)	52(7)	26(4)	49(6)	6(4)	-3(5)	-10(4)
C(13)	65(7)	53(7)	47(7)	4(5)	21(6)	10(5)
C(28)	89(9)	94(8)	47(6)	-1(6)	28(6)	39(6)
C(27)	88(10)	40(7)	39(7)	0(5)	-21(6)	-19(6)
C(16)	72(9)	58(8)	57(8)	-13(6)	29(7)	11(7)
C(15)	68(11)	95(12)	73(10)	3(8)	43(8)	2(8)
C(14)	79(9)	74(8)	54(7)	10(6)	15(6)	-12(7)

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