

https://dspace.org/

Crystallographic investigation of n-Aminopyridinium perhalometallates

Lawrence, Estee

2012-02-06
http://hdl.handle.net/10539/11247

Downloaded from a DSpace repository. https://dspace.org/

Appendix B: Detailed Crystallographic and Structural Data

Crystallographic Data for Bis(2-aminopyridinium) tetrachlorozincate(II)

Table 1. Crystal data and structure refinement for 2ampZnCl.

Identification code	2ampZnCl	
Empirical formula	C10 H14 Cl4 N4 Zn	
Formula weight	1589.32	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 8.3104(6) Å	α= 90°.
	b = 14.1150(17) Å	β= 93.641(6)°.
	c = 13.8427(10) Å	γ = 90°.
Volume	1620.5(3) $Å^3$	
Z	1	
Density (calculated)	1.629 Mg/m^3	
Absorption coefficient	2.166 mm^{-1}	
F(000)	800	
Crystal size	0.6 x 0.4 x 0.1 mm^3	
Theta range for data collection	3.99 to 26.99°.	
Index ranges	-9<=h<=10, -18<=k<=17, -16<=l<=17	
Reflections collected	6308	
Independent reflections	1772 [R(int) = 0.0219]	
Completeness to theta = 25.00°	99.6 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1772 / 0 / 88	
Goodness-of-fit on F^2	1.050	
Final R indices [I>2sigma(I)]	R1 = 0.0213, wR2 = 0.0522	
R indices (all data)	R1 = 0.0290, wR2 = 0.0559	
Extinction coefficient	0.0153(6)	
Largest diff. peak and hole	0.295 and -0.236 e.$Å^{-3}$	

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

	x	y	z	U(eq)
C(1)	4124(2)	1933(1)	558(1)	46(1)
C(2)	3293(2)	583(1)	-377(2)	59(1)
C(3)	4153(3)	854(2)	-1117(2)	64(1)
C(4)	5048(2)	1691(2)	-1022(2)	62(1)
C(5)	5043(2)	2223(1)	-208(1)	53(1)
Cl(1)	2111(1)	1318(1)	3026(1)	61(1)
Cl(2)	999(1)	-533(1)	1344(1)	68(1)
N(1)	4023(2)	2426(1)	1365(1)	60(1)
N(2)	3298(2)	1115(1)	439(1)	51(1)
Zn(1)	0	394(1)	2500	45(1)

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

C(1)-N(1)	1.322(2)
C(1)-N(2)	1.348(2)
C(1)-C(5)	1.407(2)
C(2)-C(3)	1.342(3)
C(2)-N(2)	1.355(3)
C(2)-H(2)	0.9300
C(3)-C(4)	1.398(3)
C(3)-H(3)	0.9300
C(4)-C(5)	1.354(3)
C(4)-H(4)	0.9300
C(5)-H(5)	0.9300
Cl(1)-Zn(1)	2.2688(5)
Cl(2)-Zn(1)	2.2658(5)
N(1)-H(1A)	0.8601
N(1)-H(1B)	0.8600
N(2)-H(2A)	0.8601
Zn(1)-Cl(2)#1	2.2658(5)
Zn(1)-Cl(1)#1	2.2688(5)
N(1)-C(1)-N(2)	119.67(16)
N(1)-C(1)-C(5)	123.39(18)
N(2)-C(1)-C(5)	116.94(17)

C(3)-C(2)-N(2)	120.34(19)
C(3)-C(2)-H(2)	119.8
N(2)-C(2)-H(2)	119.8
C(2)-C(3)-C(4)	118.3(2)
C(2)-C(3)-H(3)	120.8
C(4)-C(3)-H(3)	120.8
C(5)-C(4)-C(3)	121.18(19)
C(5)-C(4)-H(4)	119.4
C(3)-C(4)-H(4)	119.4
C(4)-C(5)-C(1)	119.78(18)
C(4)-C(5)-H(5)	120.1
C(1)-C(5)-H(5)	120.1
C(1)-N(1)-H(1A)	120.0
C(1)-N(1)-H(1B)	120.1
H(1A)-N(1)-H(1B)	120.0
C(1)-N(2)-C(2)	123.45(16)
C(1)-N(2)-H(2A)	118.3
C(2)-N(2)-H(2A)	118.3
Cl(2)#1-Zn(1)-Cl(2)	109.41(3)
Cl(2)#1-Zn(1)-Cl(1)	114.57(2)
Cl(2)-Zn(1)-Cl(1)	104.39(2)
Cl(2)#1-Zn(1)-Cl(1)#1	104.39(2)
Cl(2)-Zn(1)-Cl(1)#1	114.57(2)
Cl(1)-Zn(1)-Cl(1)#1	109.81(3)

Symmetry transformations used to generate equivalent atoms:

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

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

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(1)	35(1)	52(1)	51(1)	10(1)	2(1)	6(1)
C(2)	52(1)	49(1)	75(1)	4(1)	2(1)	-1(1)
C(3)	66(1)	64(1)	61(1)	-2(1)	8(1)	-1(1)
C(4)	57(1)	73(1)	57(1)	10(1)	15(1)	-3(1)

C(5)	46(1)	56(1)	59(1)	11(1)	7(1)	-7(1)
Cl(1)	59(1)	54(1)	69(1)	-2(1)	6(1)	-14(1)
Cl(2)	66(1)	61(1)	79(1)	-24(1)	32(1)	-8(1)
N(1)	59(1)	65(1)	57(1)	4(1)	11(1)	-2(1)
N(2)	42(1)	52(1)	62(1)	14(1)	12(1)	1(1)
Zn(1)	44(1)	41(1)	52(1)	0	14(1)	0

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

	x	y	z	U(eq)
H(2)	2690	28	-423	71
H(3)	4155	493	-1679	76
H(4)	5658	1886	-1526	74
H(5)	5645	2778	-156	64
H(1A)	3434	2223	1810	72
H(1B)	4547	2949	1444	72
H(2A)	2744	921	904	62

Table 6. Torsion angles [°] for 2ampZnCl.

N(2)-C(2)-C(3)-C(4)	0.1(3)
C(2)-C(3)-C(4)-C(5)	-0.5(3)
C(3)-C(4)-C(5)-C(1)	0.0(3)
N(1)-C(1)-C(5)-C(4)	-178.18(18)
N(2)-C(1)-C(5)-C(4)	0.9(3)
N(1)-C(1)-N(2)-C(2)	177.78(17)
C(5)-C(1)-N(2)-C(2)	-1.3(3)
C(3)-C(2)-N(2)-C(1)	0.8(3)

Symmetry transformations used to generate equivalent atoms:

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

Table 7. Hydrogen bonds for 2ampZnCl [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...Cl(2)	0.86	2.43	3.276	166.9
N(1)-H(1B)...Cl(2)#2	0.86	2.47	3.316	169.4
N(2)-H(2A)...Cl(2)	0.86	2.61	3.305	139.3

Symmetry transformations used to generate equivalent atoms:

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

Crystallographic Data for Bis(2-aminopyridinium) tetrabromozincate(II)

Table 1. Crystal data and structure refinement for 2ampZnBr.

Identification code	2ampZnBr	
Empirical formula	C10 H14 Br4 N4 Zn	
Formula weight	517.21	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 15.3064(11) Å	α= 90°.
	b = 7.7064(6) Å	β= 92.313(6)°.
	c = 14.7911(10) Å	γ = 90°.
Volume	1743.3(2) $Å^3$	
Z	4	
Density (calculated)	1.971 Mg/m^3	
Absorption coefficient	10.551 mm^{-1}	
F(000)	968	
Crystal size	0.4 x 0.2 x 0.2 mm^3	
Theta range for data collection	3.91 to 27.00°.	
Index ranges	-18<=h<=19, -9<=k<=9, -15<=l<=18	
Reflections collected	6551	
Independent reflections	1895 [R(int) = 0.0249]	
Completeness to theta = 27.00°	99.6 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1895 / 0 / 88	
Goodness-of-fit on F^2	1.027	
Final R indices [I>2sigma(I)]	R1 = 0.0237, wR2 = 0.0593	
R indices (all data)	R1 = 0.0324, wR2 = 0.0612	
Extinction coefficient	0.00278(18)	
Largest diff. peak and hole0.837 and -0.699 e.$Å^{-3}$		

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

	x	y	z	U(eq)

C(1)	1897(2)	1149(4)	-975(2)	31(1)
C(2)	733(2)	1816(4)	1(2)	41(1)
C(3)	1142(2)	1001(4)	701(2)	41(1)
C(4)	1948(2)	211(4)	570(2)	38(1)
C(5)	2319(2)	277(4)	-249(2)	35(1)
Zn(1)	0	4480(1)	2500	27(1)
Br(1)	-1016(1)	2927(1)	1571(1)	47(1)
Br(2)	877(1)	6496(1)	1635(1)	39(1)
N(1)	2224(2)	1316(4)	-1784(2)	46(1)
N(2)	1115(2)	1867(3)	-816(2)	37(1)

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

C(1)-N(1)	1.323(4)
C(1)-N(2)	1.347(4)
C(1)-C(5)	1.402(4)
C(2)-C(3)	1.343(4)
C(2)-N(2)	1.365(4)
C(2)-H(2)	0.9300
C(3)-C(4)	1.396(4)
C(3)-H(3)	0.9300
C(4)-C(5)	1.360(4)
C(4)-H(4)	0.9300
C(5)-H(5)	0.9300
Zn(1)-Br(1)	2.3600(4)
Zn(1)-Br(1)#1	2.3600(4)
Zn(1)-Br(2)	2.4477(4)
Zn(1)-Br(2)#1	2.4477(4)
N(1)-H(1A)	0.8600
N(1)-H(1B)	0.8600
N(2)-H(2A)	0.8600
N(1)-C(1)-N(2)	119.3(3)
N(1)-C(1)-C(5)	124.0(3)
N(2)-C(1)-C(5)	116.7(3)
C(3)-C(2)-N(2)	119.6(3)
C(3)-C(2)-H(2)	120.2

N(2)-C(2)-H(2)	120.2
C(2)-C(3)-C(4)	118.9(3)
C(2)-C(3)-H(3)	120.5
C(4)-C(3)-H(3)	120.5
C(5)-C(4)-C(3)	120.7(3)
C(5)-C(4)-H(4)	119.7
C(3)-C(4)-H(4)	119.7
C(4)-C(5)-C(1)	120.2(3)
C(4)-C(5)-H(5)	119.9
C(1)-C(5)-H(5)	119.9
Br(1)-Zn(1)-Br(1)#1	119.03(3)
Br(1)-Zn(1)-Br(2)	112.314(12)
Br(1)#1-Zn(1)-Br(2)	105.327(11)
Br(1)-Zn(1)-Br(2)#1	105.327(11)
Br(1)#1-Zn(1)-Br(2)#1	112.314(12)
Br(2)-Zn(1)-Br(2)#1	101.21(2)
C(1)-N(1)-H(1A)	120.0
C(1)-N(1)-H(1B)	120.0
H(1A)-N(1)-H(1B)	120.0
C(1)-N(2)-C(2)	123.8(3)
C(1)-N(2)-H(2A)	118.1
C(2)-N(2)-H(2A)	118.1

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for 2ampZnBr. 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}
C(1)	25(1)	28(2)	41(2)	-6(1)	-2(1)	-5(1)
C(2)	27(2)	43(2)	52(2)	-3(2)	4(1)	2(1)
C(3)	40(2)	41(2)	43(2)	3(2)	7(1)	-4(2)
C(4)	37(2)	30(2)	45(2)	9(1)	-5(1)	-4(1)
C(5)	25(2)	27(2)	53(2)	-4(1)	-2(1)	1(1)
Zn(1)	21(1)	25(1)	35(1)	0	2(1)	0

Br(1)	28(1)	60(1)	52(1)	-23(1)	0(1)	-7(1)
Br(2)	29(1)	37(1)	51(1)	13(1)	10(1)	-1(1)
N(1)	37(2)	59(2)	41(2)	0(1)	3(1)	4(1)
N(2)	30(1)	41(2)	40(1)	2(1)	-4(1)	6(1)

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

	x	y	z	U(eq)
H(2)	194	2342	74	49
H(3)	892	963	1263	50
H(4)	2234	-367	1048	45
H(5)	2855	-258	-328	42
H(1A)	1939	1878	-2202	55
H(1B)	2723	863	-1891	55
H(2A)	840	2387	-1257	44

Table 6. Torsion angles [°] for 2ampZnBr.

N(2)-C(2)-C(3)-C(4)	-0.5(5)
C(2)-C(3)-C(4)-C(5)	0.6(5)
C(3)-C(4)-C(5)-C(1)	0.2(4)
N(1)-C(1)-C(5)-C(4)	178.0(3)
N(2)-C(1)-C(5)-C(4)	-1.2(4)
N(1)-C(1)-N(2)-C(2)	-177.8(3)
C(5)-C(1)-N(2)-C(2)	1.4(4)
C(3)-C(2)-N(2)-C(1)	-0.5(4)

Symmetry transformations used to generate equivalent atoms:
#1 -x,y,-z+1/2

Table 7. Hydrogen bonds for 2ampZnBr [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)

N(1)-H(1A)...Br(2)#2	0.86	2.64	3.490(3)	172.4
N(1)-H(1B)...Br(2)#3	0.86	2.82	3.625(3)	155.6
N(2)-H(2A)...Br(2)#4	0.86	2.80	3.471(2)	136.1

Symmetry transformations used to generate equivalent atoms:

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

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

Crystallographic Data for Bis(2-aminopyridinium) tetraiodozincate(II)

Table 1. Crystal data and structure refinement for 2ampZnI.

Identification code	2ampZnI	
Empirical formula	C10 H14 I4 N4 Zn	
Formula weight	655.08	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 35.2785(8) Å	α= 90°.
	b = 7.6246(2) Å	β= 108.5920(10)°.
	c = 22.6941(5) Å	γ = 90°.
Volume	5785.8(2) $Å^3$	
Z	20	
Density (calculated)	3.760 Mg/m^3	
Absorption coefficient	12.745 mm^{-1}	
F(000)	5720	
Crystal size	0.49 x 0.44 x 0.44 mm^3	
Theta range for data collection	1.22 to 27.00°.	
Index ranges	-43<=h<=44, -9<=k<=9, -28<=l<=28	
Reflections collected	31254	
Independent reflections	6315 [R(int) = 0.1510]	
Completeness to theta = 27.00°	100.0 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6315 / 0 / 259	
Goodness-of-fit on F^2	1.097	
Final R indices [I>2sigma(I)]	R1 = 0.0582, wR2 = 0.1516	
R indices (all data)	R1 = 0.0621, wR2 = 0.1566	
Extinction coefficient	0.00032(4)	
Largest diff. peak and hole	4.497 and -2.237 $e.Å^{-3}$	

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

	x	y	z	U(eq)

C(1)	2897(2)	11222(11)	5903(4)	36(2)
C(2)	2632(3)	10695(11)	6727(4)	40(2)
C(3)	2932(3)	11538(13)	7140(4)	51(2)
C(4)	3225(3)	12265(12)	6937(4)	47(2)
C(5)	3214(2)	12123(11)	6348(5)	40(2)
C(6)	3809(2)	8601(10)	6997(4)	33(2)
C(7)	3903(3)	9246(13)	8060(4)	46(2)
C(8)	3574(3)	8331(13)	8054(4)	44(2)
C(9)	3356(3)	7499(12)	7502(4)	41(2)
C(10)	3469(2)	7633(10)	6986(4)	34(2)
C(11)	-381(2)	1007(11)	5540(4)	37(2)
C(12)	316(3)	1074(15)	6087(5)	51(2)
C(13)	408(4)	1922(15)	5668(6)	58(3)
C(14)	106(4)	2487(12)	5166(5)	57(3)
C(15)	-306(4)	2036(13)	5080(4)	56(3)
N(1)	2865(3)	11104(13)	5317(5)	55(2)
N(2)	2619(2)	10539(9)	6123(3)	36(2)
N(3)	3926(2)	8772(12)	6511(4)	48(2)
N(4)	4016(2)	9343(10)	7541(4)	41(2)
N(5)	-745(3)	462(15)	5512(6)	69(3)
N(6)	-58(2)	603(10)	6044(3)	36(2)
Zn(1)	1672(1)	6770(1)	5625(1)	26(1)
Zn(2)	0	7401(2)	7500	26(1)
I(1)	1826(1)	8852(1)	4791(1)	33(1)
I(2)	2348(1)	5489(1)	6306(1)	34(1)
I(3)	1178(1)	4356(1)	5044(1)	36(1)
I(4)	1348(1)	8731(1)	6271(1)	40(1)
I(5)	-40(1)	5485(1)	6538(1)	39(1)
I(6)	652(1)	9253(1)	7812(1)	47(1)

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

C(1)-N(1)	1.303(13)
C(1)-N(2)	1.338(11)
C(1)-C(5)	1.423(12)
C(2)-C(3)	1.333(15)
C(2)-N(2)	1.362(12)

C(2)-H(2)	0.9300
C(3)-C(4)	1.377(16)
C(3)-H(3)	0.9300
C(4)-C(5)	1.329(14)
C(4)-H(4)	0.9300
C(5)-H(5)	0.9300
C(6)-N(3)	1.301(12)
C(6)-N(4)	1.341(11)
C(6)-C(10)	1.404(11)
C(7)-C(8)	1.352(15)
C(7)-N(4)	1.361(14)
C(7)-H(7)	0.9300
C(8)-C(9)	1.395(13)
C(8)-H(8)	0.9300
C(9)-C(10)	1.355(13)
C(9)-H(9)	0.9300
C(10)-H(10)	0.9300
C(11)-N(5)	1.332(12)
C(11)-N(6)	1.368(10)
C(11)-C(15)	1.396(15)
C(12)-C(13)	1.275(16)
C(12)-N(6)	1.340(12)
C(12)-H(12)	0.9300
C(13)-C(14)	1.360(18)
C(13)-H(13)	0.9300
C(14)-C(15)	1.443(17)
C(14)-H(14)	0.9300
C(15)-H(15)	0.9300
N(1)-H(1A)	0.8600
N(1)-H(1B)	0.8600
N(2)-H(2A)	0.8600
N(3)-H(3A)	0.8600
N(3)-H(3B)	0.8600
N(4)-H(4A)	0.8600
N(5)-H(5A)	0.8600
N(5)-H(5B)	0.8600
N(6)-H(6)	0.8600

Zn(1)-I(2)	2.5845(9)
Zn(1)-I(3)	2.5886(10)
Zn(1)-I(4)	2.6003(10)
Zn(1)-I(1)	2.6549(10)
Zn(2)-I(5)	2.5923(9)
Zn(2)-I(5)#1	2.5923(9)
Zn(2)-I(6)	2.5990(8)
Zn(2)-I(6)#1	2.5990(8)

N(1)-C(1)-N(2)	121.3(9)
N(1)-C(1)-C(5)	123.3(9)
N(2)-C(1)-C(5)	115.3(8)
C(3)-C(2)-N(2)	121.0(9)
C(3)-C(2)-H(2)	119.5
N(2)-C(2)-H(2)	119.5
C(2)-C(3)-C(4)	118.0(9)
C(2)-C(3)-H(3)	121.0
C(4)-C(3)-H(3)	121.0
C(5)-C(4)-C(3)	121.4(9)
C(5)-C(4)-H(4)	119.3
C(3)-C(4)-H(4)	119.3
C(4)-C(5)-C(1)	121.0(8)
C(4)-C(5)-H(5)	119.5
C(1)-C(5)-H(5)	119.5
N(3)-C(6)-N(4)	120.8(8)
N(3)-C(6)-C(10)	122.5(8)
N(4)-C(6)-C(10)	116.7(8)
C(8)-C(7)-N(4)	120.4(8)
C(8)-C(7)-H(7)	119.8
N(4)-C(7)-H(7)	119.8
C(7)-C(8)-C(9)	118.0(9)
C(7)-C(8)-H(8)	121.0
C(9)-C(8)-H(8)	121.0
C(10)-C(9)-C(8)	120.8(8)
C(10)-C(9)-H(9)	119.6
C(8)-C(9)-H(9)	119.6
C(9)-C(10)-C(6)	120.6(8)

C(9)-C(10)-H(10)	119.7
C(6)-C(10)-H(10)	119.7
N(5)-C(11)-N(6)	120.2(9)
N(5)-C(11)-C(15)	123.3(9)
N(6)-C(11)-C(15)	116.5(8)
C(13)-C(12)-N(6)	124.0(11)
C(13)-C(12)-H(12)	118.0
N(6)-C(12)-H(12)	118.0
C(12)-C(13)-C(14)	117.9(11)
C(12)-C(13)-H(13)	121.0
C(14)-C(13)-H(13)	121.0
C(13)-C(14)-C(15)	121.6(9)
C(13)-C(14)-H(14)	119.2
C(15)-C(14)-H(14)	119.2
C(11)-C(15)-C(14)	117.1(8)
C(11)-C(15)-H(15)	121.4
C(14)-C(15)-H(15)	121.4
C(1)-N(1)-H(1A)	120.0
C(1)-N(1)-H(1B)	120.0
H(1A)-N(1)-H(1B)	120.0
C(1)-N(2)-C(2)	123.2(8)
C(1)-N(2)-H(2A)	118.4
C(2)-N(2)-H(2A)	118.4
C(6)-N(3)-H(3A)	120.0
C(6)-N(3)-H(3B)	120.0
H(3A)-N(3)-H(3B)	120.0
C(6)-N(4)-C(7)	123.4(8)
C(6)-N(4)-H(4A)	118.3
C(7)-N(4)-H(4A)	118.3
C(11)-N(5)-H(5A)	120.0
C(11)-N(5)-H(5B)	120.0
H(5A)-N(5)-H(5B)	120.0
C(12)-N(6)-C(11)	122.6(8)
C(12)-N(6)-H(6)	118.7
C(11)-N(6)-H(6)	118.7
I(2)-Zn(1)-I(3)	112.30(4)
I(2)-Zn(1)-I(4)	111.53(3)

I(3)-Zn(1)-I(4)	110.52(3)
I(2)-Zn(1)-I(1)	107.06(3)
I(3)-Zn(1)-I(1)	108.64(3)
I(4)-Zn(1)-I(1)	106.52(3)
I(5)-Zn(2)-I(5)#1	111.38(5)
I(5)-Zn(2)-I(6)	109.96(2)
I(5)#1-Zn(2)-I(6)	105.732(19)
I(5)-Zn(2)-I(6)#1	105.732(19)
I(5)#1-Zn(2)-I(6)#1	109.96(2)
I(6)-Zn(2)-I(6)#1	114.18(5)

Symmetry transformations used to generate equivalent atoms:

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

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

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(1)	35(4)	31(4)	38(4)	5(3)	8(3)	6(3)
C(2)	48(5)	34(4)	42(5)	5(3)	20(4)	5(4)
C(3)	70(6)	37(5)	33(4)	3(4)	-3(4)	14(4)
C(4)	48(5)	32(4)	41(5)	-2(4)	-13(4)	11(4)
C(5)	27(4)	24(4)	65(6)	5(4)	7(4)	3(3)
C(6)	34(4)	23(3)	39(4)	2(3)	7(3)	4(3)
C(7)	48(5)	39(5)	37(5)	-4(4)	-6(4)	4(4)
C(8)	47(5)	47(5)	37(4)	7(4)	11(4)	13(4)
C(9)	39(4)	33(4)	49(5)	3(4)	10(4)	-1(3)
C(10)	31(4)	27(4)	36(4)	-3(3)	1(3)	-5(3)
C(11)	28(4)	38(4)	36(4)	-4(3)	-1(3)	9(3)
C(12)	33(4)	62(6)	57(6)	-14(5)	12(4)	-1(4)
C(13)	68(7)	56(6)	59(6)	-13(5)	37(6)	-11(5)
C(14)	109(9)	25(4)	61(6)	-3(4)	61(7)	-5(5)
C(15)	88(8)	42(5)	22(4)	-1(4)	-4(4)	38(5)
N(1)	55(5)	57(5)	56(5)	-10(4)	20(4)	-5(4)
N(2)	35(3)	35(4)	35(4)	-5(3)	5(3)	-4(3)
N(3)	41(4)	52(5)	50(5)	3(4)	14(3)	-3(3)

N(4)	29(3)	38(4)	42(4)	-2(3)	-6(3)	-4(3)
N(5)	29(4)	86(8)	86(8)	-8(6)	11(4)	-4(4)
N(6)	39(4)	40(4)	27(3)	4(3)	9(3)	4(3)
Zn(1)	22(1)	27(1)	27(1)	2(1)	4(1)	1(1)
Zn(2)	28(1)	27(1)	21(1)	0	3(1)	0
I(1)	31(1)	35(1)	29(1)	5(1)	4(1)	-9(1)
I(2)	26(1)	39(1)	34(1)	3(1)	3(1)	10(1)
I(3)	35(1)	36(1)	37(1)	-4(1)	11(1)	-13(1)
I(4)	43(1)	41(1)	32(1)	-2(1)	7(1)	17(1)
I(5)	45(1)	42(1)	26(1)	-9(1)	4(1)	7(1)
I(6)	37(1)	48(1)	51(1)	2(1)	5(1)	-18(1)

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

	x	y	z	U(eq)
H(2)	2429	10206	6853	48
H(3)	2942	11633	7554	61
H(4)	3435	12869	7217	56
H(5)	3418	12620	6225	48
H(7)	4054	9814	8422	55
H(8)	3495	8257	8407	53
H(9)	3131	6845	7488	50
H(10)	3319	7078	6621	41
H(12)	521	762	6445	61
H(13)	674	2147	5705	69
H(14)	165	3181	4870	68
H(15)	-512	2416	4735	67
H(1A)	2663	10579	5063	66
H(1B)	3047	11551	5184	66
H(2A)	2423	9974	5871	44
H(3A)	4137	9367	6535	57
H(3B)	3791	8290	6165	57
H(4A)	4231	9910	7562	49
H(5A)	-777	-144	5812	83

H(5B)	-947	718	5195	83
H(6)	-96	25	6346	43

Table 6. Torsion angles [°] for 2ampZnI.

N(2)-C(2)-C(3)-C(4)	0.8(14)
C(2)-C(3)-C(4)-C(5)	-0.6(14)
C(3)-C(4)-C(5)-C(1)	0.5(13)
N(1)-C(1)-C(5)-C(4)	177.3(9)
N(2)-C(1)-C(5)-C(4)	-0.5(12)
N(4)-C(7)-C(8)-C(9)	0.0(14)
C(7)-C(8)-C(9)-C(10)	-1.1(13)
C(8)-C(9)-C(10)-C(6)	0.5(13)
N(3)-C(6)-C(10)-C(9)	-179.4(8)
N(4)-C(6)-C(10)-C(9)	1.1(12)
N(6)-C(12)-C(13)-C(14)	4.7(17)
C(12)-C(13)-C(14)-C(15)	-4.7(15)
N(5)-C(11)-C(15)-C(14)	-178.4(9)
N(6)-C(11)-C(15)-C(14)	3.4(12)
C(13)-C(14)-C(15)-C(11)	0.6(14)
N(1)-C(1)-N(2)-C(2)	-177.2(9)
C(5)-C(1)-N(2)-C(2)	0.6(12)
C(3)-C(2)-N(2)-C(1)	-0.8(13)
N(3)-C(6)-N(4)-C(7)	178.3(8)
C(10)-C(6)-N(4)-C(7)	-2.3(12)
C(8)-C(7)-N(4)-C(6)	1.8(14)
C(13)-C(12)-N(6)-C(11)	-0.4(16)
N(5)-C(11)-N(6)-C(12)	178.0(10)
C(15)-C(11)-N(6)-C(12)	-3.7(12)

Symmetry transformations used to generate equivalent atoms:

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

Table 7. Hydrogen bonds for 2ampZnI [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)

N(1)-H(1A)...I(1)	0.86	3.11	3.876(10)	149.5
N(1)-H(1A)...I(2)#2	0.86	3.20	3.721(9)	121.4
N(1)-H(1B)...I(3)#2	0.86	3.02	3.735(9)	141.7
N(2)-H(2A)...I(1)	0.86	2.81	3.637(7)	162.6
N(3)-H(3A)...I(5)#3	0.86	3.02	3.856(8)	164.1
N(3)-H(3B)...I(1)#2	0.86	3.02	3.843(9)	161.8
N(3)-H(3B)...I(3)#2	0.86	3.31	3.714(9)	111.7
N(4)-H(4A)...I(5)#4	0.86	2.97	3.657(7)	138.6
N(5)-H(5A)...I(6)#5	0.86	3.05	3.826(13)	151.6
N(5)-H(5B)...I(1)#6	0.86	3.13	3.691(9)	125.2
N(5)-H(5B)...I(4)#6	0.86	3.20	3.975(12)	151.0
N(6)-H(6)...I(6)#5	0.86	3.20	3.960(7)	148.4

Symmetry transformations used to generate equivalent atoms:

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

#4 -x+1/2,y+1/2,-z+3/2 #5 -x,y-1,-z+3/2 #6 -x,-y+1,-z+1

Crystallographic Data for Bis(2-aminopyridinium) tetraiodocadmate(II)

Table 1. Crystal data and structure refinement for 2ampCdI.

Identification code	2ampCdI	
Empirical formula	C10 H14 Cd I4 N4	
Formula weight	752.20	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 8.2597(3) Å	α= 81.9790(10)°.
	b = 8.7807(3) Å	β= 82.1140(10)°.
	c = 15.5171(5) Å	γ = 63.1230(10)°.
Volume	990.50(6) $Å^3$	
Z	4	
Density (calculated)	5.044 Mg/m^3	
Absorption coefficient	14.628 mm^{-1}	
F(000)	1328	
Crystal size	0.42 x 0.40 x 0.28 mm^3	
Theta range for data collection	1.33 to 27.00°.	
Index ranges	-10<=h<=10, -11<=k<=11, -19<=l<=17	
Reflections collected	9045	
Independent reflections	4261 [R(int) = 0.1019]	
Completeness to theta = 27.00°	98.3 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4261 / 0 / 172	
Goodness-of-fit on F^2	1.079	
Final R indices [I>2sigma(I)]	R1 = 0.0466, wR2 = 0.1195	
R indices (all data)	R1 = 0.0520, wR2 = 0.1255	
Largest diff. peak and hole	2.357 and -1.727 e.$Å^{-3}$	

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

	x	y	z	U(eq)
C(1)	-5080(12)	9124(10)	1348(5)	45(2)

C(2)	-3338(16)	10659(13)	876(8)	62(3)
C(3)	-2096(13)	9362(15)	373(8)	63(3)
C(4)	-2375(12)	7918(13)	387(7)	57(2)
C(5)	-3870(11)	7793(10)	861(6)	46(2)
C(6)	3830(10)	6549(9)	4125(5)	35(2)
C(7)	1497(16)	6785(16)	5241(9)	82(4)
C(8)	1542(18)	8120(16)	5534(7)	83(5)
C(9)	2743(17)	8689(12)	5130(7)	68(3)
C(10)	3875(13)	7948(11)	4419(7)	50(2)
Cd(1)	688(1)	4831(1)	2320(1)	31(1)
I(1)	2806(1)	5542(1)	954(1)	43(1)
I(2)	-1552(1)	7624(1)	3225(1)	45(1)
I(3)	-1106(1)	3090(1)	1890(1)	40(1)
I(4)	3296(1)	2363(1)	3439(1)	38(1)
N(1)	-6558(12)	9062(11)	1812(6)	60(2)
N(2)	-4740(11)	10464(10)	1342(6)	53(2)
N(3)	4895(11)	5802(10)	3452(5)	54(2)
N(4)	2660(11)	5991(10)	4535(6)	51(2)

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

C(1)-N(2)	1.326(11)
C(1)-N(1)	1.349(12)
C(1)-C(5)	1.386(11)
C(2)-N(2)	1.345(14)
C(2)-C(3)	1.390(17)
C(2)-H(2)	0.9300
C(3)-C(4)	1.384(15)
C(3)-H(3)	0.9300
C(4)-C(5)	1.389(14)
C(4)-H(4)	0.9300
C(5)-H(5)	0.9300
C(6)-N(3)	1.308(10)
C(6)-N(4)	1.324(11)
C(6)-C(10)	1.386(11)
C(7)-C(8)	1.33(2)
C(7)-N(4)	1.388(14)

C(7)-H(7)	0.9300
C(8)-C(9)	1.348(19)
C(8)-H(8)	0.9300
C(9)-C(10)	1.373(14)
C(9)-H(9)	0.9300
C(10)-H(10)	0.9300
Cd(1)-I(1)	2.7470(7)
Cd(1)-I(2)	2.7481(6)
Cd(1)-I(3)	2.7534(7)
Cd(1)-I(4)	2.8473(7)
N(1)-H(1A)	0.8600
N(1)-H(1B)	0.8600
N(2)-H(2A)	0.8600
N(3)-H(3A)	0.8600
N(3)-H(3B)	0.8600
N(4)-H(4A)	0.8600

N(2)-C(1)-N(1)	121.0(8)
N(2)-C(1)-C(5)	117.8(8)
N(1)-C(1)-C(5)	121.2(8)
N(2)-C(2)-C(3)	119.2(9)
N(2)-C(2)-H(2)	120.4
C(3)-C(2)-H(2)	120.4
C(4)-C(3)-C(2)	117.3(10)
C(4)-C(3)-H(3)	121.3
C(2)-C(3)-H(3)	121.3
C(3)-C(4)-C(5)	121.4(8)
C(3)-C(4)-H(4)	119.3
C(5)-C(4)-H(4)	119.3
C(1)-C(5)-C(4)	119.2(8)
C(1)-C(5)-H(5)	120.4
C(4)-C(5)-H(5)	120.4
N(3)-C(6)-N(4)	120.3(8)
N(3)-C(6)-C(10)	121.3(8)
N(4)-C(6)-C(10)	118.4(8)
C(8)-C(7)-N(4)	120.9(11)
C(8)-C(7)-H(7)	119.5

N(4)-C(7)-H(7)	119.5
C(7)-C(8)-C(9)	118.6(9)
C(7)-C(8)-H(8)	120.7
C(9)-C(8)-H(8)	120.7
C(8)-C(9)-C(10)	121.4(10)
C(8)-C(9)-H(9)	119.3
C(10)-C(9)-H(9)	119.3
C(9)-C(10)-C(6)	119.5(9)
C(9)-C(10)-H(10)	120.2
C(6)-C(10)-H(10)	120.2
I(1)-Cd(1)-I(2)	113.34(2)
I(1)-Cd(1)-I(3)	114.12(2)
I(2)-Cd(1)-I(3)	112.98(2)
I(1)-Cd(1)-I(4)	103.22(2)
I(2)-Cd(1)-I(4)	108.77(2)
I(3)-Cd(1)-I(4)	103.24(2)
C(1)-N(1)-H(1A)	120.0
C(1)-N(1)-H(1B)	120.0
H(1A)-N(1)-H(1B)	120.0
C(1)-N(2)-C(2)	125.0(8)
C(1)-N(2)-H(2A)	117.5
C(2)-N(2)-H(2A)	117.5
C(6)-N(3)-H(3A)	120.0
C(6)-N(3)-H(3B)	120.0
H(3A)-N(3)-H(3B)	120.0
C(6)-N(4)-C(7)	121.1(9)
C(6)-N(4)-H(4A)	119.4
C(7)-N(4)-H(4A)	119.4

Symmetry transformations used to generate equivalent atoms:

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

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(1)	55(5)	35(4)	38(4)	-5(3)	-6(3)	-13(3)

C(2)	70(6)	48(5)	76(7)	9(5)	-29(5)	-31(5)
C(3)	40(5)	77(7)	68(7)	-8(5)	-7(4)	-23(5)
C(4)	37(4)	56(5)	70(6)	-32(5)	-2(4)	-7(4)
C(5)	42(4)	33(4)	58(5)	-15(3)	-9(4)	-8(3)
C(6)	38(4)	25(3)	37(4)	-3(3)	-9(3)	-7(3)
C(7)	56(6)	71(7)	72(8)	19(6)	26(6)	-3(5)
C(8)	80(8)	61(7)	39(5)	-1(5)	10(5)	25(6)
C(9)	93(8)	38(4)	53(6)	-19(4)	-21(6)	-3(5)
C(10)	51(5)	35(4)	67(6)	-11(4)	-1(4)	-20(4)
Cd(1)	32(1)	28(1)	30(1)	-8(1)	2(1)	-10(1)
I(1)	42(1)	47(1)	40(1)	-4(1)	7(1)	-23(1)
I(2)	44(1)	32(1)	49(1)	-19(1)	-1(1)	-6(1)
I(3)	45(1)	44(1)	38(1)	-13(1)	-1(1)	-23(1)
I(4)	43(1)	29(1)	37(1)	-4(1)	-8(1)	-9(1)
N(1)	63(5)	49(4)	54(5)	-11(3)	14(4)	-17(4)
N(2)	54(4)	41(4)	60(5)	-18(3)	-5(4)	-13(3)
N(3)	58(5)	46(4)	54(4)	-23(3)	13(4)	-19(3)
N(4)	56(4)	41(4)	63(5)	-6(3)	-5(4)	-26(3)

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

	x	y	z	U(eq)
H(2)	-3201	11650	891	74
H(3)	-1116	9460	40	75
H(4)	-1543	7012	73	68
H(5)	-4056	6827	851	55
H(7)	674	6380	5513	98
H(8)	762	8648	6008	100
H(9)	2805	9604	5338	81
H(10)	4667	8382	4136	60
H(1A)	-7297	9900	2110	72
H(1B)	-6761	8185	1810	72
H(2A)	-5472	11270	1661	64
H(3A)	4836	4945	3275	65

H(3B)	5653	6169	3187	65
H(4A)	2620	5121	4362	62

Table 6. Torsion angles [°] for 2ampCdI.

N(2)-C(2)-C(3)-C(4)	-0.5(16)
C(2)-C(3)-C(4)-C(5)	2.2(16)
N(2)-C(1)-C(5)-C(4)	-0.4(13)
N(1)-C(1)-C(5)-C(4)	179.4(9)
C(3)-C(4)-C(5)-C(1)	-1.8(15)
N(4)-C(7)-C(8)-C(9)	0.1(18)
C(7)-C(8)-C(9)-C(10)	1.5(17)
C(8)-C(9)-C(10)-C(6)	-2.2(16)
N(3)-C(6)-C(10)-C(9)	-179.6(9)
N(4)-C(6)-C(10)-C(9)	1.3(13)
N(1)-C(1)-N(2)-C(2)	-177.6(10)
C(5)-C(1)-N(2)-C(2)	2.3(14)
C(3)-C(2)-N(2)-C(1)	-1.8(16)
N(3)-C(6)-N(4)-C(7)	-178.8(10)
C(10)-C(6)-N(4)-C(7)	0.3(13)
C(8)-C(7)-N(4)-C(6)	-1.0(17)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for 2ampCdI[Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...I(3)#1	0.86	3.15	3.823(8)	136.9
N(1)-H(1B)...I(1)#2	0.86	3.00	3.796(9)	154.4
N(2)-H(2A)...I(4)#1	0.86	2.94	3.690(8)	146.6
N(3)-H(3A)...I(4)	0.86	3.03	3.807(8)	151.4
N(3)-H(3B)...I(2)#3	0.86	3.11	3.886(9)	150.7
N(4)-H(4A)...I(4)	0.86	2.78	3.615(8)	163.0

Symmetry transformations used to generate equivalent atoms:

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

Crystallographic Data for Bis(2-aminopyridinium) tetrachloromercurate(II)

Table 1. Crystal data and structure refinement for 2ampHgCl.

Identification code	2ampHgCl	
Empirical formula	C10 H14 Cl4 Hg N4	
Formula weight	474.59	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 15.0298(8) Å	α= 90°.
	b = 7.4925(4) Å	β= 92.229(5)°.
	c = 14.7577(9) Å	γ = 90°.
Volume	1660.62(16) $Å^3$	
Z	4	
Density (calculated)	1.898 Mg/m^3	
Absorption coefficient	9.884 mm^{-1}	
F(000)	880	
Crystal size	0.4 x 0.4 x 0.3 mm^3	
Theta range for data collection	3.80 to 26.99°.	
Index ranges	-14<=h<=19, -9<=k<=9, -18<=l<=18	
Reflections collected	6193	
Independent reflections	1813 [R(int) = 0.0241]	
Completeness to theta = 26.99°	99.7 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1813 / 0 / 87	
Goodness-of-fit on F^2	1.061	
Final R indices [I>2sigma(I)]	R1 = 0.0177, wR2 = 0.0424	
R indices (all data)	R1 = 0.0193, wR2 = 0.0427	
Largest diff. peak and hole	0.524 and -0.609 $e.Å^{-3}$	

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

	x	y	z	U(eq)
Cl(1)	5948(1)	-1586(1)	1720(1)	48(1)

Cl(2)	3940(1)	1943(1)	1405(1)	53(1)
C(1)	6914(2)	3898(4)	-1070(2)	36(1)
C(2)	5724(2)	3129(4)	-133(3)	45(1)
C(3)	6104(2)	3962(4)	585(3)	47(1)
C(4)	6925(2)	4813(4)	486(2)	40(1)
C(5)	7327(2)	4782(4)	-325(2)	35(1)
Hg(1)	5000	880(1)	2500	36(1)
N(1)	7284(2)	3804(4)	-1871(2)	51(1)
N(2)	6122(2)	3113(3)	-936(2)	43(1)

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

Cl(1)-Hg(1)	2.6260(8)
Cl(2)-Hg(1)	2.3631(8)
C(1)-N(1)	1.327(4)
C(1)-N(2)	1.350(4)
C(1)-C(5)	1.406(4)
C(2)-C(3)	1.339(5)
C(2)-N(2)	1.348(5)
C(2)-H(2)	0.9300
C(3)-C(4)	1.401(5)
C(3)-H(3)	0.9300
C(4)-C(5)	1.362(5)
C(4)-H(4)	0.9300
C(5)-H(5)	0.9300
Hg(1)-Cl(2)#1	2.3631(8)
Hg(1)-Cl(1)#1	2.6260(8)
N(1)-H(1A)	0.8600
N(1)-H(1B)	0.8600
N(2)-H(2A)	0.8600

N(1)-C(1)-N(2)	120.7(3)
N(1)-C(1)-C(5)	122.2(3)
N(2)-C(1)-C(5)	117.1(3)
C(3)-C(2)-N(2)	120.6(3)
C(3)-C(2)-H(2)	119.7
N(2)-C(2)-H(2)	119.7

C(2)-C(3)-C(4)	118.7(3)
C(2)-C(3)-H(3)	120.6
C(4)-C(3)-H(3)	120.6
C(5)-C(4)-C(3)	120.4(3)
C(5)-C(4)-H(4)	119.8
C(3)-C(4)-H(4)	119.8
C(4)-C(5)-C(1)	119.9(3)
C(4)-C(5)-H(5)	120.1
C(1)-C(5)-H(5)	120.1
Cl(2)#1-Hg(1)-Cl(2)	140.59(5)
Cl(2)#1-Hg(1)-Cl(1)	100.03(3)
Cl(2)-Hg(1)-Cl(1)	107.48(3)
Cl(2)#1-Hg(1)-Cl(1)#1	107.48(3)
Cl(2)-Hg(1)-Cl(1)#1	100.03(3)
Cl(1)-Hg(1)-Cl(1)#1	90.58(4)
C(1)-N(1)-H(1A)	120.0
C(1)-N(1)-H(1B)	120.0
H(1A)-N(1)-H(1B)	120.0
C(2)-N(2)-C(1)	123.3(3)
C(2)-N(2)-H(2A)	118.4
C(1)-N(2)-H(2A)	118.4

Symmetry transformations used to generate equivalent atoms:

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

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

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl(1)	43(1)	45(1)	55(1)	-15(1)	1(1)	10(1)
Cl(2)	39(1)	59(1)	60(1)	20(1)	-9(1)	4(1)
C(1)	36(2)	30(1)	40(2)	1(1)	-7(1)	5(1)
C(2)	35(2)	40(2)	61(2)	3(2)	-3(1)	-3(1)
C(3)	48(2)	47(2)	47(2)	3(2)	8(2)	9(2)
C(4)	43(2)	32(2)	45(2)	-7(1)	-8(1)	7(1)
C(5)	29(1)	26(1)	50(2)	1(1)	-5(1)	1(1)

Hg(1)	30(1)	36(1)	43(1)	0	-4(1)	0
N(1)	58(2)	57(2)	39(2)	-4(1)	0(1)	-1(1)
N(2)	42(1)	36(1)	48(2)	-5(1)	-13(1)	-3(1)

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

	x	y	z	U(eq)
H(2)	5180	2555	-77	55
H(3)	5829	3976	1138	57
H(4)	7197	5403	977	48
H(5)	7873	5344	-387	42
H(1A)	7019	3239	-2310	62
H(1B)	7790	4308	-1949	62
H(2A)	5857	2576	-1386	51

Table 6. Torsion angles [°] for 2ampHgCl.

N(2)-C(2)-C(3)-C(4)	-0.2(5)
C(2)-C(3)-C(4)-C(5)	-0.3(5)
C(3)-C(4)-C(5)-C(1)	0.3(5)
N(1)-C(1)-C(5)-C(4)	-178.9(3)
N(2)-C(1)-C(5)-C(4)	0.2(4)
C(3)-C(2)-N(2)-C(1)	0.7(5)
N(1)-C(1)-N(2)-C(2)	178.4(3)
C(5)-C(1)-N(2)-C(2)	-0.7(4)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,y,-z+1/2

Table 7. Hydrogen bonds for 2ampHgCl [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...Cl(1)#2	0.86	2.45	3.286(3)	164.9

N(1)-H(1B)...Cl(1)#3	0.86	2.56	3.377(4)	158.0
N(2)-H(2A)...Cl(1)#4	0.86	2.84	3.470(3)	131.8
N(2)-H(2A)...Cl(1)#2	0.86	2.90	3.642(3)	145.6

Symmetry transformations used to generate equivalent atoms:

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

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

Crystallographic Data for Bis(2-aminopyridinium) tetrabromomercurate(II)

Table 1. Crystal data and structure refinement for 2ampHgBr.

Identification code	2ampHgBr	
Empirical formula	C10 H14 Br4 Hg N4	
Formula weight	538.45	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 6.9651(5) Å	α= 90.000(5)°.
	b = 17.7646(13) Å	β= 97.856(4)°.
	c = 14.3009(10) Å	γ = 90.000(4)°.
Volume	1752.9(2) $Å^3$	
Z	4	
Density (calculated)	2.040 Mg/m^3	
Absorption coefficient	13.616 mm^{-1}	
F(000)	964	
Crystal size	0.56 x 0.40 x 0.26 mm^3	
Theta range for data collection	1.84 to 27.00°.	
Index ranges	-7<=h<=8, -22<=k<=22, -18<=l<=18	
Reflections collected	14967	
Independent reflections	3820 [R(int) = 0.2769]	
Completeness to theta = 27.00°	100.0 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3820 / 0 / 173	
Goodness-of-fit on F^2	0.929	
Final R indices [I>2sigma(I)]	R1 = 0.0735, wR2 = 0.1684	
R indices (all data)	R1 = 0.1173, wR2 = 0.1947	
Extinction coefficient	0.0046(5)	
Largest diff. peak and hole	2.746 and -2.269 e.$Å^{-3}$	

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

	x	y	z	U(eq)

C(1)	9070(20)	3117(9)	4045(10)	52(4)
C(2)	11940(30)	3833(11)	4018(14)	76(6)
C(3)	12320(20)	3420(11)	3255(12)	63(4)
C(4)	11120(30)	2874(11)	2894(11)	66(5)
C(5)	9420(20)	2701(9)	3285(10)	56(4)
C(6)	-1560(20)	4148(9)	1383(11)	57(4)
C(7)	1260(30)	4835(11)	1358(13)	74(5)
C(8)	1830(30)	4433(11)	681(13)	74(5)
C(9)	640(30)	3825(10)	319(12)	66(5)
C(10)	-1040(30)	3689(9)	691(12)	62(4)
N(1)	7410(20)	2989(9)	4467(11)	77(4)
N(2)	10275(19)	3671(7)	4387(8)	52(3)
N(3)	-3190(20)	4063(10)	1759(12)	90(5)
N(4)	-380(20)	4716(8)	1679(9)	61(4)
Br(1)	5267(3)	6293(1)	1375(1)	63(1)
Hg(1)	4944(1)	6206(1)	3159(1)	49(1)
Br(2)	1218(2)	6039(1)	3378(1)	59(1)
Br(3)	5898(2)	7438(1)	4047(1)	56(1)
Br(4)	6605(3)	4982(1)	3836(1)	65(1)

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

C(1)-N(2)	1.343(19)
C(1)-C(5)	1.364(19)
C(1)-N(1)	1.394(19)
C(2)-C(3)	1.37(3)
C(2)-N(2)	1.37(2)
C(2)-H(2)	0.9300
C(3)-C(4)	1.34(2)
C(3)-H(3)	0.9300
C(4)-C(5)	1.41(2)
C(4)-H(4)	0.9300
C(5)-H(5)	0.9300
C(6)-N(3)	1.33(2)
C(6)-N(4)	1.33(2)
C(6)-C(10)	1.37(2)
C(7)-N(4)	1.31(2)

C(7)-C(8)	1.31(2)
C(7)-H(7)	0.9300
C(8)-C(9)	1.42(2)
C(8)-H(8)	0.9300
C(9)-C(10)	1.37(3)
C(9)-H(9)	0.9300
C(10)-H(10)	0.9300
N(1)-H(1A)	0.8600
N(1)-H(1B)	0.8600
N(2)-H(2A)	0.8600
N(3)-H(3A)	0.8600
N(3)-H(3B)	0.8600
N(4)-H(4A)	0.8600
Br(1)-Hg(1)	2.5962(15)
Hg(1)-Br(3)	2.5732(16)
Hg(1)-Br(4)	2.5874(17)
Hg(1)-Br(2)	2.6726(16)

N(2)-C(1)-C(5)	121.0(14)
N(2)-C(1)-N(1)	118.5(14)
C(5)-C(1)-N(1)	120.5(16)
C(3)-C(2)-N(2)	117.3(18)
C(3)-C(2)-H(2)	121.3
N(2)-C(2)-H(2)	121.3
C(4)-C(3)-C(2)	121.3(16)
C(4)-C(3)-H(3)	119.3
C(2)-C(3)-H(3)	119.3
C(3)-C(4)-C(5)	121.2(15)
C(3)-C(4)-H(4)	119.4
C(5)-C(4)-H(4)	119.4
C(1)-C(5)-C(4)	116.8(15)
C(1)-C(5)-H(5)	121.6
C(4)-C(5)-H(5)	121.6
N(3)-C(6)-N(4)	118.7(16)
N(3)-C(6)-C(10)	123.5(16)
N(4)-C(6)-C(10)	117.8(16)
N(4)-C(7)-C(8)	122.8(18)

N(4)-C(7)-H(7)	118.6
C(8)-C(7)-H(7)	118.6
C(7)-C(8)-C(9)	117.6(18)
C(7)-C(8)-H(8)	121.2
C(9)-C(8)-H(8)	121.2
C(10)-C(9)-C(8)	118.8(16)
C(10)-C(9)-H(9)	120.6
C(8)-C(9)-H(9)	120.6
C(9)-C(10)-C(6)	120.1(15)
C(9)-C(10)-H(10)	120.0
C(6)-C(10)-H(10)	120.0
C(1)-N(1)-H(1A)	120.0
C(1)-N(1)-H(1B)	120.0
H(1A)-N(1)-H(1B)	120.0
C(1)-N(2)-C(2)	122.4(14)
C(1)-N(2)-H(2A)	118.8
C(2)-N(2)-H(2A)	118.8
C(6)-N(3)-H(3A)	120.0
C(6)-N(3)-H(3B)	120.0
H(3A)-N(3)-H(3B)	120.0
C(7)-N(4)-C(6)	122.8(16)
C(7)-N(4)-H(4A)	118.6
C(6)-N(4)-H(4A)	118.6
Br(3)-Hg(1)-Br(4)	117.28(6)
Br(3)-Hg(1)-Br(1)	112.52(6)
Br(4)-Hg(1)-Br(1)	108.90(6)
Br(3)-Hg(1)-Br(2)	103.03(5)
Br(4)-Hg(1)-Br(2)	104.77(6)
Br(1)-Hg(1)-Br(2)	109.73(5)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for 2ampHgBr. 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}

C(1)	57(9)	57(10)	45(7)	12(8)	22(7)	14(8)
C(2)	68(12)	85(15)	77(11)	36(11)	19(10)	-10(9)
C(3)	60(10)	69(13)	64(10)	16(10)	22(9)	6(9)
C(4)	82(12)	74(13)	48(8)	0(9)	33(9)	8(10)
C(5)	72(10)	38(9)	56(9)	-12(7)	6(8)	16(7)
C(6)	58(10)	52(10)	57(9)	-2(8)	-11(8)	2(8)
C(7)	65(12)	85(14)	66(10)	-5(11)	-7(9)	-16(10)
C(8)	53(10)	104(16)	60(10)	3(11)	-5(8)	22(10)
C(9)	63(11)	81(13)	55(9)	-10(9)	15(8)	19(9)
C(10)	63(10)	49(10)	69(10)	-12(9)	-8(9)	-3(8)
N(1)	71(9)	80(11)	88(10)	3(9)	41(8)	8(8)
N(2)	71(9)	47(8)	40(6)	-1(6)	12(6)	-7(6)
N(3)	62(10)	102(13)	109(13)	-16(11)	25(10)	-13(9)
N(4)	72(9)	52(9)	60(7)	-24(7)	7(7)	-9(7)
Br(1)	70(1)	80(1)	43(1)	-3(1)	20(1)	-8(1)
Hg(1)	55(1)	48(1)	47(1)	-4(1)	14(1)	0(1)
Br(2)	49(1)	77(1)	53(1)	-7(1)	19(1)	-9(1)
Br(3)	64(1)	47(1)	60(1)	-9(1)	24(1)	-7(1)
Br(4)	65(1)	53(1)	80(1)	11(1)	17(1)	9(1)

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

	x	y	z	U(eq)
H(2)	12784	4209	4274	91
H(3)	13428	3521	2983	76
H(4)	11414	2603	2376	79
H(5)	8581	2321	3037	67
H(7)	2054	5222	1623	88
H(8)	2980	4543	445	88
H(9)	988	3524	-163	79
H(10)	-1821	3284	473	74
H(1A)	7178	3262	4937	93
H(1B)	6614	2637	4259	93
H(2A)	9993	3934	4855	63

H(3A)	-3468	4371	2185	108
H(3B)	-3969	3699	1577	108
H(4A)	-718	5018	2099	74

Table 6. Torsion angles [°] for 2ampHgBr.

N(2)-C(2)-C(3)-C(4)	-1(3)
C(2)-C(3)-C(4)-C(5)	0(3)
N(2)-C(1)-C(5)-C(4)	1(2)
N(1)-C(1)-C(5)-C(4)	179.3(15)
C(3)-C(4)-C(5)-C(1)	0(2)
N(4)-C(7)-C(8)-C(9)	-3(3)
C(7)-C(8)-C(9)-C(10)	0(3)
C(8)-C(9)-C(10)-C(6)	2(3)
N(3)-C(6)-C(10)-C(9)	178.1(18)
N(4)-C(6)-C(10)-C(9)	-1(2)
C(5)-C(1)-N(2)-C(2)	-2(2)
N(1)-C(1)-N(2)-C(2)	179.6(15)
C(3)-C(2)-N(2)-C(1)	2(2)
C(8)-C(7)-N(4)-C(6)	4(3)
N(3)-C(6)-N(4)-C(7)	179.0(17)
C(10)-C(6)-N(4)-C(7)	-2(3)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for 2ampHgBr [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...Br(2)#1	0.86	2.80	3.547(17)	145.6
N(1)-H(1A)...Br(3)#1	0.86	3.02	3.424(13)	111.3
N(1)-H(1B)...Br(1)#2	0.86	2.81	3.659(16)	167.7
N(2)-H(2A)...Br(2)#1	0.86	2.77	3.531(12)	148.1
N(3)-H(3A)...Br(4)#3	0.86	2.59	3.409(18)	158.8
N(3)-H(3B)...Br(3)#4	0.86	2.70	3.552(17)	170.8
N(4)-H(4A)...Br(2)	0.86	2.79	3.453(12)	135.2

Symmetry transformations used to generate equivalent atoms:

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

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

Crystallographic Data for Bis(2-aminopyridinium) tetraiodomercuate(II)

Table 1. Crystal data and structure refinement for 2ampHgI.

Identification code	2ampHgI	
Empirical formula	C10 H14 Hg I4 N4	
Formula weight	840.39	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.1780(4) Å	α= 82.124(2)°.
	b = 8.7740(4) Å	β= 82.261(2)°.
	c = 15.4043(7) Å	γ = 63.168(2)°.
Volume	973.69(8) $Å^3$	
Z	4	
Density (calculated)	5.733 Mg/m^3	
Absorption coefficient	28.445 mm^{-1}	
F(000)	1456	
Crystal size	0.72 x 0.55 x 0.47 mm^3	
Theta range for data collection	1.34 to 27.00°.	
Index ranges	-10<=h<=10, -11<=k<=11, -19<=l<=19	
Reflections collected	17620	
Independent reflections	4260 [R(int) = 0.2016]	
Completeness to theta = 27.00°	100.0 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4260 / 0 / 172	
Goodness-of-fit on F^2	1.051	
Final R indices [I>2sigma(I)]	R1 = 0.0763, wR2 = 0.1965	
R indices (all data)	R1 = 0.0807, wR2 = 0.2046	
Largest diff. peak and hole	6.434 and -5.970 $e.Å^{-3}$	

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

	x	y	z	U(eq)
C(1)	4912(19)	9129(16)	1354(9)	34(3)

C(2)	6690(30)	10620(20)	868(13)	55(4)
C(3)	7910(20)	9340(30)	404(12)	52(4)
C(4)	7640(19)	7900(20)	394(10)	43(3)
C(5)	6170(20)	7761(18)	893(10)	40(3)
C(6)	3819(18)	6546(17)	4126(8)	31(2)
C(7)	1500(30)	6680(20)	5233(12)	58(5)
C(8)	1490(30)	8070(30)	5542(11)	70(7)
C(9)	2680(30)	8680(20)	5118(12)	55(4)
C(10)	3810(20)	7990(19)	4411(10)	41(3)
Hg	666(1)	4858(1)	2298(1)	29(1)
I(1)	2870(1)	5511(1)	941(1)	34(1)
I(2)	-1524(1)	7647(1)	3212(1)	38(1)
I(3)	-1096(1)	3054(1)	1887(1)	32(1)
I(4)	3349(1)	2331(1)	3445(1)	31(1)
N(1)	3440(20)	9010(20)	1847(9)	55(4)
N(2)	5240(20)	10491(16)	1327(9)	46(3)
N(3)	4914(18)	5777(17)	3440(9)	42(3)
N(4)	2677(17)	5956(18)	4541(9)	45(3)

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

C(1)-N(2)	1.334(19)
C(1)-N(1)	1.37(2)
C(1)-C(5)	1.388(19)
C(2)-N(2)	1.34(2)
C(2)-C(3)	1.33(3)
C(2)-H(2)	0.9300
C(3)-C(4)	1.38(2)
C(3)-H(3)	0.9300
C(4)-C(5)	1.38(2)
C(4)-H(4)	0.9300
C(5)-H(5)	0.9300
C(6)-N(4)	1.317(18)
C(6)-N(3)	1.330(18)
C(6)-C(10)	1.394(19)
C(7)-N(4)	1.35(2)
C(7)-C(8)	1.37(3)

C(7)-H(7)	0.9300
C(8)-C(9)	1.37(3)
C(8)-H(8)	0.9300
C(9)-C(10)	1.35(2)
C(9)-H(9)	0.9300
C(10)-H(10)	0.9300
Hg-I(2)	2.7356(9)
Hg-I(1)	2.7447(9)
Hg-I(3)	2.7497(9)
Hg-I(4)	2.9031(9)
N(1)-H(1A)	0.8600
N(1)-H(1B)	0.8600
N(2)-H(2A)	0.8600
N(3)-H(3A)	0.8600
N(3)-H(3B)	0.8600
N(4)-H(4A)	0.8600

N(2)-C(1)-N(1)	122.7(14)
N(2)-C(1)-C(5)	117.6(14)
N(1)-C(1)-C(5)	119.6(14)
N(2)-C(2)-C(3)	120.4(16)
N(2)-C(2)-H(2)	119.8
C(3)-C(2)-H(2)	119.8
C(2)-C(3)-C(4)	118.9(16)
C(2)-C(3)-H(3)	120.5
C(4)-C(3)-H(3)	120.5
C(5)-C(4)-C(3)	120.0(14)
C(5)-C(4)-H(4)	120.0
C(3)-C(4)-H(4)	120.0
C(4)-C(5)-C(1)	119.2(14)
C(4)-C(5)-H(5)	120.4
C(1)-C(5)-H(5)	120.4
N(4)-C(6)-N(3)	119.5(13)
N(4)-C(6)-C(10)	118.6(14)
N(3)-C(6)-C(10)	121.9(13)
N(4)-C(7)-C(8)	119.5(17)
N(4)-C(7)-H(7)	120.2

C(8)-C(7)-H(7)	120.2
C(9)-C(8)-C(7)	117.4(16)
C(9)-C(8)-H(8)	121.3
C(7)-C(8)-H(8)	121.3
C(10)-C(9)-C(8)	122.7(18)
C(10)-C(9)-H(9)	118.6
C(8)-C(9)-H(9)	118.6
C(9)-C(10)-C(6)	118.3(15)
C(9)-C(10)-H(10)	120.8
C(6)-C(10)-H(10)	120.8
I(2)-Hg-I(1)	113.45(3)
I(2)-Hg-I(3)	114.61(3)
I(1)-Hg-I(3)	114.93(3)
I(2)-Hg-I(4)	108.34(3)
I(1)-Hg-I(4)	102.01(3)
I(3)-Hg-I(4)	101.69(3)
C(1)-N(1)-H(1A)	120.0
C(1)-N(1)-H(1B)	120.0
H(1A)-N(1)-H(1B)	120.0
C(1)-N(2)-C(2)	123.7(15)
C(1)-N(2)-H(2A)	118.2
C(2)-N(2)-H(2A)	118.2
C(6)-N(3)-H(3A)	120.0
C(6)-N(3)-H(3B)	120.0
H(3A)-N(3)-H(3B)	120.0
C(6)-N(4)-C(7)	123.3(15)
C(6)-N(4)-H(4A)	118.3
C(7)-N(4)-H(4A)	118.3

Symmetry transformations used to generate equivalent atoms:

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

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(1)	36(7)	22(6)	37(7)	2(5)	-12(5)	-5(5)

C(2)	54(10)	45(9)	76(12)	15(8)	-27(9)	-30(8)
C(3)	39(8)	62(11)	56(10)	-11(8)	-9(7)	-21(8)
C(4)	25(6)	43(8)	53(9)	-16(6)	-10(6)	-4(6)
C(5)	41(7)	24(6)	49(8)	-15(6)	-19(6)	-3(6)
C(6)	36(6)	31(6)	28(6)	3(5)	-10(5)	-18(5)
C(7)	55(10)	41(9)	56(10)	12(7)	12(8)	-11(8)
C(8)	64(12)	59(12)	35(8)	5(7)	8(7)	14(9)
C(9)	63(11)	36(8)	59(10)	-16(7)	-19(8)	-8(8)
C(10)	40(7)	36(7)	53(8)	-12(6)	-1(6)	-22(6)
Hg	27(1)	28(1)	30(1)	-7(1)	3(1)	-11(1)
I(1)	31(1)	39(1)	36(1)	-2(1)	4(1)	-21(1)
I(2)	37(1)	29(1)	41(1)	-15(1)	-5(1)	-4(1)
I(3)	32(1)	37(1)	33(1)	-10(1)	-4(1)	-19(1)
I(4)	35(1)	24(1)	32(1)	-1(1)	-11(1)	-9(1)
N(1)	54(8)	42(8)	48(8)	-6(6)	7(6)	-5(6)
N(2)	50(8)	30(6)	53(8)	-12(5)	-10(6)	-10(6)
N(3)	40(6)	32(6)	50(7)	-11(5)	4(5)	-13(5)
N(4)	33(6)	44(7)	64(8)	-2(6)	-15(6)	-20(6)

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

	x	y	z	U(eq)
H(2)	6850	11602	872	66
H(3)	8934	9419	92	62
H(4)	8445	7024	50	51
H(5)	6030	6761	921	48
H(7)	695	6231	5497	69
H(8)	696	8587	6021	84
H(9)	2714	9614	5327	67
H(10)	4575	8462	4120	49
H(1A)	2690	9828	2156	66
H(1B)	3274	8107	1848	66
H(2A)	4485	11334	1620	55
H(3A)	4873	4902	3270	51

H(3B)	5664	6156	3165	51
H(4A)	2683	5067	4362	54

Table 6. Torsion angles [°] for 2ampHgI.

N(2)-C(2)-C(3)-C(4)	1(3)
C(2)-C(3)-C(4)-C(5)	-3(2)
C(3)-C(4)-C(5)-C(1)	4(2)
N(2)-C(1)-C(5)-C(4)	-4(2)
N(1)-C(1)-C(5)-C(4)	179.6(14)
N(4)-C(7)-C(8)-C(9)	1(3)
C(7)-C(8)-C(9)-C(10)	1(3)
C(8)-C(9)-C(10)-C(6)	-3(3)
N(4)-C(6)-C(10)-C(9)	2(2)
N(3)-C(6)-C(10)-C(9)	-179.2(15)
N(1)-C(1)-N(2)-C(2)	178.3(15)
C(5)-C(1)-N(2)-C(2)	1(2)
C(3)-C(2)-N(2)-C(1)	0(3)
N(3)-C(6)-N(4)-C(7)	-178.8(15)
C(10)-C(6)-N(4)-C(7)	0(2)
C(8)-C(7)-N(4)-C(6)	-1(3)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for 2ampHgI [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(3)-H(3A)...I(4)	0.86	3.00	3.777(13)	151.5
N(3)-H(3B)...I(2)#1	0.86	3.13	3.896(14)	149.6
N(4)-H(4A)...I(4)	0.86	2.76	3.593(14)	164.8

Symmetry transformations used to generate equivalent atoms:

#1 x+1,y,z

Crystallographic Data for Bis(3-aminopyridinium) tetrachlorozincate(II)

Table 1. Crystal data and structure refinement for 3ampZnCl.

Identification code	3ampZnCl	
Empirical formula	C10 H14 Cl4 N4 Zn	
Formula weight	339.37	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 6.8921(5) Å	α= 99.008(6)°.
	b = 8.4555(6) Å	β= 89.573(5)°.
	c = 13.8003(9) Å	γ = 100.194(6)°.
Volume	781.60(9) $Å^3$	
Z	4	
Density (calculated)	2.884 Mg/m^3	
Absorption coefficient	4.450 mm^{-1}	
F(000)	680	
Crystal size	0.2 x 0.2 x 0.2 mm^3	
Theta range for data collection	3.97 to 27.00°.	
Index ranges	-7<=h<=8, -10<=k<=10, -17<=l<=17	
Reflections collected	6269	
Independent reflections	3381 [R(int) = 0.0187]	
Completeness to theta = 27.00°	99.3 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3381 / 0 / 172	
Goodness-of-fit on F^2	0.977	
Final R indices [I>2sigma(I)]	R1 = 0.0217, wR2 = 0.0444	
R indices (all data)	R1 = 0.0301, wR2 = 0.0455	
Largest diff. peak and hole	0.320 and -0.272 $e.Å^{-3}$	

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

	x	y	z	U(eq)
C(1)	23660(3)	2990(2)	4843(1)	32(1)

C(2)	24451(3)	2918(2)	5756(1)	34(1)
C(3)	27026(3)	1643(2)	5028(2)	39(1)
C(4)	26303(3)	1703(2)	4126(2)	39(1)
C(5)	24665(3)	2364(2)	4021(1)	33(1)
C(6)	24081(2)	2011(2)	1366(1)	22(1)
C(7)	25378(2)	3085(2)	898(1)	23(1)
C(8)	27659(3)	1284(2)	677(1)	28(1)
C(9)	26435(3)	193(2)	1139(1)	29(1)
C(10)	24660(2)	540(2)	1476(1)	26(1)
Cl(1)	31293(1)	3406(1)	9372(1)	25(1)
Cl(2)	30995(1)	5321(1)	7065(1)	32(1)
Cl(3)	26577(1)	3441(1)	8126(1)	26(1)
Cl(4)	29870(1)	783(1)	6948(1)	33(1)
Zn(1)	29840(1)	3242(1)	7899(1)	23(1)
N(1)	22045(2)	3650(2)	4777(1)	48(1)
N(2)	26060(2)	2270(2)	5811(1)	38(1)
N(3)	22331(2)	2368(2)	1704(1)	35(1)
N(4)	27082(2)	2685(2)	577(1)	25(1)

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

C(1)-N(1)	1.340(2)
C(1)-C(2)	1.391(2)
C(1)-C(5)	1.407(2)
C(2)-N(2)	1.329(2)
C(2)-H(2)	0.9300
C(3)-N(2)	1.351(2)
C(3)-C(4)	1.356(3)
C(3)-H(3)	0.9300
C(4)-C(5)	1.363(2)
C(4)-H(4)	0.9300
C(5)-H(5)	0.9300
C(6)-N(3)	1.357(2)
C(6)-C(7)	1.388(2)
C(6)-C(10)	1.402(2)
C(7)-N(4)	1.333(2)
C(7)-H(7)	0.9300

C(8)-N(4)	1.341(2)
C(8)-C(9)	1.368(2)
C(8)-H(8)	0.9300
C(9)-C(10)	1.369(2)
C(9)-H(9)	0.9300
C(10)-H(10)	0.9300
Cl(1)-Zn(1)	2.2473(5)
Cl(2)-Zn(1)	2.2742(5)
Cl(3)-Zn(1)	2.3001(5)
Cl(4)-Zn(1)	2.2813(5)
N(1)-H(1A)	0.8600
N(1)-H(1B)	0.8600
N(2)-H(2A)	0.8600
N(3)-H(3A)	0.8600
N(3)-H(3B)	0.8600
N(4)-H(4A)	0.8600

N(1)-C(1)-C(2)	120.45(17)
N(1)-C(1)-C(5)	123.30(17)
C(2)-C(1)-C(5)	116.24(17)
N(2)-C(2)-C(1)	119.78(17)
N(2)-C(2)-H(2)	120.1
C(1)-C(2)-H(2)	120.1
N(2)-C(3)-C(4)	117.17(18)
N(2)-C(3)-H(3)	121.4
C(4)-C(3)-H(3)	121.4
C(3)-C(4)-C(5)	120.96(18)
C(3)-C(4)-H(4)	119.5
C(5)-C(4)-H(4)	119.5
C(4)-C(5)-C(1)	121.17(17)
C(4)-C(5)-H(5)	119.4
C(1)-C(5)-H(5)	119.4
N(3)-C(6)-C(7)	121.61(15)
N(3)-C(6)-C(10)	121.28(15)
C(7)-C(6)-C(10)	117.11(15)
N(4)-C(7)-C(6)	119.60(15)
N(4)-C(7)-H(7)	120.2

C(6)-C(7)-H(7)	120.2
N(4)-C(8)-C(9)	118.40(16)
N(4)-C(8)-H(8)	120.8
C(9)-C(8)-H(8)	120.8
C(8)-C(9)-C(10)	119.82(16)
C(8)-C(9)-H(9)	120.1
C(10)-C(9)-H(9)	120.1
C(9)-C(10)-C(6)	120.98(15)
C(9)-C(10)-H(10)	119.5
C(6)-C(10)-H(10)	119.5
Cl(1)-Zn(1)-Cl(2)	115.004(18)
Cl(1)-Zn(1)-Cl(4)	111.586(18)
Cl(2)-Zn(1)-Cl(4)	111.051(18)
Cl(1)-Zn(1)-Cl(3)	108.686(17)
Cl(2)-Zn(1)-Cl(3)	103.445(17)
Cl(4)-Zn(1)-Cl(3)	106.364(18)
C(1)-N(1)-H(1A)	120.0
C(1)-N(1)-H(1B)	120.0
H(1A)-N(1)-H(1B)	120.0
C(2)-N(2)-C(3)	124.68(16)
C(2)-N(2)-H(2A)	117.7
C(3)-N(2)-H(2A)	117.7
C(6)-N(3)-H(3A)	120.0
C(6)-N(3)-H(3B)	120.0
H(3A)-N(3)-H(3B)	120.0
C(7)-N(4)-C(8)	124.07(15)
C(7)-N(4)-H(4A)	118.0
C(8)-N(4)-H(4A)	118.0

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for 3ampZnCl. 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}
C(1)	29(1)	33(1)	31(1)	5(1)	-1(1)	1(1)

C(2)	37(1)	40(1)	23(1)	5(1)	1(1)	-3(1)
C(3)	33(1)	38(1)	48(1)	16(1)	2(1)	-1(1)
C(4)	37(1)	39(1)	41(1)	7(1)	10(1)	4(1)
C(5)	38(1)	36(1)	22(1)	4(1)	0(1)	3(1)
C(6)	23(1)	23(1)	20(1)	3(1)	-2(1)	5(1)
C(7)	28(1)	19(1)	25(1)	5(1)	-1(1)	6(1)
C(8)	27(1)	29(1)	29(1)	0(1)	0(1)	9(1)
C(9)	38(1)	23(1)	30(1)	4(1)	-1(1)	13(1)
C(10)	33(1)	20(1)	25(1)	6(1)	1(1)	2(1)
Cl(1)	27(1)	25(1)	26(1)	6(1)	2(1)	8(1)
Cl(2)	38(1)	30(1)	31(1)	12(1)	11(1)	7(1)
Cl(3)	25(1)	24(1)	30(1)	4(1)	6(1)	8(1)
Cl(4)	38(1)	26(1)	35(1)	-2(1)	7(1)	10(1)
Zn(1)	26(1)	20(1)	23(1)	4(1)	5(1)	6(1)
N(1)	46(1)	66(1)	35(1)	2(1)	1(1)	23(1)
N(2)	37(1)	45(1)	32(1)	16(1)	-5(1)	-1(1)
N(3)	30(1)	35(1)	48(1)	19(1)	11(1)	15(1)
N(4)	25(1)	24(1)	25(1)	5(1)	3(1)	1(1)

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

	x	y	z	U(eq)
H(2)	23856	3322	6327	41
H(3)	28140	1191	5105	47
H(4)	26933	1286	3570	47
H(5)	24205	2402	3395	39
H(7)	25059	4077	810	28
H(8)	28862	1060	437	34
H(9)	26806	-782	1223	35
H(10)	23827	-211	1784	31
H(1A)	21491	4033	5301	58
H(1B)	21562	3691	4210	58
H(2A)	26520	2247	6385	46
H(3A)	22002	3277	1632	42

H(3B)	21550	1684	1992	42
H(4A)	27859	3368	288	30

Table 6. Torsion angles [°] for 3ampZnCl.

N(1)-C(1)-C(2)-N(2)	-179.56(17)
C(5)-C(1)-C(2)-N(2)	-0.6(2)
N(2)-C(3)-C(4)-C(5)	-0.2(3)
C(3)-C(4)-C(5)-C(1)	-0.7(3)
N(1)-C(1)-C(5)-C(4)	-179.96(18)
C(2)-C(1)-C(5)-C(4)	1.1(3)
N(3)-C(6)-C(7)-N(4)	-179.97(15)
C(10)-C(6)-C(7)-N(4)	0.2(2)
N(4)-C(8)-C(9)-C(10)	0.7(2)
C(8)-C(9)-C(10)-C(6)	-0.7(3)
N(3)-C(6)-C(10)-C(9)	-179.58(15)
C(7)-C(6)-C(10)-C(9)	0.2(2)
C(1)-C(2)-N(2)-C(3)	-0.4(3)
C(4)-C(3)-N(2)-C(2)	0.8(3)
C(6)-C(7)-N(4)-C(8)	-0.2(2)
C(9)-C(8)-N(4)-C(7)	-0.2(2)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for 3ampZnCl [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...Cl(2)#3	0.86	2.55	3.379	161.4
N(2)-H(2A)...Cl(3)	0.86	2.45	3.197	145.0
N(4)-H(4A)...Cl(1)#1	0.86	2.65	3.286	131.4
N(4)-H(4A)...Cl(1)#2	0.86	2.67	3.343	135.9

Symmetry transformations used to generate equivalent atoms:

#1 -x+6,-y+1,-z+1 #2 x, y, z-1 #3 x-1, y, z

Crystallographic Data for Bis(3-ammoniopyridinium) tetrabromozincate(II) monohydrate

Table 1. Crystal data and structure refinement for 3ampZnBr·H2O.

Identification code	3ampZnBr·H2O	
Empirical formula	C5 H10 Br4 N2 O Zn	
Formula weight	448.44	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 7.017(2) Å	α= 90°.
	b = 23.380(7) Å	β= 94.299(17)°.
	c = 7.766(2) Å	γ = 90°.
Volume	1270.5(6) Å3	
Z	6	
Density (calculated)	3.517 Mg/m3	
Absorption coefficient	21.688 mm-1	
F(000)	1228	
Crystal size	0.98 x 0.50 x 0.40 mm3	
Theta range for data collection	1.74 to 27.00°.	
Index ranges	-8<=h<=8, -29<=k<=29, -8<=l<=9	
Reflections collected	12195	
Independent reflections	2759 [R(int) = 0.5444]	
Completeness to theta = 27.00°	100.0 %	
Refinement method	Full-matrix least-squares on F2	
Data / restraints / parameters	2759 / 0 / 122	
Goodness-of-fit on F2	1.073	
Final R indices [I>2sigma(I)]	R1 = 0.1048, wR2 = 0.2113	
R indices (all data)	R1 = 0.1298, wR2 = 0.2427	
Extinction coefficient	0.028(3)	
Largest diff. peak and hole1.517 and -2.292 e.Å-3		

Table 2. Atomic coordinates (x 104) and equivalent isotropic displacement parameters (Å2x 103) for 3ampZnBr·H2O. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)

C(1)	-6309(14)	6265(5)	5520(10)	33(2)
C(2)	-4663(14)	6222(5)	4663(12)	37(2)
C(3)	-4386(17)	7202(6)	4618(13)	48(3)
C(4)	-6046(18)	7267(6)	5453(17)	51(3)
C(5)	-7001(16)	6787(5)	5917(14)	43(3)
N(1)	-7248(13)	5728(4)	5988(11)	42(2)
N(2)	-3787(12)	6683(4)	4251(9)	39(2)
O(1)	-4175(13)	5045(4)	7114(12)	57(2)
Zn(1)	340(2)	6208(1)	772(1)	36(1)
Br(1)	3697(2)	6109(1)	328(1)	43(1)
Br(2)	-1301(2)	6170(1)	-2048(1)	45(1)
Br(4)	-714(2)	5500(1)	2754(1)	46(1)
Br(5)	-261(2)	7111(1)	2098(1)	48(1)

Table 3. Bond lengths [Å] and angles [°] for 3ampZnBr·H2O.

C(1)-C(5)	1.357(15)
C(1)-C(2)	1.379(12)
C(1)-N(1)	1.475(13)
C(2)-N(2)	1.294(14)
C(2)-H(2)	0.9300
C(3)-N(2)	1.322(16)
C(3)-C(4)	1.383(17)
C(3)-H(3)	0.9300
C(4)-C(5)	1.369(17)
C(4)-H(4)	0.9300
C(5)-H(5)	0.9300
N(1)-H(1A)	0.8900
N(1)-H(1B)	0.8900
N(1)-H(1C)	0.8900
N(2)-H(2A)	0.8600
O(1)-H(1D)	1.013(9)
O(1)-H(1E)	0.954(9)
Zn(1)-Br(2)	2.3981(16)
Zn(1)-Br(5)	2.4015(18)
Zn(1)-Br(4)	2.4146(16)
Zn(1)-Br(1)	2.4163(16)

C(5)-C(1)-C(2)	120.1(10)
C(5)-C(1)-N(1)	122.3(8)
C(2)-C(1)-N(1)	117.5(10)
N(2)-C(2)-C(1)	119.3(10)
N(2)-C(2)-H(2)	120.4
C(1)-C(2)-H(2)	120.4
N(2)-C(3)-C(4)	119.6(12)
N(2)-C(3)-H(3)	120.2
C(4)-C(3)-H(3)	120.2
C(5)-C(4)-C(3)	118.7(12)
C(5)-C(4)-H(4)	120.7
C(3)-C(4)-H(4)	120.7
C(1)-C(5)-C(4)	119.1(10)
C(1)-C(5)-H(5)	120.4
C(4)-C(5)-H(5)	120.4
C(1)-N(1)-H(1A)	109.5
C(1)-N(1)-H(1B)	109.5
H(1A)-N(1)-H(1B)	109.5
C(1)-N(1)-H(1C)	109.5
H(1A)-N(1)-H(1C)	109.5
H(1B)-N(1)-H(1C)	109.5
C(2)-N(2)-C(3)	123.2(9)
C(2)-N(2)-H(2A)	118.4
C(3)-N(2)-H(2A)	118.4
H(1D)-O(1)-H(1E)	115.7(9)
Br(2)-Zn(1)-Br(5)	109.65(6)
Br(2)-Zn(1)-Br(4)	114.08(6)
Br(5)-Zn(1)-Br(4)	104.91(6)
Br(2)-Zn(1)-Br(1)	105.84(5)
Br(5)-Zn(1)-Br(1)	110.44(6)
Br(4)-Zn(1)-Br(1)	111.97(6)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 \times 10^3$)for 3ampZnBr·H2O. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(1)	40(5)	50(6)	11(3)	3(4)	5(3)	-4(5)
C(2)	34(4)	56(7)	21(4)	-3(4)	7(4)	4(5)
C(3)	53(6)	65(9)	26(4)	-2(5)	5(4)	-13(6)
C(4)	63(7)	41(7)	51(6)	3(5)	18(6)	0(6)
C(5)	41(5)	47(7)	44(5)	3(5)	17(4)	7(5)
N(1)	46(5)	42(6)	37(4)	6(4)	9(4)	-3(4)
N(2)	42(4)	54(6)	20(3)	-5(4)	7(3)	-6(4)
O(1)	63(5)	52(6)	55(5)	6(4)	-10(4)	-5(5)
Zn(1)	40(1)	48(1)	19(1)	3(1)	9(1)	-2(1)
Br(1)	39(1)	62(1)	29(1)	4(1)	9(1)	2(1)
Br(2)	44(1)	69(1)	24(1)	2(1)	3(1)	-7(1)
Br(4)	50(1)	53(1)	36(1)	13(1)	15(1)	-2(1)
Br(5)	54(1)	49(1)	43(1)	-5(1)	25(1)	-7(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 3ampZnBr·H2O.

	x	y	z	U(eq)
H(2)	-4187	5865	4385	44
H(3)	-3695	7522	4316	58
H(4)	-6504	7629	5694	61
H(5)	-8109	6818	6497	52
H(1A)	-7993	5795	6844	62
H(1B)	-6364	5471	6326	62
H(1C)	-7955	5595	5075	62
H(2A)	-2766	6651	3712	46
H(1D)	-4030	4719	7973	2000(2000)
H(1E)	-3355	5365	7353	1400(1500)

Table 6. Torsion angles [°] for 3ampZnBr·H2O.

C(5)-C(1)-C(2)-N(2)	0.2(14)
N(1)-C(1)-C(2)-N(2)	-179.2(9)

N(2)-C(3)-C(4)-C(5)	1.6(17)
C(2)-C(1)-C(5)-C(4)	0.1(16)
N(1)-C(1)-C(5)-C(4)	179.5(10)
C(3)-C(4)-C(5)-C(1)	-1.1(17)
C(1)-C(2)-N(2)-C(3)	0.4(14)
C(4)-C(3)-N(2)-C(2)	-1.3(16)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for 3ampZnBr·H2O [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...Br(2)#1	0.89	2.68	3.483(9)	150.2
N(1)-H(1A)...Br(1)#1	0.89	2.96	3.502(9)	120.6
N(1)-H(1B)...O(1)	0.89	1.89	2.772(14)	169.1
N(1)-H(1C)...Br(4)#2	0.89	2.55	3.404(10)	160.0
N(2)-H(2A)...Br(5)	0.86	2.48	3.246(8)	148.9
O(1)-H(1D)...Br(1)#3	1.013(9)	2.3453(13)	3.353(9)	173.1(6)
O(1)-H(1E)...Br(2)#4	0.954(9)	2.3946(13)	3.348(9)	179.9(7)

Symmetry transformations used to generate equivalent atoms:

#1 x-1,y,z+1 #2 x-1,y,z #3 -x,-y+1,-z+1 #4 x,y,z+1

Crystallographic Data for Bis(3-ammoniopyridinium) tetraiodomercurate(II) monohydrate

Table 1. Crystal data and structure refinement for 3ampHgI ·H2O.

Identification code	3ampHgI ·H2O	
Empirical formula	C4.97 H7.70 Hg0.98 I3.96 N1.86 O	
Formula weight	840.39	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 8.3752(2) Å	α= 90°.
	b = 14.7432(3) Å	β= 93.663(2)°.
	c = 12.1260(3) Å	γ = 90°.
Volume	1494.23(6) Å3	
Z	4	
Density (calculated)	3.736 Mg/m3	
Absorption coefficient	18.536 mm-1	
F(000)	1456	
Crystal size	0.5 x 0.5 x 0.2 mm3	
Theta range for data collection	3.64 to 27.00°.	
Index ranges	-10<=h<=10, -18<=k<=15, -15<=l<=15	
Reflections collected	11030	
Independent reflections	3261 [R(int) = 0.0380]	
Completeness to theta = 27.00°	99.7 %	
Refinement method	Full-matrix least-squares on F2	
Data / restraints / parameters	3261 / 0 / 142	
Goodness-of-fit on F2	1.076	
Final R indices [I>2sigma(I)]	R1 = 0.0402, wR2 = 0.1191	
R indices (all data)	R1 = 0.0487, wR2 = 0.1300	
Largest diff. peak and hole3.091 and -2.458 e.Å-3		

Table 2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å² x 10³) for 3ampHgI ·H2O. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(1)	7930(11)	9151(6)	2751(8)	27(3)

C(2)	6982(12)	8517(7)	3184(9)	30(4)
C(3)	7099(11)	9323(6)	4886(8)	25(3)
C(4)	8019(12)	9996(7)	4434(9)	29(3)
C(5)	8447(11)	9915(6)	3366(9)	28(3)
Hg(1)	6853(1)	7548(1)	8481(1)	29(1)
I(1)	9651(1)	8539(1)	8966(1)	24(1)
I(2)	5213(1)	7464(1)	10423(1)	27(1)
I(3)	7572(1)	5869(1)	7581(1)	27(1)
I(4)	4590(1)	8319(1)	6982(1)	32(1)
N(1)	8348(11)	9050(6)	1622(7)	24(3)
N(2)	6612(9)	8630(5)	4258(7)	20(3)
O(1)	8429(10)	5282(7)	4559(9)	50(4)

Table 3. Bond lengths [Å] and angles [°] for 3ampHgI ·H2O.

C(1)-C(2)	1.354(14)
C(1)-C(5)	1.403(14)
C(1)-N(1)	1.443(12)
C(2)-N(2)	1.368(14)
C(2)-H(2)	0.9300
C(3)-N(2)	1.324(13)
C(3)-C(4)	1.390(14)
C(3)-H(3)	0.9300
C(4)-C(5)	1.371(14)
C(4)-H(4)	0.9300
C(5)-H(5)	0.9300
Hg(1)-I(4)	2.7834(8)
Hg(1)-I(3)	2.7868(7)
Hg(1)-I(1)	2.7914(7)
Hg(1)-I(2)	2.8043(8)
N(1)-H(1A)	0.8900
N(1)-H(1B)	0.8900
N(1)-H(1C)	0.8900
N(2)-H(2A)	0.8600
O(1)-H(1D)	0.831(10)
O(1)-H(1E)	0.814(11)

C(2)-C(1)-C(5)	121.2(9)
C(2)-C(1)-N(1)	118.7(9)
C(5)-C(1)-N(1)	120.1(9)
C(1)-C(2)-N(2)	117.3(9)
C(1)-C(2)-H(2)	121.4
N(2)-C(2)-H(2)	121.4
N(2)-C(3)-C(4)	118.9(9)
N(2)-C(3)-H(3)	120.6
C(4)-C(3)-H(3)	120.6
C(5)-C(4)-C(3)	119.7(10)
C(5)-C(4)-H(4)	120.2
C(3)-C(4)-H(4)	120.2
C(4)-C(5)-C(1)	118.8(9)
C(4)-C(5)-H(5)	120.6
C(1)-C(5)-H(5)	120.6
I(4)-Hg(1)-I(3)	105.17(2)
I(4)-Hg(1)-I(1)	116.85(2)
I(3)-Hg(1)-I(1)	110.37(2)
I(4)-Hg(1)-I(2)	102.52(2)
I(3)-Hg(1)-I(2)	114.77(2)
I(1)-Hg(1)-I(2)	107.22(2)
C(1)-N(1)-H(1A)	109.5
C(1)-N(1)-H(1B)	109.5
H(1A)-N(1)-H(1B)	109.5
C(1)-N(1)-H(1C)	109.5
H(1A)-N(1)-H(1C)	109.5
H(1B)-N(1)-H(1C)	109.5
C(3)-N(2)-C(2)	124.2(8)
C(3)-N(2)-H(2A)	117.9
C(2)-N(2)-H(2A)	117.9
H(1D)-O(1)-H(1E)	111.2(11)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 \times 10^3$)for 3ampHgI ·H2O. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(1)	27(5)	29(5)	23(6)	-2(4)	0(4)	9(4)
C(2)	24(5)	32(6)	34(7)	2(4)	-3(4)	-1(4)
C(3)	28(5)	24(5)	21(6)	-2(4)	1(4)	0(4)
C(4)	37(6)	22(5)	28(6)	-2(4)	3(4)	-1(4)
C(5)	29(5)	20(5)	34(6)	1(4)	4(4)	3(4)
Hg(1)	24(1)	27(1)	35(1)	-3(1)	-2(1)	0(1)
I(1)	22(1)	20(1)	31(1)	0(1)	2(1)	-3(1)
I(2)	22(1)	28(1)	30(1)	-4(1)	-1(1)	-2(1)
I(3)	29(1)	21(1)	32(1)	-2(1)	4(1)	-1(1)
I(4)	25(1)	29(1)	41(1)	10(1)	-4(1)	-1(1)
N(1)	31(5)	21(5)	20(5)	1(3)	1(3)	2(3)
N(2)	18(4)	19(4)	22(5)	7(3)	0(3)	-3(3)
O(1)	38(5)	51(6)	58(7)	-9(4)	-9(4)	1(4)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 3ampHgI ·H2O.

	x	y	z	U(eq)
H(2)	6599	8024	2768	36
H(3)	6831	9360	5617	30
H(4)	8342	10499	4853	35
H(5)	9069	10357	3054	33
H(1A)	7962	8527	1353	36
H(1B)	9408	9054	1598	36
H(1C)	7932	9506	1218	36
H(2A)	6025	8225	4543	24
H(1D)	8771	5791	4398	74
H(1E)	7921	5304	5108	74

Table 6. Torsion angles [°] for 3ampHgI ·H2O.

C(5)-C(1)-C(2)-N(2)	-2.9(14)
N(1)-C(1)-C(2)-N(2)	179.7(8)

N(2)-C(3)-C(4)-C(5)	-2.2(15)
C(3)-C(4)-C(5)-C(1)	0.5(15)
C(2)-C(1)-C(5)-C(4)	2.1(15)
N(1)-C(1)-C(5)-C(4)	179.4(9)
C(4)-C(3)-N(2)-C(2)	1.4(15)
C(1)-C(2)-N(2)-C(3)	1.1(15)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for 3ampHgI ·H2O [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...I(2)#1	0.89	2.95	3.740(9)	149.0
N(1)-H(1A)...I(4)#2	0.89	3.12	3.662(9)	121.6
N(1)-H(1B)...I(3)#2	0.89	2.84	3.654(9)	153.3
N(1)-H(1C)...O(1)#3	0.89	1.83	2.701(13)	164.5
N(2)-H(2A)...I(1)#4	0.86	2.91	3.602(8)	138.7
N(2)-H(2A)...I(4)	0.86	3.27	3.834(8)	126.0
O(1)-H(1D)...I(2)#2	0.831(10)	3.07	3.765(9)	142.6(7)
O(1)-H(1D)...I(4)#2	0.831(10)	3.32	3.918(11)	131.1(7)
O(1)-H(1E)...I(3)	0.814(11)	3.14	3.877(11)	151.3(6)

Symmetry transformations used to generate equivalent atoms:

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

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

Crystallographic Data for Bis(4-aminopyridinium) tetrachlorozincate(II)

Table 1. Crystal data and structure refinement for 4ampZnCl.

Identification code	4ampZnCl	
Empirical formula	C10 H14 Cl4 N4 Zn	
Formula weight	339.37	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 7.1525(3) Å	α= 90°.
	b = 14.9902(12) Å	β= 90°.
	c = 14.9993(2) Å	γ = 90°.
Volume	1608.19(15) $Å^3$	
Z	4	
Density (calculated)	1.402 Mg/m^3	
Absorption coefficient	2.163 mm^{-1}	
F(000)	680	
Crystal size	0.4 x 0.4 x 0.3 mm^3	
Theta range for data collection	3.84 to 28.00°.	
Index ranges	-9<=h<=9, -17<=k<=19, -17<=l<=19	
Reflections collected	13762	
Independent reflections	3869 [R(int) = 0.0211]	
Completeness to theta = 28.00°	99.6 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3869 / 0 / 172	
Goodness-of-fit on F^2	1.348	
Final R indices [I>2sigma(I)]	R1 = 0.0962, wR2 = 0.2277	
R indices (all data)	R1 = 0.0987, wR2 = 0.2286	
Absolute structure parameter	0.05(5)	
Largest diff. peak and hole	0.992 and -1.087 e.$Å^{-3}$	

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

	x	y	z	U(eq)

C(1)	2830(20)	13084(9)	4244(9)	40(3)
C(2)	2710(20)	14032(9)	4387(11)	43(3)
C(3)	2380(20)	14330(10)	5258(9)	44(3)
C(4)	2260(20)	12900(10)	5838(12)	48(4)
C(5)	2410(20)	12527(9)	4918(10)	44(3)
C(6)	4688(15)	11835(8)	9451(7)	24(2)
C(7)	4707(16)	11923(8)	8474(7)	28(2)
C(8)	4950(20)	12763(12)	8130(10)	49(4)
C(9)	5210(20)	13397(9)	9560(13)	52(4)
C(10)	4982(16)	12608(8)	9969(8)	28(2)
Cl(5)	2904(5)	10526(2)	6327(2)	41(1)
N(1)	3075(19)	12731(8)	3477(7)	46(3)
N(2)	2113(19)	13776(9)	5932(9)	51(3)
N(3)	4510(20)	11023(7)	9795(8)	46(3)
N(4)	5238(16)	13503(8)	8721(9)	44(3)
Cl(1)	3399(5)	9368(2)	8440(2)	41(1)
Cl(3)	-669(6)	10922(2)	8182(2)	45(1)
Cl(4)	-521(5)	8794(2)	7011(2)	41(1)
Zn(1)	1261(2)	9962(1)	7490(1)	26(1)

Table 3. Bond lengths [Å] and angles [°] for 4ampZnCl.

C(1)-N(1)	1.278(16)
C(1)-C(5)	1.345(19)
C(1)-C(2)	1.441(19)
C(2)-C(3)	1.40(2)
C(2)-H(2A)	0.9300
C(3)-N(2)	1.32(2)
C(3)-H(3)	0.9300
C(4)-N(2)	1.325(19)
C(4)-C(5)	1.49(2)
C(4)-H(4)	0.9300
C(5)-H(5)	0.9300
C(6)-N(3)	1.329(15)
C(6)-C(10)	1.411(16)
C(6)-C(7)	1.471(14)
C(7)-C(8)	1.37(2)

C(7)-H(7)	0.9300
C(8)-N(4)	1.43(2)
C(8)-H(8)	0.9300
C(9)-N(4)	1.27(2)
C(9)-C(10)	1.343(18)
C(9)-H(9)	0.9300
C(10)-H(10)	0.9300
Cl(5)-Zn(1)	2.267(3)
N(1)-H(1A)	0.8600
N(1)-H(1B)	0.8600
N(2)-H(2)	0.8600
N(3)-H(3A)	0.8600
N(3)-H(3B)	0.8600
N(4)-H(4A)	0.8600
Cl(1)-Zn(1)	2.272(3)
Cl(3)-Zn(1)	2.248(3)
Cl(4)-Zn(1)	2.282(3)

N(1)-C(1)-C(5)	116.8(13)
N(1)-C(1)-C(2)	123.4(13)
C(5)-C(1)-C(2)	119.1(13)
C(3)-C(2)-C(1)	117.6(14)
C(3)-C(2)-H(2A)	121.2
C(1)-C(2)-H(2A)	121.2
N(2)-C(3)-C(2)	122.5(14)
N(2)-C(3)-H(3)	118.8
C(2)-C(3)-H(3)	118.7
N(2)-C(4)-C(5)	118.4(16)
N(2)-C(4)-H(4)	120.8
C(5)-C(4)-H(4)	120.8
C(1)-C(5)-C(4)	118.5(13)
C(1)-C(5)-H(5)	120.7
C(4)-C(5)-H(5)	120.7
N(3)-C(6)-C(10)	123.5(10)
N(3)-C(6)-C(7)	118.0(11)
C(10)-C(6)-C(7)	118.3(11)
C(8)-C(7)-C(6)	117.3(11)

C(8)-C(7)-H(7)	121.4
C(6)-C(7)-H(7)	121.4
C(7)-C(8)-N(4)	119.7(12)
C(7)-C(8)-H(8)	120.2
N(4)-C(8)-H(8)	120.2
N(4)-C(9)-C(10)	124.4(15)
N(4)-C(9)-H(9)	117.8
C(10)-C(9)-H(9)	117.8
C(9)-C(10)-C(6)	119.3(12)
C(9)-C(10)-H(10)	120.3
C(6)-C(10)-H(10)	120.4
C(1)-N(1)-H(1A)	120.0
C(1)-N(1)-H(1B)	120.0
H(1A)-N(1)-H(1B)	120.0
C(4)-N(2)-C(3)	122.0(14)
C(4)-N(2)-H(2)	119.0
C(3)-N(2)-H(2)	119.0
C(6)-N(3)-H(3A)	120.0
C(6)-N(3)-H(3B)	120.0
H(3A)-N(3)-H(3B)	120.0
C(9)-N(4)-C(8)	121.0(13)
C(9)-N(4)-H(4A)	119.5
C(8)-N(4)-H(4A)	119.5
Cl(3)-Zn(1)-Cl(5)	115.79(13)
Cl(3)-Zn(1)-Cl(1)	111.96(14)
Cl(5)-Zn(1)-Cl(1)	106.29(14)
Cl(3)-Zn(1)-Cl(4)	107.04(15)
Cl(5)-Zn(1)-Cl(4)	109.48(13)
Cl(1)-Zn(1)-Cl(4)	105.84(14)

Symmetry transformations used to generate equivalent atoms:

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

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}

C(1)	53(8)	36(6)	30(6)	-1(5)	18(6)	-5(6)
C(2)	35(7)	33(6)	62(9)	6(6)	-8(7)	0(5)
C(3)	50(8)	47(8)	34(7)	-14(6)	-10(6)	14(7)
C(4)	28(6)	41(7)	74(11)	-18(7)	-3(7)	0(6)
C(5)	62(10)	33(6)	37(7)	7(5)	-4(7)	16(7)
C(6)	14(5)	39(6)	19(5)	-1(4)	3(4)	3(4)
C(7)	26(5)	46(6)	13(5)	-9(4)	-1(4)	12(5)
C(8)	34(7)	80(11)	35(7)	-1(7)	-6(6)	22(7)
C(9)	42(8)	25(6)	88(13)	10(7)	13(8)	1(6)
C(10)	29(6)	30(6)	27(5)	6(4)	-6(5)	1(5)
Cl(5)	41(2)	40(2)	42(2)	19(1)	6(1)	0(1)
N(1)	72(9)	40(6)	25(5)	5(5)	-3(6)	-3(6)
N(2)	56(8)	52(7)	46(7)	-25(6)	-4(6)	8(6)
N(3)	64(8)	31(6)	42(6)	-2(5)	-9(6)	-6(6)
N(4)	34(6)	39(6)	59(8)	10(6)	20(6)	-3(5)
Cl(1)	51(2)	32(2)	41(2)	6(1)	-14(1)	1(1)
Cl(3)	70(2)	36(2)	27(1)	-2(1)	4(2)	20(2)
Cl(4)	57(2)	41(2)	27(1)	-9(1)	8(1)	-27(2)
Zn(1)	33(1)	21(1)	24(1)	0(1)	-1(1)	-2(1)

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

	x	y	z	U(eq)
H(2A)	2838	14432	3917	52
H(3)	2343	14940	5366	52
H(4)	2275	12527	6333	57
H(5)	2216	11922	4813	53
H(7)	4561	11429	8105	34
H(8)	4926	12853	7516	59
H(9)	5352	13901	9915	62
H(10)	5019	12571	10588	34
H(1A)	2969	12163	3412	55
H(1B)	3346	13061	3027	55
H(2)	1836	13991	6447	61

H(3A)	4570	10948	10363	55
H(3B)	4331	10572	9450	55
H(4A)	5435	14025	8503	53

Table 6. Torsion angles [°] for 4ampZnCl.

N(1)-C(1)-C(2)-C(3)	178.0(15)
C(5)-C(1)-C(2)-C(3)	8(2)
C(1)-C(2)-C(3)-N(2)	-3(2)
N(1)-C(1)-C(5)-C(4)	175.2(14)
C(2)-C(1)-C(5)-C(4)	-14(2)
N(2)-C(4)-C(5)-C(1)	16(2)
N(3)-C(6)-C(7)-C(8)	-178.1(12)
C(10)-C(6)-C(7)-C(8)	-2.2(17)
C(6)-C(7)-C(8)-N(4)	2.3(18)
N(4)-C(9)-C(10)-C(6)	-2(2)
N(3)-C(6)-C(10)-C(9)	177.8(13)
C(7)-C(6)-C(10)-C(9)	2.1(18)
C(5)-C(4)-N(2)-C(3)	-11(2)
C(2)-C(3)-N(2)-C(4)	4(2)
C(10)-C(9)-N(4)-C(8)	3(2)
C(7)-C(8)-N(4)-C(9)	-3(2)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for 4ampZnCl [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...Cl(1)#1	0.86	2.50	3.32	160.0
N(1)-H(1B)...Cl(3)#2	0.86	2.47	3.33	174.9
N(2)-H(2)...Cl(4)#3	0.86	2.51	3.29	150.5

Symmetry transformations used to generate equivalent atoms:

#1 -x+1/2, -y+2, z-1/2 #2 x+1/2, -y+5/2, -z+1 #3 -x, y+1/2, -z+3/2

Crystallographic Data for Bis(4-aminopyridinium) tetrabromozincate(II)

Table 1. Crystal data and structure refinement for 4ampZnBr.

Identification code	4ampZnBr	
Empirical formula	C10 H14 Br4 N4 Zn	
Formula weight	575.26	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 7.3747(7) Å	α= 90°.
	b = 15.4569(13) Å	β= 90°.
	c = 15.4716(15) Å	γ = 90°.
Volume	1763.6(3) $Å^3$	
Z	4	
Density (calculated)	2.167 Mg/m^3	
Absorption coefficient	10.447 mm^{-1}	
F(000)	1088	
Crystal size	0.2 x 0.2 x 0.2 mm^3	
Theta range for data collection	3.82 to 27.00°.	
Index ranges	-9<=h<=8, -19<=k<=19, -19<=l<=19	
Reflections collected	14103	
Independent reflections	3839 [R(int) = 0.0491]	
Completeness to theta = 25.00°	99.5 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3839 / 0 / 173	
Goodness-of-fit on F^2	0.889	
Final R indices [I>2sigma(I)]	R1 = 0.0264, wR2 = 0.0502	
R indices (all data)	R1 = 0.0533, wR2 = 0.0527	
Absolute structure parameter	0.002(15)	
Extinction coefficient	0.0294(5)	
Largest diff. peak and hole	0.418 and -0.352 $e.Å^{-3}$	

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

	x	y	z	U(eq)

C(1)	10254(7)	8167(3)	598(3)	56(1)
C(2)	9935(6)	7410(3)	139(4)	62(2)
C(3)	9668(7)	6661(4)	572(5)	76(2)
C(4)	10076(6)	7332(5)	1885(4)	81(2)
C(5)	10341(7)	8126(4)	1516(3)	67(1)
C(6)	7206(7)	8154(4)	4234(4)	65(2)
C(7)	7496(6)	7619(4)	4949(4)	65(2)
C(8)	7850(8)	7968(5)	5723(5)	91(2)
C(9)	7692(7)	9364(5)	5121(5)	87(2)
C(10)	7295(6)	9065(4)	4319(5)	72(2)
N(1)	10496(6)	8892(3)	200(3)	85(1)
N(2)	9750(6)	6632(3)	1432(4)	82(2)
N(3)	6834(7)	7820(3)	3511(4)	93(2)
N(4)	7955(6)	8836(6)	5798(4)	104(2)
Zn(1)	6311(1)	5067(1)	2503(1)	46(1)
Br(1)	4418(1)	4078(1)	3270(1)	69(1)
Br(2)	8557(1)	5670(1)	3468(1)	68(1)
Br(3)	4453(1)	6261(1)	2028(1)	63(1)
Br(4)	7854(1)	4446(1)	1305(1)	71(1)

Table 3. Bond lengths [Å] and angles [°] for 4ampZnBr.

C(1)-N(1)	1.291(6)
C(1)-C(2)	1.389(7)
C(1)-C(5)	1.423(7)
C(2)-C(3)	1.351(7)
C(2)-H(2)	0.9300
C(3)-N(2)	1.333(7)
C(3)-H(3)	0.9300
C(4)-N(2)	1.311(7)
C(4)-C(5)	1.367(8)
C(4)-H(4)	0.9300
C(5)-H(5)	0.9300
C(6)-N(3)	1.261(6)
C(6)-C(7)	1.398(8)
C(6)-C(10)	1.415(7)

C(7)-C(8)	1.339(8)
C(7)-H(7)	0.9300
C(8)-N(4)	1.350(8)
C(8)-H(8)	0.9300
C(9)-N(4)	1.342(8)
C(9)-C(10)	1.356(9)
C(9)-H(9)	0.9300
C(10)-H(10)	0.9300
N(1)-H(1A)	0.8600
N(1)-H(1B)	0.8600
N(2)-H(2A)	0.8600
N(3)-H(3A)	0.8600
N(3)-H(3B)	0.8600
N(4)-H(4A)	0.8600
Zn(1)-Br(4)	2.3768(7)
Zn(1)-Br(1)	2.3854(7)
Zn(1)-Br(3)	2.4138(7)
Zn(1)-Br(2)	2.4167(7)

N(1)-C(1)-C(2)	120.8(5)
N(1)-C(1)-C(5)	120.5(5)
C(2)-C(1)-C(5)	118.7(5)
C(3)-C(2)-C(1)	119.6(6)
C(3)-C(2)-H(2)	120.2
C(1)-C(2)-H(2)	120.2
N(2)-C(3)-C(2)	121.1(6)
N(2)-C(3)-H(3)	119.4
C(2)-C(3)-H(3)	119.4
N(2)-C(4)-C(5)	122.9(6)
N(2)-C(4)-H(4)	118.6
C(5)-C(4)-H(4)	118.5
C(4)-C(5)-C(1)	116.8(5)
C(4)-C(5)-H(5)	121.6
C(1)-C(5)-H(5)	121.6
N(3)-C(6)-C(7)	119.5(6)
N(3)-C(6)-C(10)	120.0(6)
C(7)-C(6)-C(10)	120.5(6)

C(8)-C(7)-C(6)	120.0(6)
C(8)-C(7)-H(7)	120.0
C(6)-C(7)-H(7)	120.0
C(7)-C(8)-N(4)	119.2(7)
C(7)-C(8)-H(8)	120.4
N(4)-C(8)-H(8)	120.4
N(4)-C(9)-C(10)	122.6(6)
N(4)-C(9)-H(9)	118.7
C(10)-C(9)-H(9)	118.7
C(9)-C(10)-C(6)	115.7(6)
C(9)-C(10)-H(10)	122.2
C(6)-C(10)-H(10)	122.1
C(1)-N(1)-H(1A)	120.0
C(1)-N(1)-H(1B)	120.0
H(1A)-N(1)-H(1B)	120.0
C(4)-N(2)-C(3)	120.9(5)
C(4)-N(2)-H(2A)	119.5
C(3)-N(2)-H(2A)	119.5
C(6)-N(3)-H(3A)	120.0
C(6)-N(3)-H(3B)	120.0
H(3A)-N(3)-H(3B)	120.0
C(9)-N(4)-C(8)	122.0(6)
C(9)-N(4)-H(4A)	119.0
C(8)-N(4)-H(4A)	119.0
Br(4)-Zn(1)-Br(1)	114.16(3)
Br(4)-Zn(1)-Br(3)	110.05(3)
Br(1)-Zn(1)-Br(3)	108.00(3)
Br(4)-Zn(1)-Br(2)	108.01(3)
Br(1)-Zn(1)-Br(2)	109.96(3)
Br(3)-Zn(1)-Br(2)	106.39(2)

Symmetry transformations used to generate equivalent atoms:

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

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}

C(1)	51(3)	48(3)	67(4)	7(3)	7(3)	8(2)
C(2)	71(4)	54(4)	60(3)	-5(3)	3(3)	-4(3)
C(3)	58(4)	81(5)	87(5)	1(4)	-3(4)	-3(3)
C(4)	62(4)	119(6)	62(4)	19(4)	7(3)	8(4)
C(5)	60(3)	82(4)	57(4)	-10(3)	5(3)	-1(3)
C(6)	51(3)	94(5)	51(4)	-23(4)	1(3)	-3(3)
C(7)	71(4)	66(4)	56(4)	3(3)	-6(3)	-2(3)
C(8)	60(4)	69(5)	144(7)	-35(5)	16(4)	-4(3)
C(9)	53(4)	93(5)	115(6)	-50(5)	-4(4)	1(3)
C(10)	51(3)	52(4)	113(6)	6(4)	1(3)	0(3)
N(1)	120(4)	67(3)	68(3)	-7(3)	5(3)	-8(3)
N(2)	71(3)	68(4)	106(5)	19(3)	3(3)	-4(3)
N(3)	123(4)	67(3)	88(4)	1(3)	7(3)	4(3)
N(4)	64(3)	185(7)	62(4)	-26(4)	-5(3)	9(4)
Zn(1)	57(1)	40(1)	41(1)	-1(1)	-1(1)	1(1)
Br(1)	99(1)	55(1)	52(1)	4(1)	11(1)	-18(1)
Br(2)	90(1)	48(1)	66(1)	1(1)	-34(1)	-5(1)
Br(3)	79(1)	62(1)	49(1)	10(1)	-1(1)	24(1)
Br(4)	86(1)	62(1)	67(1)	-21(1)	21(1)	3(1)

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

	x	y	z	U(eq)
H(2)	9905	7418	-462	74
H(3)	9424	6158	264	91
H(4)	10129	7287	2484	97
H(5)	10568	8615	1849	80
H(7)	7444	7021	4887	78
H(8)	8021	7615	6204	109
H(9)	7786	9958	5205	104
H(10)	7095	9435	3854	87
H(1A)	10461	8910	-355	102
H(1B)	10693	9357	491	102

H(2A)	9586	6148	1694	98
H(3A)	6761	7267	3461	111
H(3B)	6654	8146	3069	111
H(4A)	8198	9058	6294	124

Table 6. Torsion angles [°] for 4ampZnBr.

N(1)-C(1)-C(2)-C(3)	-179.4(5)
C(5)-C(1)-C(2)-C(3)	1.7(7)
C(1)-C(2)-C(3)-N(2)	-1.6(8)
N(2)-C(4)-C(5)-C(1)	-0.2(8)
N(1)-C(1)-C(5)-C(4)	-179.7(5)
C(2)-C(1)-C(5)-C(4)	-0.9(8)
N(3)-C(6)-C(7)-C(8)	-178.4(6)
C(10)-C(6)-C(7)-C(8)	0.5(8)
C(6)-C(7)-C(8)-N(4)	-1.3(8)
N(4)-C(9)-C(10)-C(6)	-1.1(8)
N(3)-C(6)-C(10)-C(9)	179.6(5)
C(7)-C(6)-C(10)-C(9)	0.7(8)
C(5)-C(4)-N(2)-C(3)	0.3(8)
C(2)-C(3)-N(2)-C(4)	0.6(9)
C(10)-C(9)-N(4)-C(8)	0.4(9)
C(7)-C(8)-N(4)-C(9)	0.9(9)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for 4ampZnBr [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...Br(3)#1	0.86	2.71	3.540(5)	163.9
N(1)-H(1B)...Br(2)#2	0.86	2.65	3.505(4)	173.3
N(2)-H(2A)...Br(2)	0.86	2.94	3.592(6)	134.0
N(2)-H(2A)...Br(4)	0.86	2.99	3.662(5)	137.1
N(3)-H(3A)...Br(2)	0.86	2.80	3.559(5)	147.8
N(4)-H(4A)...Br(3)#3	0.86	2.80	3.544(6)	145.7
N(4)-H(4A)...Br(1)#3	0.86	3.09	3.693(7)	128.8

Symmetry transformations used to generate equivalent atoms:

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

Crystallographic Data for Bis(4-aminopyridinium) tetraiodozincate(II)

Table 1. Crystal data and structure refinement for 4ampZnI

Identification code	4ampZnI	
Empirical formula	C10 H14 I4 N4 Zn	
Formula weight	463.36	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 7.5844(4) Å	α= 90°.
	b = 16.0413(7) Å	β= 90°.
	c = 16.041 Å	γ = 90°.
Volume	1951.64(13) $Å^3$	
Z	4	
Density (calculated)	1.577 Mg/m^3	
Absorption coefficient	4.399 mm^{-1}	
F(000)	852	
Crystal size	0.50 x 0.37 x 0.34 mm^3	
Theta range for data collection	1.80 to 26.97°.	
Index ranges	-9<=h<=9, -20<=k<=20, -18<=l<=20	
Reflections collected	10847	
Independent reflections	4001 [R(int) = 0.1539]	
Completeness to theta = 26.97°	98.6 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4001 / 0 / 162	
Goodness-of-fit on F^2	1.159	
Final R indices [I>2sigma(I)]	R1 = 0.0502, wR2 = 0.1310	
R indices (all data)	R1 = 0.0527, wR2 = 0.1377	
Absolute structure parameter	0.04(7)	
Largest diff. peak and hole	1.300 and -2.223 e.$Å^{-3}$	

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

	x	y	z	U(eq)

C(1)	5383(15)	1702(8)	698(8)	27(2)
C(2)	5308(17)	1735(11)	1583(9)	36(3)
C(3)	4831(15)	2492(10)	1936(8)	34(3)
C(4)	4530(20)	3121(10)	644(11)	45(4)
C(5)	4948(16)	2400(10)	234(11)	39(3)
C(6)	2719(15)	1868(7)	5707(8)	25(2)
C(7)	2860(14)	973(8)	5700(10)	32(3)
C(8)	2589(17)	563(9)	4985(9)	34(3)
C(9)	1980(18)	1799(10)	4259(8)	35(3)
C(10)	2200(20)	2235(9)	4957(9)	38(3)
N(1)	5844(15)	977(9)	339(8)	38(3)
N(2)	4406(14)	3138(9)	1475(9)	42(3)
N(3)	2994(15)	2308(9)	6398(8)	39(3)
N(4)	2102(12)	941(9)	4302(7)	38(3)
Zn(1)	3838(2)	5024(1)	-2586(1)	21(1)
I(1)	6218(1)	6012(1)	-3256(1)	29(1)
I(2)	1786(1)	4549(1)	-3805(1)	27(1)
I(3)	1986(1)	5901(1)	-1546(1)	29(1)
I(4)	5386(1)	3763(1)	-1914(1)	32(1)

Table 3. Bond lengths [Å] and angles [°] for 4ampZnI

C(1)-N(1)	1.344(18)
C(1)-C(5)	1.38(2)
C(1)-C(2)	1.42(2)
C(2)-C(3)	1.39(2)
C(2)-H(2)	0.9300
C(3)-N(2)	1.31(2)
C(3)-H(3)	0.9300
C(4)-N(2)	1.34(2)
C(4)-C(5)	1.37(2)
C(4)-H(4)	0.9300
C(5)-H(5)	0.9300
C(6)-N(3)	1.330(17)
C(6)-C(10)	1.396(19)
C(6)-C(7)	1.440(16)
C(7)-C(8)	1.34(2)

C(7)-H(7)	0.9300
C(8)-N(4)	1.31(2)
C(8)-H(8)	0.9300
C(9)-C(10)	1.33(2)
C(9)-N(4)	1.38(2)
C(9)-H(9)	0.9300
C(10)-H(10)	0.9300
N(1)-H(1A)	0.8600
N(1)-H(1B)	0.8600
N(2)-H(2A)	0.8600
N(3)-H(3A)	0.8600
N(3)-H(3B)	0.8600
N(4)-H(4A)	0.8600
Zn(1)-I(4)	2.5748(15)
Zn(1)-I(3)	2.5951(15)
Zn(1)-I(2)	2.6129(15)
Zn(1)-I(1)	2.6321(15)

N(1)-C(1)-C(5)	122.2(13)
N(1)-C(1)-C(2)	118.1(14)
C(5)-C(1)-C(2)	119.7(14)
C(3)-C(2)-C(1)	116.8(14)
C(3)-C(2)-H(2)	121.6
C(1)-C(2)-H(2)	121.6
N(2)-C(3)-C(2)	121.7(12)
N(2)-C(3)-H(3)	119.2
C(2)-C(3)-H(3)	119.2
N(2)-C(4)-C(5)	120.9(16)
N(2)-C(4)-H(4)	119.5
C(5)-C(4)-H(4)	119.5
C(4)-C(5)-C(1)	118.8(15)
C(4)-C(5)-H(5)	120.6
C(1)-C(5)-H(5)	120.6
N(3)-C(6)-C(10)	122.6(11)
N(3)-C(6)-C(7)	121.6(13)
C(10)-C(6)-C(7)	115.7(12)
C(8)-C(7)-C(6)	119.1(13)

C(8)-C(7)-H(7)	120.5
C(6)-C(7)-H(7)	120.5
N(4)-C(8)-C(7)	122.4(13)
N(4)-C(8)-H(8)	118.8
C(7)-C(8)-H(8)	118.8
C(10)-C(9)-N(4)	118.2(13)
C(10)-C(9)-H(9)	120.9
N(4)-C(9)-H(9)	120.9
C(9)-C(10)-C(6)	122.7(13)
C(9)-C(10)-H(10)	118.6
C(6)-C(10)-H(10)	118.6
C(1)-N(1)-H(1A)	120.0
C(1)-N(1)-H(1B)	120.0
H(1A)-N(1)-H(1B)	120.0
C(3)-N(2)-C(4)	121.8(13)
C(3)-N(2)-H(2A)	119.1
C(4)-N(2)-H(2A)	119.1
C(6)-N(3)-H(3A)	120.0
C(6)-N(3)-H(3B)	120.0
H(3A)-N(3)-H(3B)	120.0
C(8)-N(4)-C(9)	121.5(12)
C(8)-N(4)-H(4A)	119.2
C(9)-N(4)-H(4A)	119.2
I(4)-Zn(1)-I(3)	113.83(5)
I(4)-Zn(1)-I(2)	110.86(6)
I(3)-Zn(1)-I(2)	108.47(5)
I(4)-Zn(1)-I(1)	109.32(5)
I(3)-Zn(1)-I(1)	107.90(5)
I(2)-Zn(1)-I(1)	106.13(5)

Symmetry transformations used to generate equivalent atoms:

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

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}

C(1)	26(5)	26(6)	28(6)	-1(5)	1(5)	2(5)
C(2)	29(5)	47(8)	33(7)	11(6)	5(5)	-2(6)
C(3)	23(5)	56(9)	23(6)	-6(6)	-6(5)	5(5)
C(4)	52(8)	27(7)	57(10)	-8(7)	5(8)	13(7)
C(5)	24(5)	41(8)	51(9)	6(7)	-8(6)	-3(5)
C(6)	25(5)	18(5)	31(6)	-5(5)	3(5)	0(4)
C(7)	24(5)	18(6)	53(8)	0(5)	15(5)	9(4)
C(8)	38(6)	25(6)	39(7)	-5(5)	5(6)	0(5)
C(9)	37(6)	43(8)	25(6)	8(6)	-4(5)	6(6)
C(10)	58(8)	27(6)	30(6)	1(5)	13(6)	12(6)
N(2)	22(4)	44(7)	60(8)	-34(7)	4(5)	4(5)
N(4)	21(4)	61(8)	32(6)	-24(6)	2(4)	-16(5)
Zn(1)	24(1)	17(1)	23(1)	0(1)	-1(1)	0(1)
I(1)	36(1)	26(1)	24(1)	-3(1)	4(1)	-13(1)
I(2)	32(1)	19(1)	30(1)	-2(1)	-10(1)	-2(1)
I(3)	39(1)	23(1)	24(1)	-1(1)	6(1)	6(1)
I(4)	35(1)	27(1)	35(1)	8(1)	-4(1)	7(1)

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

	x	y	z	U(eq)
H(2)	5567	1272	1909	44
H(3)	4812	2543	2513	41
H(4)	4340	3607	341	54
H(5)	4937	2379	-345	46
H(7)	3134	684	6186	38
H(8)	2754	-11	4975	41
H(9)	1750	2066	3755	42
H(10)	1998	2806	4945	46
H(1A)	5876	936	-195	46
H(1B)	6107	554	644	46
H(2A)	4034	3585	1714	50
H(3A)	2851	2840	6394	46
H(3B)	3314	2061	6849	46

H(4A)	1851	648	3869	46

Table 6. Torsion angles [°] for 4ampZnI

N(1)-C(1)-C(2)-C(3)	179.9(11)
C(5)-C(1)-C(2)-C(3)	-1.5(19)
C(1)-C(2)-C(3)-N(2)	2.4(19)
N(2)-C(4)-C(5)-C(1)	-6(2)
N(1)-C(1)-C(5)-C(4)	-178.4(13)
C(2)-C(1)-C(5)-C(4)	3(2)
N(3)-C(6)-C(7)-C(8)	-179.3(11)
C(10)-C(6)-C(7)-C(8)	3.7(17)
C(6)-C(7)-C(8)-N(4)	-4.0(18)
N(4)-C(9)-C(10)-C(6)	7(2)
N(3)-C(6)-C(10)-C(9)	177.8(13)
C(7)-C(6)-C(10)-C(9)	-5(2)
C(2)-C(3)-N(2)-C(4)	-5(2)
C(5)-C(4)-N(2)-C(3)	7(2)
C(7)-C(8)-N(4)-C(9)	5.6(19)
C(10)-C(9)-N(4)-C(8)	-7(2)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for 4ampZnI [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...I(1)#1	0.86	2.95	3.689(13)	145.1
N(1)-H(1A)...I(2)#1	0.86	3.27	3.812(13)	123.8
N(1)-H(1B)...I(3)#2	0.86	2.83	3.685(14)	176.1
N(2)-H(2A)...I(3)#3	0.86	3.01	3.683(12)	136.6
N(2)-H(2A)...I(2)#3	0.86	3.17	3.844(14)	137.2
N(3)-H(3A)...I(2)#4	0.86	2.88	3.724(14)	169.1
N(3)-H(3B)...I(1)#5	0.86	2.84	3.683(13)	168.0
N(4)-H(4A)...I(1)#6	0.86	2.88	3.616(12)	144.8

Symmetry transformations used to generate equivalent atoms:

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

#4 x,y,z+1 #5 -x+1,y-1/2,-z+1/2 #6 x-1/2,-y+1/2,-z

Crystallographic Data for Catena-(bis(4-aminopyridinium) bis(μ2-chloro) dichlorocadmium(II) monohydrate)

Table 1. Crystal data and structure refinement for 4ampCdCl·H2O.

Identification code	4ampCdCl·H2O	
Empirical formula	C10 H16 Cd2 Cl8 N4 O	
Formula weight	253.09	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 7.496(5) Å	α= 90°.
	b = 24.413(5) Å	β= 101.93(4)°.
	c = 12.453(5) Å	γ = 90°.
Volume	2229.8(18) Å3	
Z	4	
Density (calculated)	0.754 Mg/m3	
Absorption coefficient	1.244 mm-1	
F(000)	474	
Crystal size	1.00 x 1.00 x 1.00 mm3	
Theta range for data collection	4.23 to 27.00°.	
Index ranges	-9<=h<=7, -31<=k<=31, -15<=l<=15	
Reflections collected	15532	
Independent reflections	4852 [R(int) = 0.3919]	
Completeness to theta = 27.00°	99.5 %	
Max. and min. transmission	0.3693 and 0.3693	
Refinement method	Full-matrix least-squares on F2	
Data / restraints / parameters	4852 / 0 / 221	
Goodness-of-fit on F2	1.881	
Final R indices [I>2sigma(I)]	R1 = 0.1997, wR2 = 0.4957	
R indices (all data)	R1 = 0.2077, wR2 = 0.5042	
Extinction coefficient	0.009(3)	
Largest diff. peak and hole5.159 and -4.067 e.Å-3		

Table 2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å2x 10³) for 4ampCdCl·H2O. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)

C(1)	-4790(40)	6486(9)	3360(20)	65(6)
C(2)	-5180(30)	6078(11)	4007(16)	65(6)
C(3)	-5670(30)	5579(10)	3682(18)	69(6)
C(4)	-5120(40)	5806(17)	1960(20)	91(10)
C(5)	-4840(40)	6366(12)	2266(18)	73(7)
C(6)	120(30)	3996(10)	7576(14)	56(5)
C(7)	430(30)	4369(9)	6805(19)	62(5)
C(8)	480(40)	4181(10)	5820(20)	75(7)
C(9)	-70(60)	3314(12)	6190(30)	108(12)
C(10)	-230(50)	3463(14)	7370(30)	91(9)
Cl(1)	-1864(6)	5703(2)	6837(3)	40(1)
Cl(2)	3869(6)	6740(2)	8940(4)	49(1)
Cl(3)	8935(6)	6668(2)	9090(3)	47(1)
Cl(4)	3125(5)	5810(2)	6637(3)	38(1)
Cl(5)	5980(20)	5485(5)	8901(10)	149(5)
Cl(6)	1934(7)	5368(2)	9320(4)	54(1)
Cl(7)	70(30)	6871(6)	6550(13)	172(6)
Cl(8)	6016(7)	7147(2)	6500(4)	54(1)
O(1)	2100(20)	7689(9)	5938(16)	88(6)
N(1)	-4440(30)	6981(8)	3702(17)	73(6)
N(2)	-5590(30)	5468(8)	2590(20)	78(6)
N(3)	160(30)	4145(9)	8647(15)	74(5)
N(4)	169(1)	3663(1)	5502(1)	84(7)
Cd(1)	1079(1)	6168(1)	7968(1)	39(1)
Cd(2)	5990(1)	6308(1)	7766(1)	38(1)

Table 3. Bond lengths [Å] and angles [°] for 4ampCdCl·H2O.

C(1)-N(1)	1.29(3)
C(1)-C(2)	1.34(3)
C(1)-C(5)	1.39(3)
C(2)-C(3)	1.31(4)
C(2)-H(2)	0.9300
C(3)-N(2)	1.40(3)
C(3)-H(3)	0.9300
C(4)-N(2)	1.24(4)

C(4)-C(5)	1.43(5)
C(4)-H(4)	0.9300
C(5)-H(5)	0.9300
C(6)-C(10)	1.34(4)
C(6)-N(3)	1.38(2)
C(6)-C(7)	1.38(3)
C(7)-C(8)	1.32(3)
C(7)-H(7)	0.9300
C(8)-N(4)	1.33(2)
C(8)-H(8)	0.9300
C(9)-N(4)	1.25(4)
C(9)-C(10)	1.54(5)
C(9)-H(9)	0.9300
C(10)-H(10)	0.9300
Cl(1)-Cd(1)	2.619(4)
Cl(1)-Cd(2)#1	2.622(4)
Cl(2)-Cd(2)	2.597(4)
Cl(2)-Cd(1)	2.597(4)
Cl(3)-Cd(2)	2.619(5)
Cl(3)-Cd(1)#2	2.637(4)
Cl(4)-Cd(2)	2.611(4)
Cl(4)-Cd(1)	2.630(3)
Cl(5)-Cd(2)	2.458(11)
Cl(6)-Cd(1)	2.572(5)
Cl(7)-Cd(1)	2.467(19)
Cl(7)-H(1D)	1.8094
Cl(8)-Cd(2)	2.588(4)
O(1)-H(1C)	0.9048
O(1)-H(1D)	0.9033
N(1)-H(1A)	0.8600
N(1)-H(1B)	0.8600
N(2)-H(2A)	0.8600
N(3)-H(3A)	0.8600
N(3)-H(3B)	0.8600
N(4)-H(4A)	0.8600
Cd(1)-Cl(3)#1	2.637(4)
Cd(2)-Cl(1)#2	2.622(4)

N(1)-C(1)-C(2)	124(2)
N(1)-C(1)-C(5)	119(2)
C(2)-C(1)-C(5)	118(2)
C(3)-C(2)-C(1)	126(2)
C(3)-C(2)-H(2)	117.1
C(1)-C(2)-H(2)	117.1
C(2)-C(3)-N(2)	114.5(18)
C(2)-C(3)-H(3)	122.8
N(2)-C(3)-H(3)	122.7
N(2)-C(4)-C(5)	121(2)
N(2)-C(4)-H(4)	119.6
C(5)-C(4)-H(4)	119.6
C(1)-C(5)-C(4)	116(2)
C(1)-C(5)-H(5)	122.1
C(4)-C(5)-H(5)	122.1
C(10)-C(6)-N(3)	114(2)
C(10)-C(6)-C(7)	124(2)
N(3)-C(6)-C(7)	122(2)
C(8)-C(7)-C(6)	118(2)
C(8)-C(7)-H(7)	121.3
C(6)-C(7)-H(7)	121.2
C(7)-C(8)-N(4)	125(2)
C(7)-C(8)-H(8)	117.6
N(4)-C(8)-H(8)	117.7
N(4)-C(9)-C(10)	123(2)
N(4)-C(9)-H(9)	118.5
C(10)-C(9)-H(9)	118.5
C(6)-C(10)-C(9)	111(2)
C(6)-C(10)-H(10)	124.4
C(9)-C(10)-H(10)	124.4
Cd(1)-Cl(1)-Cd(2)#1	92.52(12)
Cd(2)-Cl(2)-Cd(1)	92.67(12)
Cd(2)-Cl(3)-Cd(1)#2	92.16(12)
Cd(2)-Cl(4)-Cd(1)	91.60(12)
Cd(1)-Cl(7)-H(1D)	127.1
H(1C)-O(1)-H(1D)	99.7

C(1)-N(1)-H(1A)	120.0
C(1)-N(1)-H(1B)	120.0
H(1A)-N(1)-H(1B)	120.0
C(4)-N(2)-C(3)	124(2)
C(4)-N(2)-H(2A)	117.9
C(3)-N(2)-H(2A)	117.9
C(6)-N(3)-H(3A)	120.0
C(6)-N(3)-H(3B)	120.0
H(3A)-N(3)-H(3B)	120.0
C(9)-N(4)-C(8)	118.9(14)
C(9)-N(4)-H(4A)	120.5
C(8)-N(4)-H(4A)	120.6
Cl(7)-Cd(1)-Cl(6)	174.4(3)
Cl(7)-Cd(1)-Cl(2)	93.3(4)
Cl(6)-Cd(1)-Cl(2)	92.04(17)
Cl(7)-Cd(1)-Cl(1)	79.5(4)
Cl(6)-Cd(1)-Cl(1)	95.21(15)
Cl(2)-Cd(1)-Cl(1)	172.69(16)
Cl(7)-Cd(1)-Cl(4)	85.0(4)
Cl(6)-Cd(1)-Cl(4)	93.50(14)
Cl(2)-Cd(1)-Cl(4)	87.38(12)
Cl(1)-Cd(1)-Cl(4)	93.06(12)
Cl(7)-Cd(1)-Cl(3)#1	85.8(4)
Cl(6)-Cd(1)-Cl(3)#1	95.79(16)
Cl(2)-Cd(1)-Cl(3)#1	91.40(13)
Cl(1)-Cd(1)-Cl(3)#1	86.99(12)
Cl(4)-Cd(1)-Cl(3)#1	170.67(15)
Cl(5)-Cd(2)-Cl(8)	177.5(3)
Cl(5)-Cd(2)-Cl(2)	86.2(3)
Cl(8)-Cd(2)-Cl(2)	95.92(15)
Cl(5)-Cd(2)-Cl(4)	80.1(4)
Cl(8)-Cd(2)-Cl(4)	98.61(16)
Cl(2)-Cd(2)-Cl(4)	87.78(13)
Cl(5)-Cd(2)-Cl(3)	90.9(4)
Cl(8)-Cd(2)-Cl(3)	90.36(17)
Cl(2)-Cd(2)-Cl(3)	92.49(13)
Cl(4)-Cd(2)-Cl(3)	170.95(15)

Cl(5)-Cd(2)-Cl(1)#2	82.5(3)
Cl(8)-Cd(2)-Cl(1)#2	95.45(13)
Cl(2)-Cd(2)-Cl(1)#2	168.62(15)
Cl(4)-Cd(2)-Cl(1)#2	90.66(12)
Cl(3)-Cd(2)-Cl(1)#2	87.29(13)

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters ($Å^2 \times 10^3$)for 4ampCdCl·H2O. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(1)	98(16)	41(10)	75(14)	8(9)	60(13)	25(10)
C(2)	89(16)	88(17)	24(8)	13(8)	28(9)	10(12)
C(3)	78(14)	72(15)	52(12)	15(10)	3(11)	-26(11)
C(4)	82(16)	160(30)	42(12)	-11(15)	40(12)	-33(18)
C(5)	93(18)	90(20)	36(10)	20(10)	17(11)	-12(13)
C(6)	73(13)	76(13)	22(8)	-8(7)	17(8)	14(10)
C(7)	83(14)	47(11)	59(12)	2(8)	24(11)	4(9)
C(8)	104(18)	59(14)	80(16)	-13(11)	64(15)	-19(12)
C(9)	200(40)	51(15)	80(20)	-40(15)	40(20)	-25(19)
C(10)	100(20)	90(20)	72(18)	24(14)	-4(15)	-15(15)
Cl(1)	52(2)	37(2)	39(2)	-13(1)	26(2)	-3(2)
Cl(2)	55(2)	53(2)	48(2)	-25(2)	31(2)	-13(2)
Cl(3)	52(2)	63(3)	33(2)	-19(2)	22(2)	-6(2)
Cl(4)	40(2)	49(2)	30(2)	-7(1)	20(1)	0(1)
Cl(5)	241(14)	93(8)	129(9)	15(6)	76(9)	11(8)
Cl(6)	73(3)	54(3)	37(2)	11(2)	19(2)	0(2)
Cl(7)	262(17)	133(11)	150(11)	-40(8)	110(12)	-69(10)
Cl(8)	73(3)	50(3)	46(2)	11(2)	33(2)	12(2)
O(1)	60(9)	126(17)	87(13)	51(11)	36(9)	-12(9)
N(1)	109(16)	53(11)	66(12)	-2(8)	36(11)	31(10)
N(2)	94(14)	37(9)	110(17)	-27(10)	36(13)	-17(8)
N(3)	120(16)	66(13)	45(10)	-5(8)	37(10)	-3(11)
N(4)	140(20)	54(12)	71(14)	-24(10)	59(14)	-1(11)

Cd(1)	50(1)	40(1)	32(1)	-1(1)	23(1)	-2(1)
Cd(2)	47(1)	36(1)	38(1)	-2(1)	24(1)	1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for 4ampCdCl·H2O.

	x	y	z	U(eq)
H(2)	-5087	6157	4746	78
H(3)	-6034	5321	4141	83
H(4)	-4951	5691	1275	109
H(5)	-4691	6636	1763	88
H(7)	590	4739	6973	74
H(8)	759	4428	5310	90
H(9)	-156	2947	5988	130
H(10)	-523	3216	7875	109
H(1A)	-4454	7066	4371	88
H(1B)	-4206	7227	3258	88
H(2A)	-5888	5144	2346	94
H(3A)	-24	3903	9114	89
H(3B)	371	4479	8849	89
H(4A)	132	3570	4832	101
H(1C)	3218	7533	6100	126
H(1D)	1432	7415	6145	126

Table 6. Torsion angles [°] for 4ampCdCl·H2O.

N(1)-C(1)-C(2)-C(3)	175(3)
C(5)-C(1)-C(2)-C(3)	-3(4)
C(1)-C(2)-C(3)-N(2)	6(4)
N(1)-C(1)-C(5)-C(4)	177(3)
C(2)-C(1)-C(5)-C(4)	-6(4)
N(2)-C(4)-C(5)-C(1)	11(4)
C(10)-C(6)-C(7)-C(8)	-4(4)
N(3)-C(6)-C(7)-C(8)	175(2)
C(6)-C(7)-C(8)-N(4)	4(4)

N(3)-C(6)-C(10)-C(9)	-174(3)
C(7)-C(6)-C(10)-C(9)	5(4)
N(4)-C(9)-C(10)-C(6)	-7(5)
C(5)-C(4)-N(2)-C(3)	-8(5)
C(2)-C(3)-N(2)-C(4)	-1(4)
C(10)-C(9)-N(4)-C(8)	7(5)
C(7)-C(8)-N(4)-C(9)	-5(4)
Cd(2)-Cl(2)-Cd(1)-Cl(7)	-90.6(4)
Cd(2)-Cl(2)-Cd(1)-Cl(6)	87.66(17)
Cd(2)-Cl(2)-Cd(1)-Cl(1)	-99.3(8)
Cd(2)-Cl(2)-Cd(1)-Cl(4)	-5.75(15)
Cd(2)-Cl(2)-Cd(1)-Cl(3)#1	-176.49(16)
Cd(2)#1-Cl(1)-Cd(1)-Cl(7)	-78.6(4)
Cd(2)#1-Cl(1)-Cd(1)-Cl(6)	103.22(15)
Cd(2)#1-Cl(1)-Cd(1)-Cl(2)	-69.8(9)
Cd(2)#1-Cl(1)-Cd(1)-Cl(4)	-162.98(12)
Cd(2)#1-Cl(1)-Cd(1)-Cl(3)#1	7.67(14)
Cd(2)-Cl(4)-Cd(1)-Cl(7)	99.2(4)
Cd(2)-Cl(4)-Cd(1)-Cl(6)	-86.18(15)
Cd(2)-Cl(4)-Cd(1)-Cl(2)	5.71(15)
Cd(2)-Cl(4)-Cd(1)-Cl(1)	178.41(12)
Cd(2)-Cl(4)-Cd(1)-Cl(3)#1	88.3(8)
Cd(1)-Cl(2)-Cd(2)-Cl(5)	-74.5(4)
Cd(1)-Cl(2)-Cd(2)-Cl(8)	104.22(18)
Cd(1)-Cl(2)-Cd(2)-Cl(4)	5.79(15)
Cd(1)-Cl(2)-Cd(2)-Cl(3)	-165.16(16)
Cd(1)-Cl(2)-Cd(2)-Cl(1)#2	-76.5(7)
Cd(1)-Cl(4)-Cd(2)-Cl(5)	80.8(3)
Cd(1)-Cl(4)-Cd(2)-Cl(8)	-101.37(13)
Cd(1)-Cl(4)-Cd(2)-Cl(2)	-5.71(14)
Cd(1)-Cl(4)-Cd(2)-Cl(3)	86.2(7)
Cd(1)-Cl(4)-Cd(2)-Cl(1)#2	163.02(12)
Cd(1)#2-Cl(3)-Cd(2)-Cl(5)	90.1(3)
Cd(1)#2-Cl(3)-Cd(2)-Cl(8)	-87.77(15)
Cd(1)#2-Cl(3)-Cd(2)-Cl(2)	176.28(15)
Cd(1)#2-Cl(3)-Cd(2)-Cl(4)	84.8(7)
Cd(1)#2-Cl(3)-Cd(2)-Cl(1)#2	7.67(14)

Symmetry transformations used to generate equivalent atoms:

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

Table 7. Hydrogen bonds for 4ampCdCl·H2O [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...Cl(8)#1	0.86	2.61	3.45(2)	167.6
N(1)-H(1B)...Cl(8)#3	0.86	2.70	3.54(2)	166.3
N(2)-H(2A)...Cl(5)#4	0.86	2.18	2.96(2)	150.6
N(2)-H(2A)...Cl(1)#5	0.86	2.98	3.59(2)	129.7
N(3)-H(3A)...Cl(3)#6	0.86	2.62	3.40(2)	151.4
N(3)-H(3B)...Cl(6)	0.86	2.48	3.31(2)	161.9
N(4)-H(4A)...Cl(7)#4	0.86	2.01	2.841(13)	162.7
O(1)-H(1C)...Cl(8)	0.90	2.26	3.163(19)	179.6
O(1)-H(1D)...Cl(7)	0.90	1.81	2.71(2)	179.3

Symmetry transformations used to generate equivalent atoms:

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

#4 -x,-y+1,-z+1 #5 -x-1,-y+1,-z+1 #6 -x+1,-y+1,-z+2

Crystallographic Data for Bis(4-aminopyridinium) tetrabromocadmate(II) monohydrate

Table 1. Crystal data and structure refinement for 4ampCdBr·H2O.

Identification code	4ampCdBr·H2O	
Empirical formula	C10 H16 Br4 Cd N4 O	
Formula weight	640.31	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P b c m	
Unit cell dimensions	a = 6.8746(12) Å	α= 90°.
	b = 14.082(2) Å	β= 90°.
	c = 18.842(3) Å	γ = 90°.
Volume	1824.1(5) Å^3	
Z	4	
Density (calculated)	2.332 Mg/m^3	
Absorption coefficient	9.959 mm^{-1}	
F(000)	1200	
Crystal size	0.3 x 0.2 x 0.2 mm^3	
Theta range for data collection	2.16 to 27.00°.	
Index ranges	-8<=h<=8, -17<=k<=17, -24<=l<=24	
Reflections collected	21740	
Independent reflections	2049 [R(int) = 0.0945]	
Completeness to theta = 25.00°	100.0 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2049 / 3 / 102	
Goodness-of-fit on F^2	1.068	
Final R indices [I>2sigma(I)]	R1 = 0.0296, wR2 = 0.0650	
R indices (all data)	R1 = 0.0372, wR2 = 0.0687	
Extinction coefficient	0.0109(4)	
Largest diff. peak and hole	0.836 and -0.527 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for 4ampCdBr·H2O. U(eq) is defined as one third of the trace of the orthogonalized U$_{ij}$ tensor.

	x	y	z	U(eq)

C(1)	8586(5)	8723(3)	170(2)	38(1)
C(2)	6867(6)	9026(3)	-177(2)	51(1)
C(3)	6932(8)	9366(4)	-835(3)	63(1)
C(4)	10256(8)	9101(3)	-896(2)	57(1)
C(5)	10308(6)	8765(3)	-224(2)	45(1)
N(1)	8551(5)	8422(3)	842(2)	50(1)
N(2)	8599(7)	9414(3)	-1193(2)	61(1)
O(1)	9128(8)	372(3)	7500	55(1)
Br(1)	8578(1)	7404(1)	2500	40(1)
Br(2)	3947(1)	5417(1)	2500	45(1)
Br(3)	3581(1)	7997(1)	1342(1)	48(1)
Cd(1)	4828(1)	7208(1)	2500	38(1)

Table 3. Bond lengths [Å] and angles [°] for 4ampCdBr·H2O.

C(1)-N(1)	1.335(5)
C(1)-C(5)	1.399(6)
C(1)-C(2)	1.416(6)
C(2)-C(3)	1.331(7)
C(2)-H(2)	0.9300
C(3)-N(2)	1.331(7)
C(3)-H(3)	0.9300
C(4)-N(2)	1.343(7)
C(4)-C(5)	1.352(6)
C(4)-H(4)	0.9300
C(5)-H(5)	0.9300
N(1)-H(1A)	0.8600
N(1)-H(1B)	0.8600
N(2)-H(2A)	0.8600
O(1)-H(1D)	0.843(19)
O(1)-H(1E)	0.838(19)
Br(1)-Cd(1)	2.5926(8)
Br(2)-Cd(1)	2.5934(8)
Br(3)-Cd(1)	2.5944(6)
Cd(1)-Br(3)#1	2.5944(6)
N(1)-C(1)-C(5)	122.2(4)

N(1)-C(1)-C(2)	121.2(4)
C(5)-C(1)-C(2)	116.6(4)
C(3)-C(2)-C(1)	120.7(5)
C(3)-C(2)-H(2)	119.6
C(1)-C(2)-H(2)	119.6
C(2)-C(3)-N(2)	121.2(5)
C(2)-C(3)-H(3)	119.4
N(2)-C(3)-H(3)	119.4
N(2)-C(4)-C(5)	121.7(4)
N(2)-C(4)-H(4)	119.1
C(5)-C(4)-H(4)	119.1
C(4)-C(5)-C(1)	119.4(4)
C(4)-C(5)-H(5)	120.3
C(1)-C(5)-H(5)	120.3
C(1)-N(1)-H(1A)	120.0
C(1)-N(1)-H(1B)	120.0
H(1A)-N(1)-H(1B)	120.0
C(3)-N(2)-C(4)	120.2(4)
C(3)-N(2)-H(2A)	119.9
C(4)-N(2)-H(2A)	119.9
H(1D)-O(1)-H(1E)	126(5)
Br(1)-Cd(1)-Br(2)	109.61(2)
Br(1)-Cd(1)-Br(3)#1	106.436(15)
Br(2)-Cd(1)-Br(3)#1	109.845(17)
Br(1)-Cd(1)-Br(3)	106.436(15)
Br(2)-Cd(1)-Br(3)	109.845(16)
Br(3)#1-Cd(1)-Br(3)	114.49(3)

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters ($Å^2 \times 10^3$)for 4ampCdBr·H2O. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(1)	41(2)	36(2)	36(2)	0(2)	-2(2)	-4(2)

C(2)	48(2)	55(3)	49(2)	3(2)	-6(2)	-2(2)
C(3)	76(3)	66(3)	48(3)	3(2)	-19(2)	-2(3)
C(4)	78(3)	45(2)	49(2)	-5(2)	26(2)	-8(2)
C(5)	47(2)	42(2)	47(2)	-1(2)	7(2)	1(2)
N(1)	50(2)	63(2)	37(2)	13(2)	2(2)	0(2)
N(2)	107(4)	49(2)	28(2)	-2(2)	-3(2)	-4(2)
O(1)	68(3)	56(3)	42(2)	0	0	1(2)
Br(1)	35(1)	48(1)	36(1)	0	0	-4(1)
Br(2)	47(1)	42(1)	46(1)	0	0	-5(1)
Br(3)	38(1)	64(1)	42(1)	15(1)	-5(1)	-1(1)
Cd(1)	38(1)	43(1)	32(1)	0	0	-1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 4ampCdBr·H2O.

	x	y	z	U(eq)
H(2)	5680	8986	58	61
H(3)	5791	9573	-1050	76
H(4)	11399	9116	-1160	69
H(5)	11476	8565	-26	55
H(1A)	9610	8246	1046	60
H(1B)	7469	8404	1071	60
H(2A)	8615	9645	-1615	74
H(1D)	10350(30)	410(50)	7500	67
H(1E)	8340(70)	830(30)	7500	67

Table 6. Torsion angles [°] for 4ampCdBr·H2O.

N(1)-C(1)-C(2)-C(3)	176.9(4)
C(5)-C(1)-C(2)-C(3)	-2.5(7)
C(1)-C(2)-C(3)-N(2)	1.4(8)
N(2)-C(4)-C(5)-C(1)	1.3(7)
N(1)-C(1)-C(5)-C(4)	-178.2(4)
C(2)-C(1)-C(5)-C(4)	1.2(6)
C(2)-C(3)-N(2)-C(4)	1.2(8)

C(5)-C(4)-N(2)-C(3)	-2.6(7)

Symmetry transformations used to generate equivalent atoms:

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

Table 7. Hydrogen bonds for 4ampCdBr·H2O [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...Br(3)#2	0.86	2.81	3.634(4)	161.4
N(1)-H(1B)...Br(3)	0.86	2.78	3.594(4)	158.4
N(2)-H(2A)...O(1)#3	0.86	1.99	2.832(5)	166.8
O(1)-H(1D)...Br(2)#4	0.843(19)	2.74(3)	3.494(5)	151(6)
O(1)-H(1E)...Br(3)#5	0.838(19)	3.042(14)	3.675(4)	134.1(3)
O(1)-H(1E)...Br(3)#6	0.838(19)	3.042(14)	3.675(4)	134.1(3)

Symmetry transformations used to generate equivalent atoms:

#1 x,y,-z+1/2 #2 x+1,y,z #3 x,y+1,z-1 #4 x+1,-y+1/2,-z+1

#5 -x+1,-y+1,-z+1 #6 -x+1,-y+1,z+1/2

Crystallographic Data for Bis(4-aminopyridinium) tetraiodocadmate(II) monohydrate

Table 1. Crystal data and structure refinement for 4ampCdI·H2O.

Identification code	4ampCdI·H2O	
Empirical formula	C10 H16 Cd I4 N4 O	
Formula weight	828.27	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P b c m	
Unit cell dimensions	a = 7.3983(3) Å	α= 90°.
	b = 14.7586(7) Å	β= 90°.
	c = 18.7562(10) Å	γ = 90°.
Volume	2047.96(17) Å3	
Z	4	
Density (calculated)	2.686 Mg/m3	
Absorption coefficient	7.097 mm-1	
F(000)	1488	
Crystal size	0.3 x 0.2 x 0.2 mm3	
Theta range for data collection	3.77 to 27.00°.	
Index ranges	-9<=h<=9, -18<=k<=18, -19<=l<=23	
Reflections collected	15153	
Independent reflections	2305 [R(int) = 0.0279]	
Completeness to theta = 27.00°	99.7 %	
Refinement method	Full-matrix least-squares on F2	
Data / restraints / parameters	2305 / 3 / 98	
Goodness-of-fit on F2	1.062	
Final R indices [I>2sigma(I)]	R1 = 0.0231, wR2 = 0.0560	
R indices (all data)	R1 = 0.0296, wR2 = 0.0584	
Extinction coefficient	0.00845(19)	
Largest diff. peak and hole0.949 and -0.902 e.Å-3		

Table 2. Atomic coordinates (x 104) and equivalent isotropic displacement parameters (Å2x 103) for 4ampCdI·H2O. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)

C(1)	8535(5)	8751(2)	126(2)	40(1)
C(2)	6942(6)	9105(3)	-188(3)	54(1)
C(3)	7054(8)	9525(3)	-826(3)	62(1)
C(4)	10141(7)	9245(3)	-900(2)	57(1)
C(5)	10139(6)	8824(3)	-255(2)	45(1)
N(1)	8485(5)	8365(3)	767(2)	61(1)
N(2)	8635(6)	9594(2)	-1171(2)	63(1)
O(1)	9002(6)	570(3)	7500	55(1)
I(1)	8544(1)	7251(1)	2500	39(1)
I(2)	3860(1)	5191(1)	2500	44(1)
I(3)	3547(1)	7828(1)	1253(1)	46(1)
Cd(1)	4818(1)	7019(1)	2500	38(1)

Table 3. Bond lengths [Å] and angles [°] for 4ampCdI·H2O.

C(1)-N(1)	1.332(5)
C(1)-C(5)	1.389(5)
C(1)-C(2)	1.417(6)
C(2)-C(3)	1.351(6)
C(2)-H(2)	0.9300
C(3)-N(2)	1.340(7)
C(3)-H(3)	0.9300
C(4)-N(2)	1.329(6)
C(4)-C(5)	1.360(6)
C(4)-H(4)	0.9300
C(5)-H(5)	0.9300
N(1)-H(1A)	0.8600
N(1)-H(1B)	0.8600
N(2)-H(2A)	0.8600
O(1)-H(1D)	0.893(4)
O(1)-H(1C)	0.828(4)
I(1)-Cd(1)	2.7774(5)
I(2)-Cd(1)	2.7902(5)
I(3)-Cd(1)	2.7886(3)
Cd(1)-I(3)#1	2.7886(3)
N(1)-C(1)-C(5)	121.4(4)

N(1)-C(1)-C(2)	120.7(4)
C(5)-C(1)-C(2)	117.9(4)
C(3)-C(2)-C(1)	119.1(4)
C(3)-C(2)-H(2)	120.5
C(1)-C(2)-H(2)	120.5
N(2)-C(3)-C(2)	121.1(4)
N(2)-C(3)-H(3)	119.5
C(2)-C(3)-H(3)	119.5
N(2)-C(4)-C(5)	121.1(4)
N(2)-C(4)-H(4)	119.4
C(5)-C(4)-H(4)	119.4
C(4)-C(5)-C(1)	119.6(4)
C(4)-C(5)-H(5)	120.2
C(1)-C(5)-H(5)	120.2
C(1)-N(1)-H(1A)	120.0
C(1)-N(1)-H(1B)	120.0
H(1A)-N(1)-H(1B)	120.0
C(4)-N(2)-C(3)	121.2(4)
C(4)-N(2)-H(2A)	119.4
C(3)-N(2)-H(2A)	119.4
H(1D)-O(1)-H(1C)	139.2(5)
I(1)-Cd(1)-I(3)	106.385(11)
I(1)-Cd(1)-I(3)#1	106.385(11)
I(3)-Cd(1)-I(3)#1	113.984(18)
I(1)-Cd(1)-I(2)	111.784(16)
I(3)-Cd(1)-I(2)	109.151(11)
I(3)#1-Cd(1)-I(2)	109.151(11)

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters ($Å^2 \times 10^3$)for 4ampCdI·H2O. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(1)	45(2)	35(2)	40(2)	0(2)	-3(2)	-3(2)

C(2)	42(2)	55(2)	64(3)	6(2)	-8(2)	0(2)
C(3)	74(3)	55(3)	56(3)	2(2)	-20(2)	3(2)
C(4)	72(3)	46(2)	52(2)	-8(2)	15(2)	-3(2)
C(5)	46(2)	42(2)	48(2)	-5(2)	4(2)	1(2)
N(1)	61(2)	69(2)	54(2)	18(2)	5(2)	4(2)
N(2)	113(4)	45(2)	30(2)	4(2)	-4(2)	-3(2)
O(1)	62(3)	55(2)	46(2)	0	0	-4(2)
I(1)	34(1)	42(1)	42(1)	0	0	-3(1)
I(2)	44(1)	37(1)	51(1)	0	0	-5(1)
I(3)	40(1)	53(1)	44(1)	10(1)	-6(1)	-2(1)
Cd(1)	37(1)	39(1)	38(1)	0	0	-1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 4ampCdI·H2O.

	x	y	z	U(eq)
H(2)	5834	9048	42	64
H(3)	6018	9770	-1030	74
H(4)	11214	9290	-1155	68
H(5)	11205	8587	-69	54
H(1A)	9459	8154	954	73
H(1B)	7478	8326	994	73
H(2A)	8675	9869	-1575	75
H(1D)	7916	306	7500	65
H(1C)	10084	426	7500	65

Table 6. Torsion angles [°] for 4ampCdI·H2O.

N(1)-C(1)-C(2)-C(3)	177.3(4)
C(5)-C(1)-C(2)-C(3)	-2.4(6)
C(1)-C(2)-C(3)-N(2)	1.4(7)
N(2)-C(4)-C(5)-C(1)	0.4(6)
N(1)-C(1)-C(5)-C(4)	-178.3(4)
C(2)-C(1)-C(5)-C(4)	1.5(6)
C(5)-C(4)-N(2)-C(3)	-1.6(7)

C(2)-C(3)-N(2)-C(4)	0.6(7)

Symmetry transformations used to generate equivalent atoms:

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

Table 7. Hydrogen bonds for 4ampCdI·H2O [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...I(3)#2	0.86	3.11	3.935(4)	160.7
N(1)-H(1B)...I(3)	0.86	3.04	3.848(4)	157.5
N(2)-H(2A)...O(1)#3	0.86	2.04	2.892(4)	174.5
O(1)-H(1D)...I(2)#4	0.893(4)	3.09	3.967(4)	167.9(3)
O(1)-H(1C)...I(2)#5	0.828(4)	2.94	3.765(4)	176.9(3)

Symmetry transformations used to generate equivalent atoms:

#1 x,y,-z+1/2 #2 x+1,y,z #3 x,y+1,z-1 #4 x,-y+1/2,z+1/2

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

Crystallographic Data for Bis(4-aminopyridinium) tetrachloromercurate(II) monohydrate

Table 1. Crystal data and structure refinement for 4ampHgCl·H2O.

Identification code	4ampHgCl·H2O	
Empirical formula	C10 H16 Cl4 Hg N4 O	
Formula weight	550.53	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P b c m	
Unit cell dimensions	a = 6.5735(5) Å	α= 90°.
	b = 13.6799(10) Å	β= 90°.
	c = 18.7593(14) Å	γ = 90°.
Volume	1686.9(2) Å^3	
Z	4	
Density (calculated)	2.168 Mg/m^3	
Absorption coefficient	9.757 mm^{-1}	
F(000)	1040	
Crystal size	0.3 x 0.2 x 0.2 mm^3	
Theta range for data collection	3.79 to 27.00°.	
Index ranges	-8<=h<=8, -17<=k<=17, -20<=l<=23	
Reflections collected	12670	
Independent reflections	1895 [R(int) = 0.0489]	
Completeness to theta = 25.00°	99.5 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1895 / 0 / 99	
Goodness-of-fit on F^2	0.842	
Final R indices [I>2sigma(I)]	R1 = 0.0219, wR2 = 0.0350	
R indices (all data)	R1 = 0.0440, wR2 = 0.0369	
Largest diff. peak and hole	0.876 and -0.798 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for 4ampHgCl·H2O. U(eq) is defined as one third of the trace of the orthogonalized U$_{ij}$ tensor.

	x	y	z	U(eq)
C(1)	6426(6)	3717(2)	4802(2)	36(1)

C(2)	4631(6)	3736(2)	5202(2)	47(1)
C(3)	4699(7)	4020(2)	5894(2)	56(1)
C(4)	8161(7)	4256(3)	5836(2)	62(1)
C(5)	8210(6)	3969(3)	5152(2)	47(1)
Cl(1)	6412(2)	2523(1)	2500	46(1)
Cl(2)	10995(2)	568(1)	2500	55(1)
Cl(3)	11406(1)	3109(1)	1382(1)	56(1)
Hg(1)	10181(1)	2340(1)	2500	50(1)
N(1)	6433(5)	3466(2)	4122(2)	51(1)
N(2)	6426(6)	4292(2)	6197(2)	61(1)
O(1)	4261(7)	4728(3)	2500	67(1)

Table 3. Bond lengths [Å] and angles [°] for 4ampHgCl·H2O.

C(1)-N(1)	1.322(4)
C(1)-C(5)	1.387(5)
C(1)-C(2)	1.398(5)
C(2)-C(3)	1.356(5)
C(2)-H(2)	0.9300
C(3)-N(2)	1.323(5)
C(3)-H(3)	0.9300
C(4)-N(2)	1.328(5)
C(4)-C(5)	1.342(5)
C(4)-H(4)	0.9300
C(5)-H(5)	0.9300
Cl(1)-Hg(1)	2.4903(12)
Cl(2)-Hg(1)	2.4826(14)
Cl(3)-Hg(1)	2.4796(9)
Hg(1)-Cl(3)#1	2.4796(9)
N(1)-H(1A)	0.8600
N(1)-H(1B)	0.8600
N(2)-H(2A)	0.8600
O(1)-H(1C)	0.942(4)
O(1)-H(1D)	0.747(5)
N(1)-C(1)-C(5)	121.2(4)
N(1)-C(1)-C(2)	121.7(3)

C(5)-C(1)-C(2)	117.0(3)
C(3)-C(2)-C(1)	119.4(4)
C(3)-C(2)-H(2)	120.3
C(1)-C(2)-H(2)	120.3
N(2)-C(3)-C(2)	121.3(4)
N(2)-C(3)-H(3)	119.3
C(2)-C(3)-H(3)	119.3
N(2)-C(4)-C(5)	121.3(4)
N(2)-C(4)-H(4)	119.4
C(5)-C(4)-H(4)	119.4
C(4)-C(5)-C(1)	120.3(4)
C(4)-C(5)-H(5)	119.8
C(1)-C(5)-H(5)	119.8
Cl(3)#1-Hg(1)-Cl(3)	115.44(5)
Cl(3)#1-Hg(1)-Cl(2)	110.14(3)
Cl(3)-Hg(1)-Cl(2)	110.14(3)
Cl(3)#1-Hg(1)-Cl(1)	106.27(3)
Cl(3)-Hg(1)-Cl(1)	106.27(3)
Cl(2)-Hg(1)-Cl(1)	108.21(4)
C(1)-N(1)-H(1A)	120.0
C(1)-N(1)-H(1B)	120.0
H(1A)-N(1)-H(1B)	120.0
C(3)-N(2)-C(4)	120.5(3)
C(3)-N(2)-H(2A)	119.7
C(4)-N(2)-H(2A)	119.7
H(1C)-O(1)-H(1D)	119.0(5)

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for 4ampHgCl·H2O. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(1)	43(2)	30(2)	34(2)	1(2)	-1(2)	1(2)
C(2)	45(2)	45(2)	50(2)	-1(2)	2(2)	1(2)

C(3)	71(3)	43(2)	54(3)	6(2)	25(2)	10(2)
C(4)	61(3)	64(3)	60(3)	1(2)	-20(2)	0(2)
C(5)	46(2)	56(3)	39(2)	-6(2)	-4(2)	2(2)
Cl(1)	44(1)	60(1)	35(1)	0	0	5(1)
Cl(2)	61(1)	54(1)	50(1)	0	0	5(1)
Cl(3)	46(1)	79(1)	44(1)	17(1)	5(1)	0(1)
Hg(1)	54(1)	62(1)	35(1)	0	0	4(1)
N(1)	55(2)	63(2)	35(2)	-8(2)	1(2)	0(2)
N(2)	96(3)	59(2)	28(2)	-1(2)	-7(2)	5(2)
O(1)	108(4)	60(3)	34(2)	0	0	16(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 4ampHgCl·H2O.

	x	y	z	U(eq)
H(2)	3402	3554	4995	56
H(3)	3507	4025	6161	67
H(4)	9366	4433	6061	74
H(5)	9445	3938	4911	56
H(1A)	7558	3457	3888	61
H(1B)	5313	3312	3913	61
H(2A)	6425	4493	6632	73
H(1C)	4871	4105	2500	200(40)
H(1D)	4926	5171	2500	250(70)

Table 6. Torsion angles [°] for 4ampHgCl·H2O.

N(1)-C(1)-C(2)-C(3)	-178.5(3)
C(5)-C(1)-C(2)-C(3)	1.9(5)
C(1)-C(2)-C(3)-N(2)	0.8(5)
N(2)-C(4)-C(5)-C(1)	1.1(6)
N(1)-C(1)-C(5)-C(4)	177.6(3)
C(2)-C(1)-C(5)-C(4)	-2.8(5)
C(2)-C(3)-N(2)-C(4)	-2.6(5)
C(5)-C(4)-N(2)-C(3)	1.7(6)

Symmetry transformations used to generate equivalent atoms:

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

Table 7. Hydrogen bonds for 4ampHgCl·H2O [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...Cl(3)#1	0.86	2.62	3.437(3)	158.5
N(1)-H(1B)...Cl(3)#2	0.86	2.64	3.472(3)	162.4
N(2)-H(2A)...O(1)#3	0.86	2.00	2.824(4)	160.6
O(1)-H(1C)...Cl(1)	0.942(4)	2.3891(12)	3.331(4)	179.9(3)
O(1)-H(1D)...Cl(2)#4	0.747(5)	2.7358(13)	3.324(5)	137.3(3)

Symmetry transformations used to generate equivalent atoms:

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

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

Crystallographic Data for Bis(4-aminopyridinium) tetrabromomercurate(II) monohydrate

Table 1. Crystal data and structure refinement for 4ampHgBr·H2O.

Identification code	4ampHgBr·H2O	
Empirical formula	C10 H16 Br4 Hg N4 O	
Formula weight	728.50	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P b c m	
Unit cell dimensions	a = 6.8625(3) Å	α= 90°.
	b = 14.0041(6) Å	β= 90°.
	c = 18.8161(9) Å	γ = 90°.
Volume	1808.29(14) Å3	
Z	4	
Density (calculated)	2.676 Mg/m3	
Absorption coefficient	17.350 mm-1	
F(000)	1328	
Crystal size	0.3 x 0.3 x 0.1 mm3	
Theta range for data collection	2.16 to 27.00°.	
Index ranges	-8<=h<=8, -17<=k<=17, -24<=l<=18	
Reflections collected	12149	
Independent reflections	2031 [R(int) = 0.0837]	
Completeness to theta = 27.00°	100.0 %	
Refinement method	Full-matrix least-squares on F2	
Data / restraints / parameters	2031 / 3 / 101	
Goodness-of-fit on F2	1.104	
Final R indices [I>2sigma(I)]	R1 = 0.0330, wR2 = 0.0630	
R indices (all data)	R1 = 0.0522, wR2 = 0.0676	
Largest diff. peak and hole1.746 and -1.376 e.Å-3		

Table 2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å² x 10³) for 4ampHgBr·H2O. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(1)	8573(8)	8727(4)	174(3)	34(1)

C(2)	6855(9)	9022(5)	-169(3)	50(2)
C(3)	6935(12)	9355(5)	-837(4)	61(2)
C(4)	10245(11)	9103(5)	-892(3)	56(2)
C(5)	10295(9)	8761(5)	-220(3)	44(2)
N(1)	8531(8)	8425(4)	840(2)	53(2)
N(2)	8601(11)	9410(4)	-1188(3)	60(2)
O(1)	9031(11)	389(5)	7500	57(2)
Br(1)	8624(1)	7397(1)	2500	41(1)
Br(2)	3901(1)	5372(1)	2500	47(1)
Br(3)	3576(1)	7982(1)	1338(1)	49(1)
Hg(1)	4860(1)	7168(1)	2500	43(1)

Table 3. Bond lengths [Å] and angles [°] for 4ampHgBr·H2O.

C(1)-N(1)	1.323(7)
C(1)-C(5)	1.396(8)
C(1)-C(2)	1.406(8)
C(2)-C(3)	1.342(9)
C(2)-H(2)	0.9300
C(3)-N(2)	1.323(9)
C(3)-H(3)	0.9300
C(4)-N(2)	1.331(9)
C(4)-C(5)	1.352(9)
C(4)-H(4)	0.9300
C(5)-H(5)	0.9300
N(1)-H(1A)	0.8600
N(1)-H(1B)	0.8600
N(2)-H(2A)	0.8600
O(1)-H(1D)	0.84(2)
O(1)-H(1E)	0.85(2)
Br(1)-Hg(1)	2.6027(9)
Br(2)-Hg(1)	2.5996(11)
Br(3)-Hg(1)	2.6193(6)
Hg(1)-Br(3)#1	2.6193(6)
N(1)-C(1)-C(5)	122.2(5)
N(1)-C(1)-C(2)	120.7(5)

C(5)-C(1)-C(2)	117.1(5)
C(3)-C(2)-C(1)	119.8(6)
C(3)-C(2)-H(2)	120.1
C(1)-C(2)-H(2)	120.1
N(2)-C(3)-C(2)	121.6(7)
N(2)-C(3)-H(3)	119.2
C(2)-C(3)-H(3)	119.2
N(2)-C(4)-C(5)	121.9(6)
N(2)-C(4)-H(4)	119.1
C(5)-C(4)-H(4)	119.1
C(4)-C(5)-C(1)	119.2(6)
C(4)-C(5)-H(5)	120.4
C(1)-C(5)-H(5)	120.4
C(1)-N(1)-H(1A)	120.0
C(1)-N(1)-H(1B)	120.0
H(1A)-N(1)-H(1B)	120.0
C(3)-N(2)-C(4)	120.3(6)
C(3)-N(2)-H(2A)	119.9
C(4)-N(2)-H(2A)	119.9
H(1D)-O(1)-H(1E)	124(6)
Br(2)-Hg(1)-Br(1)	111.76(3)
Br(2)-Hg(1)-Br(3)#1	109.64(2)
Br(1)-Hg(1)-Br(3)#1	106.265(19)
Br(2)-Hg(1)-Br(3)	109.64(2)
Br(1)-Hg(1)-Br(3)	106.265(19)
Br(3)#1-Hg(1)-Br(3)	113.23(3)

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for 4ampHgBr·H2O. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(1)	37(3)	27(3)	37(3)	-3(2)	-2(2)	-1(2)
C(2)	39(3)	62(5)	48(3)	3(4)	-6(3)	-4(3)

C(3)	69(5)	66(5)	48(4)	3(4)	-20(4)	-1(4)
C(4)	71(5)	49(5)	49(3)	-9(3)	24(4)	-8(4)
C(5)	42(3)	44(4)	48(3)	-5(3)	9(3)	-2(3)
N(1)	45(3)	76(5)	36(3)	12(3)	2(2)	4(3)
N(2)	102(6)	50(4)	29(3)	3(2)	-2(3)	-6(4)
O(1)	68(5)	60(5)	42(3)	0	0	5(4)
Br(1)	35(1)	52(1)	36(1)	0	0	-4(1)
Br(2)	46(1)	46(1)	48(1)	0	0	-6(1)
Br(3)	37(1)	67(1)	43(1)	14(1)	-5(1)	-1(1)
Hg(1)	42(1)	51(1)	37(1)	0	0	-2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for 4ampHgBr·H2O.

	x	y	z	U(eq)
H(2)	5666	8987	67	59
H(3)	5792	9552	-1058	73
H(4)	11393	9124	-1154	67
H(5)	11462	8552	-23	53
H(1A)	9588	8241	1044	63
H(1B)	7447	8412	1069	63
H(2A)	8620	9646	-1610	72
H(1D)	10250(30)	400(60)	7500	68
H(1E)	8330(100)	890(40)	7500	68

Table 6. Torsion angles [°] for 4ampHgBr·H2O.

N(1)-C(1)-C(2)-C(3)	177.9(6)
C(5)-C(1)-C(2)-C(3)	-2.6(10)
C(1)-C(2)-C(3)-N(2)	0.3(12)
N(2)-C(4)-C(5)-C(1)	0.2(10)
N(1)-C(1)-C(5)-C(4)	-178.1(6)
C(2)-C(1)-C(5)-C(4)	2.3(9)
C(2)-C(3)-N(2)-C(4)	2.3(11)
C(5)-C(4)-N(2)-C(3)	-2.5(11)

Symmetry transformations used to generate equivalent atoms:

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

Table 7. Hydrogen bonds for 4ampHgBr·H2O [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...Br(3)#2	0.86	2.81	3.639(5)	161.1
N(1)-H(1B)...Br(3)	0.86	2.77	3.581(5)	157.8
N(2)-H(2A)...O(1)#3	0.86	1.99	2.838(7)	168.2
O(1)-H(1D)...Br(2)#4	0.84(2)	2.73(4)	3.508(8)	156(8)
O(1)-H(1E)...Br(3)#5	0.85(2)	2.996(14)	3.632(6)	132.9(7)
O(1)-H(1E)...Br(3)#6	0.85(2)	2.996(14)	3.632(6)	132.9(7)

Symmetry transformations used to generate equivalent atoms:

#1 x,y,-z+1/2 #2 x+1,y,z #3 x,y+1,z-1 #4 x+1,-y+1/2,z+1/2

#5 -x+1,-y+1,-z+1 #6 -x+1,-y+1,z+1/2

Crystallographic Data for Bis(4-aminopyridinium) tetraiodomercurate(II) monohydrate

Table 1. Crystal data and structure refinement for 4ampHgI·H2O.

Identification code	4ampHgI·H2O	
Empirical formula	C10 H16 Hg I4 N4 O	
Formula weight	916.46	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P b c m	
Unit cell dimensions	a = 7.2736(4) Å	α= 90°.
	b = 14.4831(7) Å	β= 90°.
	c = 18.5793(8) Å	γ = 90°.
Volume	1957.22(17) Å3	
Z	4	
Density (calculated)	3.110 Mg/m3	
Absorption coefficient	14.174 mm-1	
F(000)	1616	
Crystal size	0.49 x 0.40 x 0.24 mm3	
Theta range for data collection	2.19 to 27.00°.	
Index ranges	-8<=h<=9, -18<=k<=15, -23<=l<=23	
Reflections collected	13205	
Independent reflections	2211 [R(int) = 0.0485]	
Completeness to theta = 27.00°	100.0 %	
Refinement method	Full-matrix least-squares on F2	
Data / restraints / parameters	2211 / 3 / 102	
Goodness-of-fit on F2	1.108	
Final R indices [I>2sigma(I)]	R1 = 0.0224, wR2 = 0.0475	
R indices (all data)	R1 = 0.0262, wR2 = 0.0487	
Extinction coefficient	0.00128(5)	
Largest diff. peak and hole1.547 and -0.912 e.Å-3		

Table 2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å² x 10³) for 4ampHgI·H2O. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)

C(1)	8534(7)	8751(3)	129(2)	21(1)
C(2)	6934(8)	9114(3)	-184(3)	28(1)
C(3)	7034(9)	9546(4)	-821(3)	34(1)
C(4)	10171(9)	9261(4)	-903(3)	33(1)
C(5)	10176(7)	8827(3)	-260(2)	24(1)
N(1)	8488(7)	8347(3)	778(2)	32(1)
N(2)	8627(7)	9629(3)	-1170(2)	34(1)
O(1)	8910(8)	607(4)	7500	30(1)
I(1)	8641(1)	7217(1)	2500	21(1)
I(2)	3826(1)	5111(1)	2500	23(1)
I(3)	3572(1)	7794(1)	1250(1)	24(1)
Hg(1)	4879(1)	6945(1)	2500	24(1)

Table 3. Bond lengths [Å] and angles [°] for 4ampHgI·H2O.

C(1)-N(1)	1.339(6)
C(1)-C(5)	1.401(7)
C(1)-C(2)	1.403(7)
C(2)-C(3)	1.342(7)
C(2)-H(2)	0.9300
C(3)-N(2)	1.333(8)
C(3)-H(3)	0.9300
C(4)-N(2)	1.338(8)
C(4)-C(5)	1.349(7)
C(4)-H(4)	0.9300
C(5)-H(5)	0.9300
N(1)-H(1A)	0.8600
N(1)-H(1B)	0.8600
N(2)-H(2A)	0.8600
O(1)-H(1D)	0.823(19)
O(1)-H(1C)	0.83(2)
I(1)-Hg(1)	2.7642(6)
I(2)-Hg(1)	2.7650(5)
I(3)-Hg(1)	2.7940(3)
Hg(1)-I(3)#1	2.7940(3)
N(1)-C(1)-C(5)	121.3(5)

N(1)-C(1)-C(2)	121.1(5)
C(5)-C(1)-C(2)	117.6(4)
C(3)-C(2)-C(1)	119.7(5)
C(3)-C(2)-H(2)	120.1
C(1)-C(2)-H(2)	120.1
N(2)-C(3)-C(2)	121.2(5)
N(2)-C(3)-H(3)	119.4
C(2)-C(3)-H(3)	119.4
N(2)-C(4)-C(5)	121.0(5)
N(2)-C(4)-H(4)	119.5
C(5)-C(4)-H(4)	119.5
C(4)-C(5)-C(1)	119.5(5)
C(4)-C(5)-H(5)	120.3
C(1)-C(5)-H(5)	120.3
C(1)-N(1)-H(1A)	120.0
C(1)-N(1)-H(1B)	120.0
H(1A)-N(1)-H(1B)	120.0
C(3)-N(2)-C(4)	120.9(5)
C(3)-N(2)-H(2A)	119.5
C(4)-N(2)-H(2A)	119.6
H(1D)-O(1)-H(1C)	148(7)
I(1)-Hg(1)-I(2)	114.256(16)
I(1)-Hg(1)-I(3)	105.927(10)
I(2)-Hg(1)-I(3)	109.177(11)
I(1)-Hg(1)-I(3)#1	105.927(10)
I(2)-Hg(1)-I(3)#1	109.177(11)
I(3)-Hg(1)-I(3)#1	112.396(17)

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for 4ampHgI·H2O. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(1)	26(3)	17(2)	20(2)	-1(2)	-1(2)	2(2)

C(2)	25(3)	25(3)	35(3)	5(2)	-3(2)	-1(2)
C(3)	43(3)	27(3)	31(3)	0(2)	-14(2)	2(3)
C(4)	47(4)	25(3)	27(2)	-7(2)	13(2)	-3(3)
C(5)	29(3)	21(2)	22(2)	0(2)	2(2)	2(2)
N(1)	30(3)	35(3)	30(2)	9(2)	2(2)	2(2)
N(2)	59(3)	25(2)	17(2)	1(2)	-1(2)	-2(2)
O(1)	34(3)	27(3)	30(2)	0	0	3(3)
I(1)	22(1)	22(1)	21(1)	0	0	-2(1)
I(2)	25(1)	20(1)	25(1)	0	0	-2(1)
I(3)	23(1)	27(1)	23(1)	5(1)	-3(1)	-1(1)
Hg(1)	26(1)	23(1)	23(1)	0	0	-1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 4ampHgI·H2O.

	x	y	z	U(eq)
H(2)	5809	9056	50	34
H(3)	5972	9792	-1024	40
H(4)	11258	9305	-1164	40
H(5)	11260	8581	-77	29
H(1A)	9480	8128	963	38
H(1B)	7467	8307	1009	38
H(2A)	8664	9923	-1572	40
H(1D)	7780(30)	640(60)	7500	36
H(1C)	9840(60)	270(50)	7500	36

Table 6. Torsion angles [°] for 4ampHgI·H2O.

N(1)-C(1)-C(2)-C(3)	177.5(5)
C(5)-C(1)-C(2)-C(3)	-2.5(7)
C(1)-C(2)-C(3)-N(2)	0.8(8)
N(2)-C(4)-C(5)-C(1)	0.8(8)
N(1)-C(1)-C(5)-C(4)	-178.2(5)
C(2)-C(1)-C(5)-C(4)	1.7(7)
C(2)-C(3)-N(2)-C(4)	1.8(8)

C(5)-C(4)-N(2)-C(3)	-2.6(8)

Symmetry transformations used to generate equivalent atoms:

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

Table 7. Hydrogen bonds for 4ampHgI·H2O [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...I(3)#2	0.86	3.06	3.884(5)	160.6
N(1)-H(1A)...I(1)	0.86	3.20	3.596(4)	110.4
N(1)-H(1B)...I(3)	0.86	2.96	3.769(5)	156.7
N(2)-H(2A)...O(1)#3	0.86	2.00	2.856(5)	176.6
O(1)-H(1D)...I(2)#4	0.823(19)	3.07(3)	3.841(6)	156(7)
O(1)-H(1C)...I(2)#5	0.83(2)	2.95(3)	3.724(6)	155(7)

Symmetry transformations used to generate equivalent atoms:

#1 x,y,-z+1/2 #2 x+1,y,z #3 x,y+1,z-1 #4 x,-y+1/2,z+1/2

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