Table 1. Crystal data and structure refinement

Compound	$[(HgI_2)_2(TPyP)]*2(TCE)$
Color / Shape	violet / parallelepiped
Empirical formula	$C_{44}H_{30}Cl_8Hg_2I_4N_8$
Formula weight	1863.14
Temperature	173(2) K
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 10.0350(7) Å α = 98.935(1)°
(4277 reflections	b = 11.9656(8) Å β = 101.752(1)°
in full θ range)	c = 12.9198(8) Å γ = 113.669(1)°
Volume	1341.6(2) $Å^3$
Z	1
Density (calculated)	2.306 Mg/m^3
Absorption coefficient	8.455 mm^{-1}
Diffractometer / scan	Siemens SMART / CCD area detector
Radiation / wavelength	MoKα (graphite monochrom.) / 0.71073 Å
F(000)	858
Crystal size	0.38 x 0.20 x 0.18 mm
θ range for data collection	1.67 to 27.91°
Index ranges	$-10 \le h \le 13$, $-15 \le k \le 15$, $-16 \le \ell \le 15$
Reflections collected	8612
Independent / observed refls.	5987(R_{int} = 0.0294) / 4397([I>2σ(I)])
Absorption correction	SADABS[1]
Refinement method	Full-matrix least-squares on F^2
Computing	SHELXTL, Ver. 5[2]
Data / restraints / parameters	5981 / 0 / 299
Goodness-of-fit on F^2	0.960
SHELX-93 weight parameters	0.0723, 0.000
Final R indices [I>2σ(I)]	R1 = 0.0516, wR2 = 0.1206
R indices (all data)	R1 = 0.0719, wR2 = 0.1303
Extinction coefficient	0.0000(2)
Largest diff. peak and hole	3.461 and -3.134 $eÅ^{-3}$

Table 2. Atomic Coordinates [x 10^4] and Equivalent Isotropic Displacement Parameters [$Å^2$ x 10^3] for $[(HgI_2)_2(TPyP)]$* 2(TCE)

Atom	x/a	y/b	z/c	U(eq)
Hg	8222(1)	9272(1)	3174(1)	25(1)
I(1)	5693(1)	7992(1)	3655(1)	43(1)
I(2)	10357(1)	11507(1)	3258(1)	35(1)
Cl(1)	3396(8)	9681(4)	12040(4)	126(2)
Cl(2)	483(4)	7352(4)	11214(2)	70(1)
Cl(3)	2115(7)	8388(5)	9369(4)	110(2)
Cl(4)	2087(4)	6087(4)	9888(3)	67(1)
N(1)	15695(8)	3939(7)	4076(5)	22(2)
N(2)	13307(9)	4801(7)	3649(5)	23(2)
N(3)	12576(9)	1804(7)	-1178(6)	28(2)
N(4)	9636(8)	8122(7)	3701(5)	23(2)
C(1)	16764(10)	3529(8)	4396(6)	21(2)
C(2)	16879(11)	2762(9)	3462(6)	28(2)
C(3)	15860(11)	2709(9)	2561(7)	26(2)
C(4)	15137(10)	3443(8)	2945(7)	24(2)
C(5)	13922(10)	3542(9)	2256(6)	24(2)
C(6)	13105(10)	4174(8)	2587(7)	23(2)
C(7)	11925(11)	4322(9)	1898(6)	28(2)
C(8)	11460(11)	5034(8)	2503(6)	26(2)
C(9)	12347(10)	5356(8)	3616(6)	22(2)
C(10)	12319(10)	6164(8)	4523(6)	20(2)
C(11)	13447(10)	2928(8)	1066(6)	23(2)
C(12)	12217(13)	1794(10)	604(8)	42(3)
C(13)	11797(13)	1244(10)	-546(8)	41(3)
C(14)	13780(13)	2898(11)	-718(8)	46(3)
C(15)	14255(14)	3470(11)	391(8)	49(3)
C(16)	11345(10)	6822(8)	4266(6)	22(2)
C(17)	9765(10)	6199(9)	3919(7)	27(2)
C(18)	8940(10)	6869(10)	3643(7)	29(2)
C(19)	11143(10)	8718(8)	4061(6)	24(2)
C(20)	12043(10)	8110(9)	4361(7)	25(2)

C(21)	2462(22)	7972(18)	11389(14)	97(6)
C(22)	2911(23)	7826(20)	10454(17)	106(7)

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 3. Bond Lengths [Å] and Angles [°] for $[(HgI_2)_2(TPyP)]*2(TCE)$

Hg-N(4)	2.416(7)	Hg-N(3)#1	2.500(7)
Hg-I(2)	2.6401(8)	Hg-I(1)	2.6429(8)
Cl(1)-C(21)	1.84(2)	Cl(2)-C(21)	1.77(2)
Cl(3)-C(22)	1.82(2)	Cl(4)-C(22)	1.86(2)
N(1)-C(1)	1.367(10)	N(1)-C(4)	1.390(10)
N(2)-C(9)	1.370(10)	N(2)-C(6)	1.389(10)
N(3)-C(14)	1.312(13)	N(3)-C(13)	1.318(12)
N(3)-Hg#1	2.500(7)	N(4)-C(19)	1.325(11)
N(4)-C(18)	1.357(12)	C(1)-C(10)#2	1.406(10)
C(1)-C(2)	1.452(11)	C(2)-C(3)	1.358(11)
C(3)-C(4)	1.437(12)	C(4)-C(5)	1.414(11)
C(5)-C(6)	1.403(12)	C(5)-C(11)	1.484(10)
C(6)-C(7)	1.419(11)	C(7)-C(8)	1.348(12)
C(8)-C(9)	1.427(10)	C(9)-C(10)	1.412(11)
C(10)-C(1)#2	1.406(10)	C(10)-C(16)	1.501(11)
C(11)-C(12)	1.350(14)	C(11)-C(15)	1.371(14)
C(12)-C(13)	1.426(13)	C(14)-C(15)	1.379(13)
C(16)-C(20)	1.386(12)	C(16)-C(17)	1.389(13)
C(17)-C(18)	1.399(12)	C(19)-C(20)	1.403(12)
C(21)-C(22)	1.38(2)		

N(4)-Hg-N(3)#1	93.7(2)	N(4)-Hg-I(2)	103.5(2)
N(3)#1-Hg-I(2)	100.8(2)	N(4)-Hg-I(1)	100.2(2)
N(3)#1-Hg-I(1)	99.8(2)	I(2)-Hg-I(1)	147.27(3)
C(1)-N(1)-C(4)	104.5(6)	C(9)-N(2)-C(6)	108.8(7)
C(14)-N(3)-C(13)	118.0(8)	C(14)-N(3)-Hg#1	122.5(6)
C(13)-N(3)-Hg#1	119.5(6)	C(19)-N(4)-C(18)	118.0(7)
C(19)-N(4)-Hg	119.7(6)	C(18)-N(4)-Hg	122.2(6)
N(1)-C(1)-C(10)#2	125.1(7)	N(1)-C(1)-C(2)	111.1(7)
C(10)#2-C(1)-C(2)	123.7(7)	C(3)-C(2)-C(1)	106.8(7)
C(2)-C(3)-C(4)	106.2(7)	N(1)-C(4)-C(5)	125.1(8)
N(1)-C(4)-C(3)	111.4(7)	C(5)-C(4)-C(3)	123.3(7)
C(6)-C(5)-C(4)	126.3(7)	C(6)-C(5)-C(11)	115.8(7)
C(4)-C(5)-C(11)	117.9(8)	N(2)-C(6)-C(5)	127.0(7)
N(2)-C(6)-C(7)	106.3(7)	C(5)-C(6)-C(7)	126.7(8)
C(8)-C(7)-C(6)	109.7(7)	C(7)-C(8)-C(9)	107.0(7)

N(2)-C(9)-C(10)	125.2(7)	N(2)-C(9)-C(8)	108.1(7)
C(10)-C(9)-C(8)	126.6(7)	C(1)#2-C(10)-C(9)	124.6(7)
C(1)#2-C(10)-C(16)	119.2(7)	C(9)-C(10)-C(16)	115.9(7)
C(12)-C(11)-C(15)	117.0(8)	C(12)-C(11)-C(5)	121.3(9)
C(15)-C(11)-C(5)	121.6(8)	C(11)-C(12)-C(13)	119.4(10)
N(3)-C(13)-C(12)	122.1(9)	N(3)-C(14)-C(15)	122.6(10)
C(11)-C(15)-C(14)	120.8(10)	C(20)-C(16)-C(17)	117.8(8)
C(20)-C(16)-C(10)	119.0(8)	C(17)-C(16)-C(10)	123.2(8)
C(16)-C(17)-C(18)	119.7(9)	N(4)-C(18)-C(17)	122.0(8)
N(4)-C(19)-C(20)	123.0(8)	C(16)-C(20)-C(19)	119.4(8)
C(22)-C(21)-Cl(2)	117(2)	C(22)-C(21)-Cl(1)	105.9(14)
Cl(2)-C(21)-Cl(1)	109.9(11)	C(21)-C(22)-Cl(3)	114.9(14)
C(21)-C(22)-Cl(4)	104.6(13)	Cl(3)-C(22)-Cl(4)	105.2(11)

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic Displacement Parameters [$Å^2$ x 10^3] for $[(HgI_2)_2(TPyP)]*2(TCE)$

Atom	U11	U22	U33	U23	U13	U12
Hg	25(1)	34(1)	17(1)	4(1)	2(1)	16(1)
I(1)	25(1)	59(1)	35(1)	7(1)	9(1)	13(1)
I(2)	44(1)	31(1)	27(1)	6(1)	9(1)	14(1)
Cl(1)	174(6)	63(3)	96(3)	14(3)	8(4)	27(3)
Cl(2)	70(2)	114(3)	34(2)	15(2)	9(2)	53(2)
Cl(3)	181(5)	118(4)	76(3)	58(3)	61(3)	88(4)
Cl(4)	65(2)	79(2)	58(2)	16(2)	12(2)	38(2)
N(1)	28(4)	33(4)	11(3)	3(3)	-1(3)	22(4)
N(2)	32(4)	30(4)	16(3)	7(3)	2(3)	24(4)
N(3)	37(5)	34(5)	14(3)	3(3)	2(3)	20(4)
N(4)	24(4)	30(4)	14(3)	1(3)	1(3)	14(3)
C(1)	25(5)	26(5)	14(4)	2(3)	0(3)	17(4)
C(2)	38(6)	40(6)	13(4)	2(4)	3(4)	28(5)
C(3)	31(5)	31(5)	17(4)	1(4)	1(4)	19(4)
C(4)	27(5)	28(5)	14(4)	0(3)	-1(4)	16(4)
C(5)	29(5)	35(5)	7(4)	4(3)	0(3)	16(4)
C(6)	27(5)	23(5)	18(4)	3(3)	-3(4)	14(4)
C(7)	39(6)	38(6)	8(4)	1(4)	-6(4)	27(5)
C(8)	34(5)	33(5)	11(4)	0(4)	-7(4)	23(5)
C(9)	23(5)	33(5)	15(4)	7(4)	-1(3)	19(4)
C(10)	21(4)	27(5)	11(4)	3(3)	0(3)	14(4)
C(11)	32(5)	28(5)	9(4)	0(3)	-2(3)	19(4)
C(12)	45(7)	41(6)	18(5)	2(4)	6(4)	2(5)
C(13)	41(6)	40(6)	19(5)	-5(4)	8(4)	0(5)
C(14)	48(7)	50(7)	20(5)	9(5)	11(5)	4(6)
C(15)	47(7)	43(7)	19(5)	-4(5)	-1(5)	-5(6)
C(16)	30(5)	27(5)	13(4)	7(3)	5(3)	16(4)
C(17)	24(5)	30(5)	28(5)	7(4)	4(4)	15(4)
C(18)	18(5)	45(6)	23(4)	5(4)	2(4)	15(5)
C(19)	27(5)	23(5)	17(4)	2(4)	1(4)	9(4)
C(20)	19(4)	36(5)	20(4)	5(4)	3(4)	16(4)
C(21)	103(14)	119(16)	81(12)	56(11)	20(11)	54(13)
C(22)	106(15)	135(18)	134(18)	86(15)	67(14)	75(14)

The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$.

Table 5. Hydrogen Coordinates (x 10^4) and Isotropic Displacement Parameters ($Å^2$ x 10^3) for $[(HgI_2)_2(TPyP)]$* 2(TCE)

Atom	x	y	z	U(eq)
H(2B)	13956(9)	4832(7)	4260(5)	27
H(2A)	17540(11)	2373(9)	3478(6)	34
H(3A)	15665(11)	2275(9)	1825(7)	40
H(7A)	11524(11)	3973(9)	1126(6)	34
H(8A)	10687(11)	5275(8)	2240(6)	32
H(12A)	11636(13)	1368(10)	1040(8)	50
H(13A)	10928(13)	448(10)	-866(8)	50
H(14A)	14347(13)	3312(11)	-1166(8)	55
H(15A)	15153(14)	4249(11)	691(8)	58
H(17A)	9247(10)	5322(9)	3870(7)	33
H(18A)	7860(10)	6434(10)	3407(7)	35
H(19A)	11637(10)	9599(8)	4119(6)	29
H(20A)	13120(10)	8577(9)	4627(7)	30
H(21A)	2882(22)	7560(18)	11893(14)	116
H(22A)	4046(23)	8223(20)	10640(17)	127

Table 1. Crystal data and structure refinement

Compound	$[(HgI_2)_2(TPyP)_{0.25}(ZnTPyP)_{0.75}]*2(TCE)$
Color / Shape	violet / parallalepiped
Empirical formula	$C_{44}H_{28.5}Cl_8Hg_2I_4N_8Zn_{0.75}$
Formula weight	1910.15
Temperature	173(2) K
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 10.1734(6) Å α = 97.884(1)°
(2983 reflections	b = 11.7880(7) Å β = 102.216(1)°
in full θ range)	c = 12.8166(6) Å γ = 113.594(2)°
Volume	1333.73(13) Å^3
Z	1
Density (calculated)	2.378 Mg/m^3
Absorption coefficient	8.834 mm^{-1}
Diffractometer / scan	Siemens SMART / CCD area detector
Radiation / wavelength	MoKα (graphite monochrom.) / 0.71073 Å
F(000)	879
Crystal size	0.12 x 0.20 x 0.22 mm
θ range for data collection	1.68 to 27.89°
Index ranges	$-10 \le h \le 13$, $-15 \le k \le 10$, $-16 \le \ell \le 16$
Reflections collected	8374
Independent / observed refls.	5834(R_{int} = 0.0565) / 3540([I>2σ(I)])
Absorption correction	SADABS[1]
Refinement method	Full-matrix least-squares on F^2
Computing	SHELXTL, Ver. 5[2]
Data / restraints / parameters	5831 / 0 / 285
Goodness-of-fit on F^2	1.051
SHELX-93 weight parameters	0.0358, 32.3472
Final R indices [I>2σ(I)]	R1 = 0.0873, wR2 = 0.1487
R indices (all data)	R1 = 0.1584, wR2 = 0.1975
Extinction coefficient	0.0000(2)
Largest diff. peak and hole	2.484 and -2.210 eÅ^{-3}

Table 2. Atomic Coordinates [x 10^4] and Equivalent Isotropic Displacement Parameters [$Å^2$ x 10^3] for [$(HgI_2)_2$ $(TPyP)_{0.25}(ZnTPyP)_{0.75}$]*2(TCE)

Atom	x/a	y/b	z/c	U(eq)
Hg	8224(1)	9258(1)	3198(1)	25(1)
I(1)	5754(1)	7946(2)	3704(1)	43(1)
I(2)	10293(2)	11528(1)	3263(1)	35(1)
Zn	15000	5000	5000	28(1)
Cl(1)	3464(11)	9663(8)	12071(7)	105(3)
Cl(2)	565(7)	7407(8)	11213(5)	66(2)
Cl(3)	2272(13)	8454(10)	9380(7)	118(4)
Cl(4)	2120(8)	6090(7)	9858(5)	65(2)
N(1)	15671(15)	3945(13)	4060(11)	20(3)
N(2)	13331(16)	4784(15)	3667(11)	28(4)
N(3)	12565(17)	1816(14)	-1194(12)	27(4)
N(4)	9626(16)	8068(15)	3680(10)	25(3)
C(1)	16759(19)	3548(16)	4411(13)	21(4)
C(2)	16875(19)	2799(17)	3481(13)	24(4)
C(3)	15869(19)	2744(19)	2563(13)	28(5)
C(4)	15099(18)	3434(15)	2927(11)	16(3)
C(5)	13913(19)	3529(17)	2249(14)	25(4)
C(6)	13099(20)	4187(17)	2595(13)	29(4)
C(7)	11911(22)	4292(19)	1889(14)	34(5)
C(8)	11474(23)	5006(20)	2504(15)	38(5)
C(9)	12360(17)	5322(15)	3600(12)	14(3)
C(10)	12354(16)	6142(16)	4518(12)	16(4)
C(11)	13435(19)	2896(17)	1047(12)	21(4)
C(12)	12198(22)	1772(18)	574(13)	33(5)
C(13)	11809(23)	1191(21)	-532(14)	38(5)
C(14)	13810(23)	2855(21)	-734(14)	36(5)
C(15)	14300(20)	3457(19)	375(13)	31(5)
C(16)	11381(20)	6816(20)	4273(12)	29(5)
C(17)	9806(19)	6149(18)	3903(13)	26(4)
C(18)	8996(20)	6831(20)	3644(15)	34(5)

C(19)	11140(20)	8694(18)	4011(13)	27(4)
C(20)	12019(18)	8116(17)	4343(13)	23(4)
C(21)	2450(28)	7990(29)	11400(22)	69(8)
C(22)	2895(40)	7774(43)	10419(28)	116(15)

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 3. Bond Lengths [Å] and Angles [°] for $[(HgI_2)_2(TPyP)_{0.25}(ZnTPyP)_{0.75}]*2(TCE)$

Hg-N(4)	2.42(2)	Hg-N(3)#1	2.503(14)
Hg-I(2)	2.636(2)	Hg-I(1)	2.643(2)
Zn-N(1)	2.020(14)	Zn-N(1)#2	2.020(14)
Zn-N(2)#2	2.043(14)	Zn-N(2)	2.043(14)
Cl(1)-C(21)	1.80(3)	Cl(2)-C(21)	1.71(3)
Cl(3)-C(22)	1.78(3)	Cl(4)-C(22)	1.79(5)
N(1)-C(1)	1.38(2)	N(1)-C(4)	1.39(2)
N(2)-C(9)	1.37(2)	N(2)-C(6)	1.38(2)
N(3)-C(14)	1.30(2)	N(3)-C(13)	1.36(2)
N(3)-Hg#1	2.503(14)	N(4)-C(18)	1.33(2)
N(4)-C(19)	1.35(2)	C(1)-C(10)#2	1.38(2)
C(1)-C(2)	1.44(2)	C(2)-C(3)	1.36(2)
C(3)-C(4)	1.43(2)	C(4)-C(5)	1.38(2)
C(5)-C(6)	1.44(3)	C(5)-C(11)	1.50(2)
C(6)-C(7)	1.41(2)	C(7)-C(8)	1.34(3)
C(8)-C(9)	1.41(2)	C(9)-C(10)	1.42(2)
C(10)-C(1)#2	1.38(2)	C(10)-C(16)	1.51(2)
C(11)-C(12)	1.35(2)	C(11)-C(15)	1.40(2)
C(12)-C(13)	1.38(2)	C(14)-C(15)	1.38(2)
C(16)-C(20)	1.39(3)	C(16)-C(17)	1.41(2)
C(17)-C(18)	1.39(3)	C(19)-C(20)	1.36(2)
C(21)-C(22)	1.45(4)		

N(4)-Hg-N(3)#1	91.8(5)	N(4)-Hg-I(2)	104.1(4)
N(3)#1-Hg-I(2)	100.9(4)	N(4)-Hg-I(1)	100.4(3)
N(3)#1-Hg-I(1)	100.0(4)	I(2)-Hg-I(1)	147.02(6)
N(1)-Zn-N(1)#2	180.000(4)	N(1)-Zn-N(2)#2	88.9(6)
N(1)#2-Zn-N(2)#2	91.1(6)	N(1)-Zn-N(2)	91.1(6)
N(1)#2-Zn-N(2)	88.9(6)	N(2)#2-Zn-N(2)	180.000(2)
C(1)-N(1)-C(4)	105.7(14)	C(1)-N(1)-Zn	127.3(10)
C(4)-N(1)-Zn	127.0(11)	C(9)-N(2)-C(6)	105(2)
C(9)-N(2)-Zn	128.8(11)	C(6)-N(2)-Zn	125.4(13)
C(14)-N(3)-C(13)	118(2)	C(14)-N(3)-Hg#1	121.9(12)
C(13)-N(3)-Hg#1	118.8(12)	C(18)-N(4)-C(19)	118(2)
C(18)-N(4)-Hg	123.9(12)	C(19)-N(4)-Hg	118.5(13)

C(10)#2-C(1)-N(1)	126(2)	C(10)#2-C(1)-C(2)	125(2)
N(1)-C(1)-C(2)	109.6(14)	C(3)-C(2)-C(1)	108(2)
C(2)-C(3)-C(4)	106.5(14)	C(5)-C(4)-N(1)	125(2)
C(5)-C(4)-C(3)	124.5(14)	N(1)-C(4)-C(3)	110.4(14)
C(4)-C(5)-C(6)	126(2)	C(4)-C(5)-C(11)	118(2)
C(6)-C(5)-C(11)	117(2)	N(2)-C(6)-C(7)	110(2)
N(2)-C(6)-C(5)	126(2)	C(7)-C(6)-C(5)	125(2)
C(8)-C(7)-C(6)	108(2)	C(7)-C(8)-C(9)	107(2)
N(2)-C(9)-C(8)	110(2)	N(2)-C(9)-C(10)	123.0(14)
C(8)-C(9)-C(10)	127(2)	C(1)#2-C(10)-C(9)	126(2)
C(1)#2-C(10)-C(16)	118(2)	C(9)-C(10)-C(16)	116.3(13)
C(12)-C(11)-C(15)	118(2)	C(12)-C(11)-C(5)	122(2)
C(15)-C(11)-C(5)	120(2)	C(11)-C(12)-C(13)	121(2)
N(3)-C(13)-C(12)	120(2)	N(3)-C(14)-C(15)	124(2)
C(14)-C(15)-C(11)	118(2)	C(20)-C(16)-C(17)	117(2)
C(20)-C(16)-C(10)	121(2)	C(17)-C(16)-C(10)	122(2)
C(18)-C(17)-C(16)	118(2)	N(4)-C(18)-C(17)	124(2)
N(4)-C(19)-C(20)	123(2)	C(19)-C(20)-C(16)	120(2)
C(22)-C(21)-Cl(2)	116(2)	C(22)-C(21)-Cl(1)	108(3)
Cl(2)-C(21)-Cl(1)	113(2)	C(21)-C(22)-Cl(3)	114(2)
C(21)-C(22)-Cl(4)	109(3)	Cl(3)-C(22)-Cl(4)	108(2)

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic Displacement Parameters [$Å^2$ x 10^3] for $[(HgI_2)_2(TPyP)_{0.25}(ZnTPyP)_{0.75}]*2(TCE)$

Atom	U11	U22	U33	U23	U13	U12
Hg	24(1)	30(1)	19(1)	1(1)	3(1)	14(1)
I(1)	27(1)	56(1)	37(1)	6(1)	11(1)	12(1)
I(2)	41(1)	30(1)	28(1)	3(1)	11(1)	12(1)
Zn	34(2)	33(3)	19(2)	-1(2)	5(2)	22(2)
Cl(1)	133(8)	60(6)	82(6)	6(4)	8(5)	19(5)
Cl(2)	57(4)	106(6)	39(3)	5(3)	9(3)	46(4)
Cl(3)	212(11)	152(9)	81(5)	77(6)	84(7)	132(9)
Cl(4)	71(4)	70(5)	57(4)	9(4)	17(3)	37(4)
N(2)	26(8)	32(10)	22(7)	-7(7)	3(6)	14(7)
N(3)	29(8)	21(9)	27(8)	-5(7)	-4(7)	15(7)
N(4)	25(8)	33(10)	11(6)	0(6)	5(6)	9(7)
C(1)	28(9)	20(10)	23(9)	2(7)	9(7)	20(8)
C(3)	34(10)	55(14)	5(7)	-2(8)	5(7)	34(10)
C(4)	28(9)	15(9)	3(6)	-2(6)	1(6)	9(7)
C(6)	34(11)	20(10)	15(8)	-16(7)	-6(8)	6(9)
C(7)	51(13)	36(12)	19(9)	11(9)	-4(9)	29(10)
C(8)	45(12)	50(14)	31(10)	0(10)	2(9)	40(11)
C(10)	8(7)	27(10)	15(8)	11(7)	4(6)	8(7)
C(11)	32(10)	24(10)	10(8)	1(7)	-1(7)	18(8)
C(12)	51(13)	21(11)	11(8)	1(8)	-5(8)	8(10)
C(13)	41(12)	44(14)	13(8)	0(9)	2(8)	7(10)
C(14)	45(12)	56(15)	19(9)	17(10)	17(9)	28(12)
C(15)	31(10)	32(12)	17(8)	-3(8)	12(8)	0(9)
C(16)	28(10)	50(14)	6(7)	1(8)	0(7)	18(10)
C(17)	27(10)	23(11)	22(9)	0(8)	6(8)	8(8)
C(18)	17(9)	39(13)	31(10)	-1(9)	-3(8)	6(9)
C(19)	28(10)	27(11)	16(8)	1(8)	-4(7)	10(9)
C(20)	12(8)	22(10)	21(9)	-1(8)	1(7)	-3(7)
C(21)	59(17)	91(23)	58(16)	26(16)	19(14)	30(16)
C(22)	107(27)	226(49)	97(25)	89(30)	46(22)	130(32)

The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^*b^* U_{12}]$.

Table 5. Hydrogen Coordinates (x 10^4) and Isotropic Displacement Parameters ($Å^2$ x 10^3) for [$(HgI_2)_2$ $(TPyP)_{0.25}(ZnTPyP)_{0.75}$]*2(TCE)

Atom	x	y	z	U(eq)
H(2A)	17536(19)	2412(17)	3504(13)	28
H(3A)	15709(19)	2329(19)	1826(13)	33
H(7A)	11495(22)	3923(19)	1118(14)	41
H(8A)	10707(23)	5254(20)	2247(15)	46
H(12A)	11586(22)	1374(18)	1009(13)	40
H(13A)	11012(23)	354(21)	-830(14)	46
H(14A)	14414(23)	3218(21)	-1185(14)	43
H(15A)	15199(20)	4231(19)	673(13)	37
H(17A)	9310(19)	5255(18)	3833(13)	31
H(18A)	7932(20)	6388(20)	3429(15)	41
H(19A)	11609(20)	9572(18)	4012(13)	32
H(20A)	13076(18)	8607(17)	4623(13)	28
H(21A)	2815(28)	7535(29)	11907(22)	83
H(22A)	4015(40)	8144(43)	10627(28)	139

Table 1. Crystal data and structure refinement

Compound	$[(HgI_2)_2(ZnTPyP)_{0.3}(TPyP)_{0.7}]*4(TCE)$
Color / Shape	violet / fragment
Empirical formula	$C_{48}H_{33.4}Cl_{16}Hg_2I_4N_8Zn_{0.30}$
Formula weight	2216.41
Temperature	173(2) K
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 14.6129(5) Å α = 62.053(1)°
(6091 reflections	b = 16.2090(5) Å β = 80.372(1)°
in full θ range)	c = 16.3263(5) Å γ = 73.281(1)°
Volume	3269.3(2) Å^3
Z	2
Density (calculated)	2.252 Mg/m^3
Absorption coefficient	7.381 mm^{-1}
Diffractometer / scan	Siemens SMART / CCD area detector
Radiation / wavelength	MoKα (graphite monochrom.) / 0.71073 Å
F(000)	2058
Crystal size	0.10 x 0.20 x 0.20 mm
θ range for data collection	1.41 to 27.99°
Index ranges	$-18 \le h \le 18$, $-21 \le k \le 21$, $-20 \le \ell \le 21$
Reflections collected	20627
Independent / observed refls.	14427(R_{int} = 0.0352) / 8155([I>2σ(I)])
Absorption correction	SADABS[1]
Refinement method	Full-matrix least-squares on F^2
Computing	SHELXTL, Ver. 5[2]
Data / restraints / parameters	14423 / 0 / 712
Goodness-of-fit on F^2	0.935
SHELX-93 weight parameters	0.0458, 0.0000
Final R indices [I>2σ(I)]	R1 = 0.0496, wR2 = 0.0958
R indices (all data)	R1 = 0.1092, wR2 = 0.1290
Largest diff. peak and hole	1.796 and -2.363 eÅ^{-3}

Table 2. Atomic Coordinates [x 10^4] and Equivalent Isotropic Displacement Parameters [$Å^2$ x 10^3] for [$(HgI_2)_2(ZnTPyP)_{0.3}(TPyP)_{0.7}$]*4(TCE)

Atom	x/a	y/b	z/c	U(eq)
Hg(1)	8835(1)	9309(1)	2914(1)	25(1)
Hg(2)	-3998(1)	18157(1)	3332(1)	26(1)
I(1)	8892(1)	7978(1)	4655(1)	41(1)
I(2)	9262(1)	9561(1)	1183(1)	39(1)
I(3)	-4090(1)	19529(1)	1615(1)	33(1)
I(4)	-4290(1)	17752(1)	5095(1)	42(1)
Zn	2447(3)	13788(4)	2936(4)	53(1)
Cl(1)	2226(2)	7984(2)	6465(2)	52(1)
Cl(2)	2894(2)	9153(3)	4618(3)	77(1)
Cl(3)	1507(2)	7728(3)	4822(2)	64(1)
Cl(4)	3004(2)	6140(3)	5936(2)	62(1)
Cl(5)	5306(3)	7856(3)	-48(3)	82(1)
Cl(6)	5935(2)	5941(3)	117(3)	79(1)
Cl(7)	8148(3)	6256(3)	-222(3)	92(1)
Cl(8)	7046(3)	6318(4)	1417(3)	126(2)
Cl(9)	1872(2)	-872(3)	2312(2)	71(1)
Cl(10)	2673(3)	-1640(3)	977(4)	99(2)
Cl(11)	3520(2)	89(3)	906(3)	80(1)
Cl(12)	1590(2)	1279(3)	480(3)	70(1)
Cl(13)	8973(3)	2565(3)	9601(3)	74(1)
Cl(14)	9562(2)	4234(3)	9432(3)	79(1)
Cl(15)	6778(2)	3818(3)	9516(2)	60(1)
Cl(16)	7910(2)	3523(3)	11001(2)	55(1)
N(1)	1006(4)	13853(5)	2910(5)	18(2)
N(2)	2814(5)	12618(6)	2722(5)	23(2)
N(3)	3833(4)	13926(5)	2666(5)	20(2)
N(4)	2033(5)	15055(6)	3045(5)	24(2)
N(5)	-363(5)	10453(6)	2903(6)	24(2)
N(6)	7281(5)	10405(6)	2754(6)	25(2)
N(7)	5153(5)	17081(6)	3252(6)	29(2)

N(8)	-2439(5)	17102(6)	3333(6)	27(2)
C(1)	234(6)	14531(7)	3021(7)	26(2)
C(2)	-600(6)	14299(8)	2951(8)	35(3)
C(3)	-354(6)	13484(7)	2846(7)	27(2)
C(4)	659(6)	13192(7)	2832(6)	22(2)
C(5)	1208(6)	12371(7)	2776(6)	22(2)
C(6)	2222(6)	12106(7)	2729(6)	22(2)
C(7)	2766(6)	11217(6)	2678(6)	20(2)
C(8)	3692(6)	11227(7)	2633(7)	26(2)
C(9)	3716(6)	12103(7)	2653(6)	21(2)
C(10)	4564(5)	12395(7)	2568(6)	20(2)
C(11)	4610(6)	13267(7)	2519(6)	20(2)
C(12)	5438(6)	13600(7)	2422(6)	24(2)
C(13)	5179(6)	14411(7)	2534(6)	25(2)
C(14)	4167(6)	14607(7)	2712(6)	21(2)
C(15)	3629(6)	15331(7)	2939(6)	22(2)
C(16)	2635(6)	15539(6)	3112(7)	22(2)
C(17)	2094(6)	16300(7)	3350(7)	27(2)
C(18)	1165(6)	16306(7)	3392(7)	29(2)
C(19)	1134(6)	15525(7)	3205(6)	21(2)
C(20)	291(6)	15303(6)	3162(6)	21(2)
C(21)	673(5)	11684(6)	2812(7)	20(2)
C(22)	630(6)	10863(7)	3614(7)	25(2)
C(23)	112(6)	10248(7)	3641(7)	29(2)
C(24)	-317(6)	11227(7)	2152(7)	28(2)
C(25)	173(6)	11890(7)	2056(7)	27(2)
C(26)	5500(6)	11693(7)	2603(7)	22(2)
C(27)	6143(6)	11857(7)	1865(7)	22(2)
C(28)	7025(6)	11209(7)	1955(7)	26(2)
C(29)	6658(6)	10244(7)	3467(7)	25(2)
C(30)	5761(6)	10864(7)	3418(7)	25(2)
C(31)	4162(6)	15945(7)	3032(7)	24(2)
C(32)	4524(9)	16622(8)	2311(8)	58(4)
C(33)	4978(9)	17203(9)	2410(9)	59(4)
C(34)	4843(8)	16415(9)	3953(9)	59(4)
C(35)	4345(9)	15824(9)	3898(8)	60(4)
C(36)	-652(6)	15946(7)	3245(7)	23(2)
C(37)	-987(6)	16801(7)	2502(7)	33(3)
C(38)	-1890(6)	17349(7)	2585(7)	32(2)

C(39)	-2103(7)	16278(8)	4066(8)	41(3)
C(40)	-1219(7)	15659(8)	4048(8)	41(3)
C(41)	2969(7)	7957(8)	5511(8)	46(3)
C(42)	2727(8)	7380(10)	5122(9)	57(4)
C(43)	6273(8)	6998(9)	-239(9)	61(4)
C(44)	7160(10)	6895(11)	182(11)	88(5)
C(45)	1974(8)	-612(9)	1130(9)	54(4)
C(46)	2404(7)	202(10)	538(9)	52(3)
C(47)	8597(9)	3782(11)	9294(10)	74(4)
C(48)	7789(8)	4080(10)	9794(9)	63(4)

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 3. Bond Lengths [Å] and Angles [°] for $[(HgI_2)_2(ZnTPyP)_{0.3}(TPyP)_{0.7}]*4(TCE)$

Hg(1)-N(6)	2.413(7)	Hg(1)-N(5)#1	2.454(7)
Hg(1)-I(1)	2.6395(9)	Hg(1)-I(2)	2.6503(8)
Hg(2)-N(8)	2.424(7)	Hg(2)-N(7)#2	2.472(8)
Hg(2)-I(4)	2.6220(8)	Hg(2)-I(3)	2.6337(9)
Zn-N(2)	1.996(8)	Zn-N(4)	2.051(8)
Zn-N(3)	2.053(8)	Zn-N(1)	2.084(8)
Cl(1)-C(41)	1.754(11)	Cl(2)-C(41)	1.783(12)
Cl(3)-C(42)	1.786(11)	Cl(4)-C(42)	1.783(14)
Cl(5)-C(43)	1.776(13)	Cl(6)-C(43)	1.724(13)
Cl(7)-C(44)	1.75(2)	Cl(8)-C(44)	1.78(2)
Cl(9)-C(45)	1.761(13)	Cl(10)-C(45)	1.790(11)
Cl(11)-C(46)	1.763(11)	Cl(12)-C(46)	1.778(12)
Cl(13)-C(47)	1.73(2)	Cl(14)-C(47)	1.852(14)
Cl(15)-C(48)	1.826(13)	Cl(16)-C(48)	1.758(13)
N(1)-C(4)	1.373(10)	N(1)-C(1)	1.385(11)
N(2)-C(6)	1.356(10)	N(2)-C(9)	1.361(10)
N(3)-C(14)	1.365(10)	N(3)-C(11)	1.392(10)
N(4)-C(19)	1.367(10)	N(4)-C(16)	1.383(10)
N(5)-C(24)	1.289(12)	N(5)-C(23)	1.348(11)
N(5)-Hg(1)#2	2.454(7)	N(6)-C(29)	1.322(11)
N(6)-C(28)	1.352(12)	N(7)-C(34)	1.278(14)
N(7)-C(33)	1.352(13)	N(7)-Hg(2)#1	2.472(8)
N(8)-C(38)	1.301(11)	N(8)-C(39)	1.333(13)
C(1)-C(20)	1.400(12)	C(1)-C(2)	1.412(11)
C(2)-C(3)	1.350(12)	C(3)-C(4)	1.419(11)
C(4)-C(5)	1.378(12)	C(5)-C(6)	1.418(11)
C(5)-C(21)	1.509(11)	C(6)-C(7)	1.465(11)
C(7)-C(8)	1.347(11)	C(8)-C(9)	1.446(12)
C(9)-C(10)	1.415(11)	C(10)-C(11)	1.398(12)
C(10)-C(26)	1.497(11)	C(11)-C(12)	1.417(11)
C(12)-C(13)	1.350(12)	C(13)-C(14)	1.430(10)
C(14)-C(15)	1.383(11)	C(15)-C(16)	1.404(11)
C(15)-C(31)	1.500(12)	C(16)-C(17)	1.443(11)
C(17)-C(18)	1.346(12)	C(18)-C(19)	1.447(12)
C(19)-C(20)	1.401(11)	C(20)-C(36)	1.500(11)

C(21)-C(22)	1.370(13)	C(21)-C(25)	1.395(12)
C(22)-C(23)	1.395(12)	C(24)-C(25)	1.393(12)
C(26)-C(27)	1.367(12)	C(26)-C(30)	1.385(13)
C(27)-C(28)	1.388(11)	C(29)-C(30)	1.393(11)
C(31)-C(32)	1.335(14)	C(31)-C(35)	1.396(14)
C(32)-C(33)	1.375(14)	C(34)-C(35)	1.399(14)
C(36)-C(37)	1.365(14)	C(36)-C(40)	1.382(13)
C(37)-C(38)	1.389(12)	C(39)-C(40)	1.395(13)
C(41)-C(42)	1.49(2)	C(43)-C(44)	1.50(2)
C(45)-C(46)	1.47(2)	C(47)-C(48)	1.42(2)

N(6)-Hg(1)-N(5)#1	92.5(2)	N(6)-Hg(1)-I(1)	106.1(2)
N(5)#1-Hg(1)-I(1)	104.3(2)	N(6)-Hg(1)-I(2)	101.3(2)
N(5)#1-Hg(1)-I(2)	99.0(2)	I(1)-Hg(1)-I(2)	142.90(3)
N(8)-Hg(2)-N(7)#2	93.1(2)	N(8)-Hg(2)-I(4)	101.6(2)
N(7)#2-Hg(2)-I(4)	100.3(2)	N(8)-Hg(2)-I(3)	102.7(2)
N(7)#2-Hg(2)-I(3)	101.8(2)	I(4)-Hg(2)-I(3)	145.96(3)
N(2)-Zn-N(4)	175.3(4)	N(2)-Zn-N(3)	90.8(3)
N(4)-Zn-N(3)	89.9(3)	N(2)-Zn-N(1)	90.1(3)
N(4)-Zn-N(1)	88.2(3)	N(3)-Zn-N(1)	167.7(4)
C(4)-N(1)-C(1)	108.1(6)	C(4)-N(1)-Zn	125.4(5)
C(1)-N(1)-Zn	126.5(6)	C(6)-N(2)-C(9)	105.7(7)
C(6)-N(2)-Zn	127.0(6)	C(9)-N(2)-Zn	126.9(5)
C(14)-N(3)-C(11)	108.4(6)	C(14)-N(3)-Zn	125.9(5)
C(11)-N(3)-Zn	125.3(6)	C(19)-N(4)-C(16)	104.8(7)
C(19)-N(4)-Zn	128.6(6)	C(16)-N(4)-Zn	126.0(6)
C(24)-N(5)-C(23)	118.7(8)	C(24)-N(5)-Hg(1)#2	119.7(6)
C(23)-N(5)-Hg(1)#2	121.3(7)	C(29)-N(6)-C(28)	117.8(8)
C(29)-N(6)-Hg(1)	120.2(7)	C(28)-N(6)-Hg(1)	122.0(6)
C(34)-N(7)-C(33)	116.1(9)	C(34)-N(7)-Hg(2)#1	125.0(7)
C(33)-N(7)-Hg(2)#1	118.9(7)	C(38)-N(8)-C(39)	117.7(8)
C(38)-N(8)-Hg(2)	118.8(7)	C(39)-N(8)-Hg(2)	123.5(6)
N(1)-C(1)-C(20)	125.5(7)	N(1)-C(1)-C(2)	107.0(8)
C(20)-C(1)-C(2)	127.4(8)	C(3)-C(2)-C(1)	109.4(8)
C(2)-C(3)-C(4)	106.9(8)	N(1)-C(4)-C(5)	125.4(7)
N(1)-C(4)-C(3)	108.5(7)	C(5)-C(4)-C(3)	126.1(8)
C(4)-C(5)-C(6)	125.4(8)	C(4)-C(5)-C(21)	116.3(7)
C(6)-C(5)-C(21)	118.2(8)	N(2)-C(6)-C(5)	126.1(8)
N(2)-C(6)-C(7)	111.1(7)	C(5)-C(6)-C(7)	122.9(8)

C(8)-C(7)-C(6)	105.3(8)	C(7)-C(8)-C(9)	107.3(8)
N(2)-C(9)-C(10)	125.2(8)	N(2)-C(9)-C(8)	110.6(7)
C(10)-C(9)-C(8)	124.1(8)	C(11)-C(10)-C(9)	125.6(8)
C(11)-C(10)-C(26)	116.3(7)	C(9)-C(10)-C(26)	118.0(8)
N(3)-C(11)-C(10)	124.7(7)	N(3)-C(11)-C(12)	107.1(7)
C(10)-C(11)-C(12)	127.8(8)	C(13)-C(12)-C(11)	108.8(7)
C(12)-C(13)-C(14)	107.4(8)	N(3)-C(14)-C(15)	126.0(7)
N(3)-C(14)-C(13)	108.1(7)	C(15)-C(14)-C(13)	125.8(8)
C(14)-C(15)-C(16)	126.8(8)	C(14)-C(15)-C(31)	116.8(7)
C(16)-C(15)-C(31)	116.4(7)	N(4)-C(16)-C(15)	124.1(8)
N(4)-C(16)-C(17)	110.4(7)	C(15)-C(16)-C(17)	125.4(8)
C(18)-C(17)-C(16)	107.1(8)	C(17)-C(18)-C(19)	106.3(8)
N(4)-C(19)-C(20)	124.4(8)	N(4)-C(19)-C(18)	111.2(7)
C(20)-C(19)-C(18)	124.3(7)	C(1)-C(20)-C(19)	125.9(8)
C(1)-C(20)-C(36)	115.1(7)	C(19)-C(20)-C(36)	119.0(7)
C(22)-C(21)-C(25)	118.5(8)	C(22)-C(21)-C(5)	120.1(8)
C(25)-C(21)-C(5)	121.3(9)	C(21)-C(22)-C(23)	119.3(9)
N(5)-C(23)-C(22)	121.6(10)	N(5)-C(24)-C(25)	124.2(9)
C(24)-C(25)-C(21)	117.7(9)	C(27)-C(26)-C(30)	117.7(8)
C(27)-C(26)-C(10)	122.3(9)	C(30)-C(26)-C(10)	119.9(8)
C(26)-C(27)-C(28)	119.8(9)	N(6)-C(28)-C(27)	122.4(8)
N(6)-C(29)-C(30)	122.5(9)	C(26)-C(30)-C(29)	119.8(9)
C(32)-C(31)-C(35)	114.6(9)	C(32)-C(31)-C(15)	123.8(9)
C(35)-C(31)-C(15)	121.6(9)	C(31)-C(32)-C(33)	122.8(11)
N(7)-C(33)-C(32)	122.1(11)	N(7)-C(34)-C(35)	124.4(12)
C(31)-C(35)-C(34)	119.8(11)	C(37)-C(36)-C(40)	119.2(8)
C(37)-C(36)-C(20)	119.9(9)	C(40)-C(36)-C(20)	120.8(9)
C(36)-C(37)-C(38)	118.3(10)	N(8)-C(38)-C(37)	124.0(10)
N(8)-C(39)-C(40)	123.0(10)	C(36)-C(40)-C(39)	117.8(10)
C(42)-C(41)-Cl(1)	113.2(8)	C(42)-C(41)-Cl(2)	108.8(8)
Cl(1)-C(41)-Cl(2)	109.7(6)	C(41)-C(42)-Cl(4)	109.4(8)
C(41)-C(42)-Cl(3)	114.4(8)	Cl(4)-C(42)-Cl(3)	108.8(7)
C(44)-C(43)-Cl(6)	115.1(10)	C(44)-C(43)-Cl(5)	110.5(10)
Cl(6)-C(43)-Cl(5)	109.9(7)	C(43)-C(44)-Cl(7)	109.5(10)
C(43)-C(44)-Cl(8)	110.7(10)	Cl(7)-C(44)-Cl(8)	111.1(8)
C(46)-C(45)-Cl(9)	113.6(8)	C(46)-C(45)-Cl(10)	108.2(8)
Cl(9)-C(45)-Cl(10)	110.5(8)	C(45)-C(46)-Cl(11)	113.8(9)
C(45)-C(46)-Cl(12)	108.9(7)	Cl(11)-C(46)-Cl(12)	110.2(6)
C(48)-C(47)-Cl(13)	117.0(11)	C(48)-C(47)-Cl(14)	105.5(10)

Cl(13)-C(47)-Cl(14)	110.8(7)	C(47)-C(48)-Cl(16)	114.4(10)
C(47)-C(48)-Cl(15)	106.4(10)	Cl(16)-C(48)-Cl(15)	110.3(7)

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic Displacement Parameters [$Å^2$ x 10^3] for $[(HgI_2)_2(ZnTPyP)_{0.3}(TPyP)_{0.7}]*4(TCE)$

Atom	U11	U22	U33	U23	U13	U12
Hg(1)	19(1)	29(1)	35(1)	-20(1)	1(1)	-7(1)
Hg(2)	20(1)	31(1)	35(1)	-21(1)	3(1)	-8(1)
I(1)	42(1)	39(1)	39(1)	-10(1)	-8(1)	-16(1)
I(2)	32(1)	62(1)	42(1)	-37(1)	11(1)	-21(1)
I(3)	29(1)	33(1)	38(1)	-15(1)	-1(1)	-9(1)
I(4)	40(1)	61(1)	35(1)	-29(1)	9(1)	-20(1)
Zn	43(3)	47(3)	81(4)	-39(3)	4(3)	-14(2)
Cl(1)	32(2)	75(2)	65(2)	-45(2)	5(1)	-17(2)
Cl(2)	63(2)	59(3)	78(3)	-1(2)	-13(2)	-14(2)
Cl(3)	47(2)	84(3)	73(2)	-47(2)	-25(2)	3(2)
Cl(4)	47(2)	58(2)	77(2)	-29(2)	-9(2)	-5(2)
Cl(5)	87(3)	54(3)	88(3)	-16(2)	-29(2)	-6(2)
Cl(6)	57(2)	77(3)	123(4)	-55(3)	-1(2)	-26(2)
Cl(7)	59(2)	100(4)	121(4)	-42(3)	3(2)	-38(2)
Cl(8)	110(4)	171(5)	109(4)	-77(4)	-67(3)	7(4)
Cl(9)	59(2)	91(3)	65(2)	-38(2)	11(2)	-23(2)
Cl(10)	77(3)	94(3)	161(5)	-95(4)	-2(3)	-4(2)
Cl(11)	48(2)	151(4)	68(2)	-58(3)	8(2)	-51(2)
Cl(12)	64(2)	77(3)	95(3)	-60(2)	10(2)	-24(2)
Cl(13)	77(2)	78(3)	71(3)	-46(2)	-4(2)	0(2)
Cl(14)	52(2)	111(3)	67(2)	-22(2)	1(2)	-43(2)
Cl(15)	49(2)	72(3)	54(2)	-12(2)	-14(2)	-26(2)
Cl(16)	45(2)	77(3)	36(2)	-21(2)	2(1)	-13(2)
N(1)	11(3)	16(4)	26(4)	-9(4)	1(3)	-4(3)
N(2)	14(4)	31(5)	36(5)	-24(4)	-2(3)	-6(4)
N(3)	9(3)	19(4)	33(5)	-14(4)	-7(3)	5(3)
N(4)	20(4)	29(5)	37(5)	-24(4)	1(4)	-10(4)
N(5)	17(4)	29(5)	36(5)	-21(5)	-2(4)	-6(4)
N(6)	17(4)	34(5)	31(5)	-22(4)	1(4)	-6(4)
N(7)	30(5)	25(5)	36(5)	-13(4)	0(4)	-13(4)
N(8)	16(4)	34(6)	38(5)	-23(5)	3(4)	-6(4)
C(1)	16(5)	36(6)	31(6)	-16(5)	-1(4)	-13(4)
C(2)	8(4)	39(7)	65(8)	-33(6)	-1(5)	0(4)

C(3)	12(4)	27(6)	50(7)	-24(5)	-4(4)	-2(4)
C(4)	11(4)	27(6)	31(6)	-17(5)	1(4)	-2(4)
C(5)	15(4)	29(6)	28(6)	-14(5)	-2(4)	-9(4)
C(6)	21(5)	21(6)	25(5)	-11(5)	-5(4)	-5(4)
C(7)	21(5)	16(5)	27(5)	-12(4)	-6(4)	-3(4)
C(8)	10(4)	33(6)	41(6)	-26(5)	-1(4)	-1(4)
C(9)	14(4)	25(6)	30(6)	-15(5)	0(4)	-10(4)
C(10)	11(4)	30(6)	23(5)	-14(5)	-2(4)	-4(4)
C(11)	15(4)	24(6)	24(5)	-11(5)	0(4)	-10(4)
C(12)	13(4)	25(6)	38(6)	-20(5)	7(4)	-4(4)
C(13)	12(4)	28(6)	37(6)	-15(5)	8(4)	-10(4)
C(14)	14(4)	29(6)	31(6)	-21(5)	6(4)	-10(4)
C(15)	27(5)	16(5)	24(5)	-9(4)	-4(4)	-5(4)
C(16)	19(5)	13(5)	39(6)	-12(5)	-3(4)	-8(4)
C(17)	25(5)	22(6)	43(6)	-22(5)	2(5)	-8(4)
C(18)	28(5)	26(6)	42(7)	-25(5)	-3(5)	-2(5)
C(19)	10(4)	23(6)	33(6)	-16(5)	2(4)	-1(4)
C(20)	17(4)	15(5)	25(5)	-6(4)	1(4)	-4(4)
C(21)	10(4)	15(5)	37(6)	-14(5)	1(4)	-2(4)
C(22)	22(5)	33(6)	31(6)	-19(5)	2(4)	-14(5)
C(23)	30(5)	29(6)	28(6)	-13(5)	-4(5)	-6(5)
C(24)	29(5)	31(7)	32(6)	-16(5)	-5(5)	-11(5)
C(25)	30(5)	19(6)	32(6)	-8(5)	-7(5)	-7(4)
C(26)	13(4)	24(6)	34(6)	-20(5)	-3(4)	-1(4)
C(27)	18(5)	20(6)	28(6)	-8(5)	-5(4)	-9(4)
C(28)	13(5)	36(7)	35(6)	-23(6)	7(4)	-9(4)
C(29)	23(5)	29(6)	28(6)	-15(5)	-3(4)	-7(5)
C(30)	19(5)	26(6)	31(6)	-14(5)	2(4)	-7(4)
C(31)	23(5)	13(5)	36(6)	-12(5)	-6(4)	1(4)
C(32)	102(10)	38(8)	43(8)	0(6)	-25(7)	-47(8)
C(33)	98(10)	58(9)	42(8)	-16(7)	1(7)	-61(8)
C(34)	69(9)	60(10)	62(9)	-23(8)	-24(7)	-32(8)
C(35)	96(10)	55(9)	41(8)	-10(7)	-5(7)	-55(8)
C(36)	15(4)	22(6)	39(6)	-20(5)	0(4)	-2(4)
C(37)	24(5)	28(6)	35(6)	-7(5)	4(5)	-1(5)
C(38)	22(5)	25(6)	37(6)	-9(5)	-4(5)	6(5)
C(39)	25(6)	47(8)	39(7)	-22(6)	11(5)	4(5)
C(40)	34(6)	36(7)	42(7)	-13(6)	9(5)	-4(5)
C(41)	28(6)	45(8)	39(7)	-3(6)	-4(5)	1(6)

C(42)	43(7)	78(11)	52(8)	-36(8)	7(6)	-13(7)
C(43)	55(8)	58(10)	49(8)	-4(7)	-11(7)	-13(7)
C(44)	85(11)	60(11)	126(15)	-26(10)	-52(10)	-28(9)
C(45)	33(6)	68(10)	84(10)	-52(9)	6(6)	-18(6)
C(46)	34(6)	84(11)	58(9)	-49(8)	1(6)	-14(7)
C(47)	73(10)	75(12)	55(9)	-14(8)	-14(8)	-10(9)
C(48)	49(8)	56(10)	57(9)	-11(8)	-2(7)	-2(7)

The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^*b^* U_{12}]$.

Table 5. Hydrogen Coordinates (x 10^4) and Isotropic Displacement Parameters ($Å^2$ x 10^3) for $[(HgI_2)_2(ZnTPyP)_{0.3}(TPyP)_{0.7}]*4(TCE)$

Atom	x	y	z	U(eq)
H(2A)	-1236(6)	14659(8)	2975(8)	42
H(3A)	-779(6)	13166(7)	2791(7)	32
H(7A)	2518(6)	10736(6)	2676(6)	24
H(8A)	4229(6)	10747(7)	2595(7)	31
H(12A)	6071(6)	13301(7)	2298(6)	29
H(13A)	5593(6)	14784(7)	2501(6)	30
H(17A)	2347(6)	16717(7)	3458(7)	32
H(18A)	634(6)	16738(7)	3518(7)	34
H(22A)	948(6)	10713(7)	4146(7)	30
H(23A)	95(6)	9671(7)	4193(7)	35
H(24A)	-639(6)	11354(7)	1631(7)	34
H(25A)	168(6)	12462(7)	1494(7)	33
H(27A)	5987(6)	12414(7)	1293(7)	26
H(28A)	7464(6)	11333(7)	1436(7)	31
H(29A)	6829(6)	9683(7)	4033(7)	30
H(30A)	5328(6)	10720(7)	3941(7)	30
H(32A)	4466(9)	16704(8)	1705(8)	70
H(33A)	5174(9)	17707(9)	1869(9)	71
H(34A)	4958(8)	16314(9)	4553(9)	71
H(35A)	4132(9)	15343(9)	4449(8)	72
H(37A)	-611(6)	17016(7)	1942(7)	40
H(38A)	-2122(6)	17941(7)	2064(7)	38
H(39A)	-2483(7)	16106(8)	4626(8)	49
H(40A)	-1014(7)	15060(8)	4571(8)	49
H(41A)	3643(7)	7668(8)	5715(8)	55
H(42A)	3138(8)	7455(10)	4548(9)	68
H(43A)	6405(8)	7261(9)	-925(9)	73
H(44A)	7252(10)	7552(11)	-19(11)	105
H(45A)	1317(8)	-454(9)	911(9)	65
H(46A)	2501(7)	248(10)	-102(9)	63
H(47A)	8444(9)	4123(11)	8623(10)	89

H(48A)	7665(8)	4792(10)	9561(9)	75

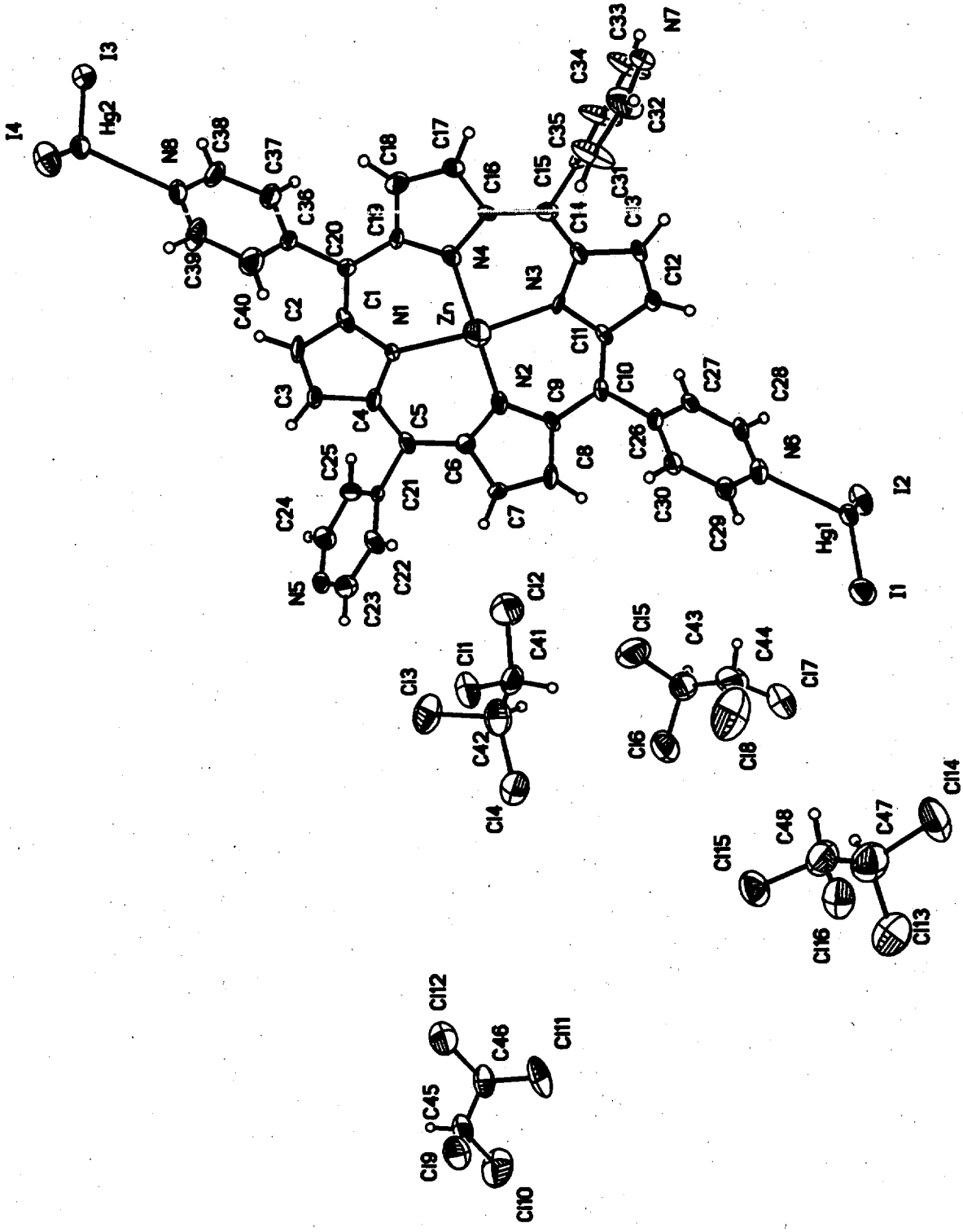
I3
I4
Hg2
N8
C38
C37
C36
C39
C40
C20
C19
C18
C17
C16
C15
C35
C34
C33
N7
C32
C31
C13
C14
C12
N4
N3
C1
C2
N1
Zn
C11
C3
C4
C5
N2
C9
C10
C27
C28
C25
C21
C6
C8
C26
N6
C24
C7
C30
C29
I2
Hg1
N5
C22
C23
I1
Cl2
C41
Cl1
Cl3
C42
Cl4
C43
Cl5
C44
Cl7
Cl6
Cl8
Cl4
C48
C47
Cl5
Cl6
Cl3
C46
Cl2
Cl1
C45
Cl9
Cl10

Table 1. Crystal data and structure refinement

Compound	$[(HgBr_2)_2(TPyP)]*6(TCE)$
Color / Shape	purple / parallelepiped
Empirical formula	$C_{52}H_{38}Br_4Cl_{24}Hg_2N_8$
Formula weight	2346.52
Temperature	173(2) K
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 10.8167(6) Å α = 104.591(1)°
(3235 reflections	b = 11.6757(7) Å β = 95.899(2)°
in full θ range)	c = 16.1584(9) Å γ = 101.073(1)°
Volume	1913.4(2) $Å^3$
Z	1
Density (calculated)	2.036 Mg/m^3
Absorption coefficient	6.975 mm^{-1}
Diffractometer / scan	Siemens SMART / CCD area detector
Radiation / wavelength	MoKα (graphite monochrom.) / 0.71073 Å
F(000)	1114
Crystal size	0.25 x 0.30 x 0.45 mm
θ range for data collection	1.32 to 27.94°
Index ranges	$-14 \le h \le 13$, $-15 \le k \le 14$, $-10 \le \ell \le 20$
Reflections collected	12316
Independent / observed refls.	8543(R_{int} = 0.0604) / 4095([I>2σ(I)])
Absorption correction	SADABS[1]
Refinement method	Full-matrix least-squares on F^2
Computing	SHELXTL, Ver. 5[2]
Data / restraints / parameters	8535 / 0 / 407
Goodness-of-fit on F^2	0.851
SHELX-93 weight parameters	0.0575, 0.0000
Final R indices [I>2σ(I)]	R1 = 0.0655, wR2 = 0.1249
R indices (all data)	R1 = 0.1420, wR2 = 0.1563
Extinction coefficient	0.0001(2)
Largest diff. peak and hole	2.243 and -3.064 $eÅ^{-3}$

Table 2. Atomic Coordinates [x 10^4] and Equivalent Isotropic Displacement Parameters [$Å^2$ x 10^3] for [$(HgBr_2)_2$(TPyP)] *6(TCE)

Atom	x/a	y/b	z/c	U(eq)
Hg	8270(1)	8739(1)	412(1)	33(1)
Br(1)	6606(1)	9784(1)	43(1)	60(1)
Br(2)	9501(1)	7261(1)	-238(1)	45(1)
Cl(1)	5112(3)	3628(3)	53(3)	76(1)
Cl(2)	7147(4)	3234(3)	1226(3)	77(1)
Cl(3)	7935(3)	4207(3)	-445(3)	76(1)
Cl(4)	6267(4)	1900(3)	-1503(3)	77(1)
Cl(5)	10494(7)	8085(5)	3058(6)	204(4)
Cl(6)	13068(4)	8018(5)	3685(3)	130(2)
Cl(7)	10735(7)	6022(7)	3998(4)	205(4)
Cl(8)	10043(4)	5147(4)	2159(3)	96(2)
Cl(9)	7730(4)	3803(4)	3673(3)	96(2)
Cl(10)	7940(3)	1369(3)	3983(3)	79(1)
Cl(11)	5680(4)	1522(4)	2527(3)	87(1)
Cl(12)	5059(4)	1003(4)	4202(3)	93(1)
N(1)	6443(7)	6495(7)	5033(6)	30(2)
N(2)	4451(7)	4765(7)	3708(6)	31(2)
N(3)	7531(8)	7969(8)	1574(6)	41(3)
N(4)	-155(8)	310(8)	1439(6)	29(2)
C(1)	7290(9)	7193(9)	5771(7)	31(3)
C(2)	8100(10)	8106(10)	5500(8)	43(3)
C(3)	7772(10)	7946(10)	4666(8)	44(3)
C(4)	6692(9)	6914(9)	4341(7)	33(3)
C(5)	6035(9)	6436(9)	3484(7)	31(3)
C(6)	4992(10)	5423(9)	3216(7)	31(3)
C(7)	4288(10)	4991(10)	2344(7)	39(3)
C(8)	3378(10)	4033(9)	2307(7)	34(3)
C(9)	3471(9)	3891(9)	3160(7)	32(3)
C(10)	2647(9)	2967(9)	3404(7)	29(3)
C(11)	6565(9)	7000(9)	2836(7)	34(3)
C(12)	7105(12)	6348(11)	2210(8)	49(3)

C(13)	7595(11)	6841(10)	1607(8)	44(3)
C(14)	6991(10)	8614(10)	2196(8)	40(3)
C(15)	6511(10)	8167(11)	2811(7)	39(3)
C(16)	1684(9)	2073(9)	2699(7)	28(3)
C(17)	1983(10)	1087(11)	2167(8)	49(4)
C(18)	1040(11)	230(10)	1545(8)	43(3)
C(19)	-442(10)	1263(10)	1941(8)	40(3)
C(20)	424(10)	2155(10)	2565(8)	46(3)
C(21)	6208(12)	2726(11)	174(10)	71(5)
C(22)	7122(12)	2744(11)	-479(10)	63(4)
C(23)	11643(16)	7282(18)	2905(12)	121(8)
C(24)	11245(14)	5991(13)	3033(12)	86(6)
C(25)	6872(19)	2346(19)	4180(14)	148(11)
C(26)	5903(18)	2256(18)	3612(12)	117(8)

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 3. Bond Lengths [Å] and Angles [°] for $[(HgBr_2)_2(TPyP)]*6(TCE)$

Hg-N(4)#1	2.389(8)	Hg-N(3)	2.419(10)
Hg-Br(1)	2.4647(13)	Hg-Br(2)	2.4719(12)
Cl(1)-C(21)	1.757(13)	Cl(2)-C(21)	1.78(2)
Cl(3)-C(22)	1.749(12)	Cl(4)-C(22)	1.75(2)
Cl(5)-C(23)	1.70(2)	Cl(6)-C(23)	1.80(2)
Cl(7)-C(24)	1.70(2)	Cl(8)-C(24)	1.76(2)
Cl(9)-C(25)	2.16(3)	Cl(10)-C(25)	1.77(2)
Cl(11)-C(26)	1.72(2)	Cl(12)-C(26)	2.06(2)
N(1)-C(4)	1.359(13)	N(1)-C(1)	1.388(12)
N(2)-C(6)	1.341(13)	N(2)-C(9)	1.373(12)
N(3)-C(13)	1.346(14)	N(3)-C(14)	1.351(13)
N(4)-C(18)	1.311(12)	N(4)-C(19)	1.311(13)
N(4)-Hg#2	2.389(8)	C(1)-C(10)#3	1.390(14)
C(1)-C(2)	1.432(14)	C(2)-C(3)	1.31(2)
C(3)-C(4)	1.451(13)	C(4)-C(5)	1.411(14)
C(5)-C(6)	1.409(13)	C(5)-C(11)	1.479(14)
C(6)-C(7)	1.446(14)	C(7)-C(8)	1.325(14)
C(8)-C(9)	1.42(2)	C(9)-C(10)	1.424(14)
C(10)-C(1)#3	1.390(14)	C(10)-C(16)	1.487(13)
C(11)-C(12)	1.36(2)	C(11)-C(15)	1.38(2)
C(12)-C(13)	1.35(2)	C(14)-C(15)	1.34(2)
C(16)-C(17)	1.368(14)	C(16)-C(20)	1.383(13)
C(17)-C(18)	1.393(14)	C(19)-C(20)	1.371(14)
C(21)-C(22)	1.52(2)	C(23)-C(24)	1.56(2)
C(25)-C(26)	1.29(2)		

N(4)#1-Hg-N(3)	90.0(3)	N(4)#1-Hg-Br(1)	103.8(2)
N(3)-Hg-Br(1)	102.8(2)	N(4)#1-Hg-Br(2)	103.5(2)
N(3)-Hg-Br(2)	102.4(2)	Br(1)-Hg-Br(2)	142.49(5)
C(4)-N(1)-C(1)	110.5(8)	C(6)-N(2)-C(9)	105.6(9)
C(13)-N(3)-C(14)	116.7(10)	C(13)-N(3)-Hg	120.7(8)
C(14)-N(3)-Hg	122.5(8)	C(18)-N(4)-C(19)	117.0(9)
C(18)-N(4)-Hg#2	120.7(7)	C(19)-N(4)-Hg#2	122.3(7)
N(1)-C(1)-C(10)#3	127.4(9)	N(1)-C(1)-C(2)	105.4(9)
C(10)#3-C(1)-C(2)	127.2(9)	C(3)-C(2)-C(1)	109.6(10)
C(2)-C(3)-C(4)	108.6(11)	N(1)-C(4)-C(5)	126.8(9)

N(1)-C(4)-C(3)	105.9(10)	C(5)-C(4)-C(3)	127.3(10)
C(6)-C(5)-C(4)	124.1(10)	C(6)-C(5)-C(11)	119.7(10)
C(4)-C(5)-C(11)	116.0(8)	N(2)-C(6)-C(5)	127.2(10)
N(2)-C(6)-C(7)	109.6(9)	C(5)-C(6)-C(7)	123.1(10)
C(8)-C(7)-C(6)	107.9(10)	C(7)-C(8)-C(9)	106.0(10)
N(2)-C(9)-C(10)	125.1(10)	N(2)-C(9)-C(8)	110.8(10)
C(10)-C(9)-C(8)	124.1(9)	C(1)#3-C(10)-C(9)	125.5(9)
C(1)#3-C(10)-C(16)	118.0(9)	C(9)-C(10)-C(16)	116.5(9)
C(12)-C(11)-C(15)	117.0(11)	C(12)-C(11)-C(5)	119.5(10)
C(15)-C(11)-C(5)	123.4(10)	C(13)-C(12)-C(11)	120.8(11)
N(3)-C(13)-C(12)	122.3(11)	C(15)-C(14)-N(3)	122.9(11)
C(14)-C(15)-C(11)	120.2(11)	C(17)-C(16)-C(20)	115.9(10)
C(17)-C(16)-C(10)	121.7(9)	C(20)-C(16)-C(10)	122.3(9)
C(16)-C(17)-C(18)	120.2(10)	N(4)-C(18)-C(17)	123.0(10)
N(4)-C(19)-C(20)	124.0(10)	C(19)-C(20)-C(16)	119.9(10)
C(22)-C(21)-Cl(1)	111.2(11)	C(22)-C(21)-Cl(2)	107.3(9)
Cl(1)-C(21)-Cl(2)	112.1(8)	C(21)-C(22)-Cl(3)	113.6(9)
C(21)-C(22)-Cl(4)	107.8(9)	Cl(3)-C(22)-Cl(4)	113.8(8)
C(24)-C(23)-Cl(5)	112.8(11)	C(24)-C(23)-Cl(6)	105(2)
Cl(5)-C(23)-Cl(6)	111.1(10)	C(23)-C(24)-Cl(7)	112.7(11)
C(23)-C(24)-Cl(8)	106.4(13)	Cl(7)-C(24)-Cl(8)	111.4(8)
C(26)-C(25)-Cl(10)	122(2)	C(26)-C(25)-Cl(9)	83(2)
Cl(10)-C(25)-Cl(9)	101.3(11)	C(25)-C(26)-Cl(11)	127(2)
C(25)-C(26)-Cl(12)	82(2)	Cl(11)-C(26)-Cl(12)	106.3(10)

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic Displacement Parameters [$Å^2$ x 10^3] for $[(HgBr_2)_2(TPyP)]*6(TCE)$

Atom	U11	U22	U33	U23	U13	U12
Hg	32(1)	29(1)	36(1)	14(1)	0(1)	-2(1)
Br(1)	38(1)	45(1)	105(1)	40(1)	3(1)	9(1)
Br(2)	45(1)	35(1)	53(1)	9(1)	10(1)	6(1)
Cl(1)	56(2)	43(2)	124(4)	21(2)	-5(2)	16(2)
Cl(2)	114(3)	53(2)	55(3)	10(2)	-21(2)	19(2)
Cl(3)	66(2)	47(2)	118(4)	42(2)	12(2)	-6(2)
Cl(4)	87(3)	72(3)	61(3)	24(2)	-10(2)	-8(2)
Cl(5)	175(6)	73(4)	313(11)	28(5)	-91(7)	7(4)
Cl(6)	99(3)	145(5)	95(4)	7(3)	15(3)	-56(3)
Cl(7)	238(7)	195(7)	93(5)	32(5)	-8(5)	-136(6)
Cl(8)	77(3)	77(3)	101(4)	-19(3)	8(3)	-2(2)
Cl(9)	93(3)	57(2)	140(4)	39(3)	36(3)	-1(2)
Cl(10)	70(2)	73(3)	90(3)	11(2)	-5(2)	29(2)
Cl(11)	78(3)	91(3)	82(3)	20(3)	-13(2)	16(2)
Cl(12)	75(3)	69(3)	131(4)	34(3)	37(3)	-8(2)
N(1)	34(5)	21(5)	28(6)	7(4)	-1(4)	-8(4)
N(2)	35(5)	20(5)	32(6)	11(4)	0(4)	-10(4)
N(3)	38(5)	32(6)	47(7)	16(5)	6(5)	-14(4)
N(4)	27(5)	27(5)	27(6)	7(4)	4(4)	-8(4)
C(1)	35(6)	21(6)	33(7)	16(5)	2(5)	-15(5)
C(2)	45(7)	39(7)	30(8)	5(6)	7(6)	-23(5)
C(3)	44(7)	42(7)	31(8)	7(6)	-4(6)	-17(5)
C(4)	39(6)	25(6)	31(7)	16(5)	9(5)	-13(5)
C(5)	40(6)	26(6)	20(7)	4(5)	4(5)	-6(5)
C(6)	38(6)	23(6)	29(7)	7(5)	6(5)	-2(5)
C(7)	45(7)	40(7)	24(7)	12(6)	-4(6)	-5(6)
C(8)	48(7)	28(6)	18(7)	8(5)	-1(5)	-4(5)
C(9)	26(5)	32(6)	32(7)	11(5)	-5(5)	-6(5)
C(10)	27(5)	29(6)	25(7)	9(5)	-9(5)	-2(5)
C(11)	30(6)	26(6)	39(8)	13(6)	7(5)	-16(5)
C(12)	88(10)	25(7)	37(8)	8(6)	26(7)	12(6)
C(13)	57(8)	31(7)	42(9)	9(6)	20(6)	2(6)
C(14)	46(7)	32(7)	45(9)	9(6)	12(6)	15(6)

C(15)	47(7)	47(8)	26(7)	15(6)	15(6)	6(6)
C(16)	34(6)	22(6)	26(7)	11(5)	6(5)	-4(5)
C(17)	25(6)	50(8)	63(10)	9(7)	-2(6)	1(6)
C(18)	48(7)	25(6)	46(9)	-2(6)	0(6)	3(5)
C(19)	28(6)	41(7)	42(8)	13(6)	-14(6)	-6(5)
C(20)	39(7)	31(6)	56(9)	-3(6)	-15(6)	10(5)
C(21)	57(9)	33(7)	117(14)	28(8)	-11(9)	1(6)
C(22)	56(8)	33(7)	111(14)	33(8)	27(9)	12(6)
C(23)	88(13)	130(17)	93(15)	-12(13)	45(11)	-56(12)
C(24)	65(10)	45(9)	126(16)	-10(10)	28(10)	0(7)
C(25)	143(18)	174(22)	107(19)	-37(16)	-25(15)	115(17)
C(26)	128(15)	136(17)	71(14)	-28(12)	-24(12)	90(14)

The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$.

Table 5. Hydrogen Coordinates (x 10^4) and Isotropic Displacement Parameters ($Å^2$ x 10^3) for $[(HgBr_2)_2(TPyP)]$ *6(TCE)

Atom	x	y	z	U(eq)
H(1)	5875(7)	5761(7)	4975(6)	45
H(2A)	8772(10)	8731(10)	5867(8)	52
H(3A)	8174(10)	8425(10)	4331(8)	53
H(7A)	4448(10)	5334(10)	1881(7)	46
H(8A)	2784(10)	3541(9)	1813(7)	40
H(12A)	7138(12)	5536(11)	2195(8)	59
H(13A)	7999(11)	6375(10)	1192(8)	53
H(14A)	6949(10)	9419(10)	2196(8)	48
H(15A)	6133(10)	8652(11)	3232(7)	47
H(17A)	2835(10)	985(11)	2221(8)	59
H(18A)	1274(11)	-443(10)	1180(8)	52
H(19A)	-1302(10)	1339(10)	1867(8)	48
H(20A)	159(10)	2828(10)	2905(8)	56
H(21A)	5726(12)	1870(11)	79(10)	85
H(22A)	7779(12)	2301(11)	-329(10)	75
H(23A)	11851(16)	7206(18)	2307(12)	145
H(24A)	11996(14)	5607(13)	3004(12)	103
H(25A)	6737(19)	2607(19)	4796(14)	177
H(26A)	5552(18)	3003(18)	3731(12)	140

Table 1. Crystal data and structure refinement

Compound	$[(CdI_2)(TPyP)]*4(TCE)$
Color / Shape	violet / fragment
Empirical formula	$C_{48}H_{34}CdCl_{16}I_2N_8$
Formula weight	1656.23
Temperature	173(2) K
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	a = 20.467(2) Å α = 90°
(3440 reflections	b = 20.406(2) Å β = 112.787(1)°
in full θ range)	c = 15.167(1) Å γ = 90°
Volume	5839.9(8) $Å^3$
Z	4
Density (calculated)	1.884 Mg/m^3
Absorption coefficient	2.207 mm^{-1}
Diffractometer / scan	Siemens SMART / CCD area detector
Radiation / wavelength	MoKα (graphite monochrom.) / 0.71073 Å
F(000)	3216
Crystal size	0.08 x 0.18 x 0.30 mm
θ range for data collection	1.47 to 27.92°
Index ranges	$-22 \le h \le 26$, $-26 \le k \le 26$, $-19 \le \ell \le 15$
Reflections collected	18403
Independent / observed refls.	6782(R_{int} = 0.1554) / 3151([I>2σ(I)])
Absorption correction	SADABS[1]
Refinement method	Full-matrix least-squares on F^2
Computing	SHELXTL, Ver. 5[2]
Data / restraints / parameters	6779 / 0 / 336
Goodness-of-fit on F^2	0.965
SHELX-93 weight parameters	0.1289, 0.0000
Final R indices [I>2σ(I)]	R1 = 0.1029, wR2 = 0.2225
R indices (all data)	R1 = 0.2013, wR2 = 0.2731
Extinction coefficient	0.00000(8)
Largest diff. peak and hole	2.794 and -2.174 $eÅ^{-3}$

Table 2. Atomic Coordinates [x 10^4] and Equivalent Isotropic Displacement Parameters [$Å^2$ x 10^3] for [(CdI_2)(TPyP)]*4(TCE)

Atom	x/a	y/b	z/c	U(eq)
I	5500(1)	8094(1)	9597(1)	27(1)
Cd	5000	8090(1)	7500	22(1)
Cl(1)	3461(4)	7436(4)	10126(4)	126(3)
Cl(2)	3175(4)	6038(6)	10015(5)	201(6)
Cl(3)	4753(4)	5832(3)	10024(4)	98(2)
Cl(4)	3726(2)	6627(2)	8465(3)	40(1)
Cl(5)	1380(3)	5546(3)	9958(4)	83(2)
Cl(6)	1887(3)	4718(3)	11619(4)	90(2)
Cl(7)	2669(3)	3829(2)	10605(4)	82(2)
Cl(8)	2014(3)	4625(2)	8870(4)	66(1)
N(1)	676(5)	7390(4)	7407(7)	17(2)
N(2)	683(5)	8810(5)	7411(8)	23(2)
N(3)	0	4296(6)	7500	26(4)
N(4)	3744(5)	8109(5)	7374(8)	23(2)
N(5)	0	11888(7)	7500	27(4)
C(1)	623(6)	6726(5)	7545(10)	22(3)
C(2)	1284(6)	6412(6)	7688(10)	28(3)
C(3)	1716(6)	6867(6)	7600(10)	28(3)
C(4)	1363(6)	7499(6)	7440(9)	22(3)
C(5)	1629(6)	8107(6)	7332(9)	23(3)
C(6)	1308(6)	8703(6)	7279(9)	24(3)
C(7)	1581(6)	9330(6)	7163(9)	25(3)
C(8)	1140(7)	9798(6)	7240(10)	27(3)
C(9)	570(5)	9475(6)	7373(9)	19(3)
C(10)	0	9789(7)	7500	19(4)
C(11)	0	6413(9)	7500	29(4)
C(12)	0	5666(9)	7500	27(4)
C(13)	160(6)	5324(6)	6828(11)	33(3)
C(14)	155(6)	4647(6)	6865(11)	33(3)
C(15)	2359(5)	8109(6)	7319(9)	21(3)
C(16)	2520(6)	7833(6)	6584(9)	25(3)

C(17)	3203(6)	7830(6)	6621(10)	30(3)
C(18)	3594(6)	8363(6)	8076(10)	25(3)
C(19)	2919(6)	8370(6)	8068(9)	24(3)
C(20)	0	10509(7)	7500	26(4)
C(21)	-474(6)	10876(6)	6731(9)	25(3)
C(22)	-443(7)	11547(6)	6764(10)	27(3)
C(23)	3824(12)	6664(13)	10284(19)	106(9)
C(24)	4208(10)	6631(8)	9722(12)	57(5)
C(25)	2031(9)	4958(9)	10575(13)	55(5)
C(26)	1974(8)	4390(8)	9979(14)	62(5)

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.