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Supporting information for article:

Coordination polymers of Cd^{II} and Pb^{II} derived from bipyridine–glycoluril ligand: influence of metal ion size and counter-ions

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poly[aqua[bis(4b,5,7,7a-tetrahydro-4b,7a-epiminomethanoimino-6H-imidazo[4,5-f] [1,10]-phenanthroline-6,13-dione)]-cadmium(II) diperchlorate dihydrate (CP 1)

Crystal data

$C_{28}H_{22}CdN_{12}O_5 \cdot 2(ClO_4) \cdot 2(H_2O)$	$F(000) = 1920$
$M_r = 953.91$	$D_x = 1.960$ Mg m^{-3}
Monoclinic, *I*2/*a*	Mo *K*α radiation, λ = 0.71073 Å
a = 15.146 (3) Å	Cell parameters from 9068 reflections
b = 12.2411 (11) Å	θ = 3.0–25.1°
c = 17.6555 (16) Å	μ = 0.94 mm^{-1}
β = 99.104 (2)°	*T* = 293 K
V = 3232.2 (8) Å^3	Rectangle, pale yellow
Z = 4	0.4 × 0.4 × 0.2 mm

Data collection

Bruker APEX-II CCD diffractometer	2683 reflections with $I > 2\sigma(I)$
ϕ and ω scans	$R_{int} = 0.037$
Absorption correction: multi-scan *SADABS* (Bruker, 2013)	$\theta_{max} = 25.1°$, $\theta_{min} = 3.0°$
$T_{min} = 0.685$, $T_{max} = 0.745$	*h* = -18→18
52684 measured reflections	*k* = -14→14
2886 independent reflections	*l* = -21→21

Refinement

Refinement on F^2	Primary atom site location: dual
Least-squares matrix: full	Hydrogen site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.026$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.064$	$w = 1/[\sigma^2(F_o^2) + (0.026P)^2 + 12.5975P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.11	$(\Delta/\sigma)_{max} = 0.001$
2886 reflections	$\Delta\rho_{max} = 0.60$ e Å^{-3}
316 parameters	$\Delta\rho_{min} = -0.54$ e Å^{-3}
0 restraints	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used

when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*Z*	U_{iso}*/U_{eq}	Occ. (<1)
Cd1	0.750000	0.30737 (2)	0.500000	0.01258 (9)	
O1	0.37182 (11)	0.76446 (14)	0.60525 (10)	0.0173 (4)	
O2	0.76411 (11)	0.84787 (14)	0.66612 (10)	0.0158 (4)	
O2W	0.7336 (3)	0.1334 (3)	0.5187 (2)	0.0257 (10)	0.5
H2WA	0.714757	0.122456	0.561996	0.039*	0.5
H2WB	0.784769	0.100096	0.524708	0.039*	0.5
N1	0.66664 (13)	0.37167 (16)	0.59002 (11)	0.0123 (4)	
N2	0.65803 (13)	0.46488 (16)	0.44986 (11)	0.0130 (4)	
N3	0.50303 (14)	0.67836 (17)	0.65646 (13)	0.0143 (4)	
H3	0.490 (2)	0.666 (3)	0.6973 (19)	0.021 (8)*	
N4	0.65267 (14)	0.79246 (17)	0.56882 (12)	0.0142 (4)	
H4	0.658 (2)	0.842 (3)	0.5350 (18)	0.021 (8)*	
N5	0.66208 (14)	0.71383 (17)	0.68209 (12)	0.0143 (4)	
H5	0.687 (2)	0.691 (3)	0.726 (2)	0.032 (9)*	
N6	0.49283 (14)	0.74908 (18)	0.54115 (12)	0.0142 (4)	
H6	0.475 (2)	0.790 (2)	0.5084 (18)	0.015 (8)*	
C1	0.63275 (15)	0.52730 (19)	0.50528 (13)	0.0107 (5)	
C2	0.66847 (16)	0.3219 (2)	0.65770 (15)	0.0157 (5)	
H2	0.6919 (18)	0.248 (2)	0.6607 (15)	0.013 (7)*	
C3	0.64942 (16)	0.5047 (2)	0.37848 (14)	0.0146 (5)	
H3A	0.6715 (18)	0.458 (2)	0.3422 (16)	0.012 (7)*	
C4	0.63718 (15)	0.47609 (19)	0.58194 (13)	0.0111 (5)	
C5	0.44929 (16)	0.73508 (19)	0.60191 (14)	0.0131 (5)	
C6	0.58955 (16)	0.6540 (2)	0.63680 (13)	0.0117 (5)	
C7	0.60242 (15)	0.63367 (19)	0.49133 (13)	0.0124 (5)	
C8	0.61586 (17)	0.6078 (2)	0.35898 (14)	0.0166 (5)	
H8	0.6053 (19)	0.633 (2)	0.3017 (17)	0.018 (7)*	
C9	0.64030 (16)	0.3720 (2)	0.71990 (14)	0.0159 (5)	
H9	0.6434 (18)	0.332 (2)	0.7748 (16)	0.014 (7)*	
C10	0.69842 (16)	0.79081 (19)	0.64124 (14)	0.0134 (5)	
C11	0.61116 (15)	0.53276 (19)	0.64262 (13)	0.0118 (5)	
C12	0.59320 (17)	0.6733 (2)	0.41651 (14)	0.0159 (5)	
H12	0.573 (2)	0.744 (3)	0.4060 (17)	0.021 (7)*	
C13	0.61223 (16)	0.4796 (2)	0.71210 (14)	0.0141 (5)	
H13	0.5949 (18)	0.513 (2)	0.7524 (16)	0.012 (7)*	
C14	0.58391 (16)	0.70852 (19)	0.55526 (14)	0.0125 (5)	

Cl1	0.56731 (4)	1.05285 (5)	0.65385 (3)	0.01767 (14)
O3	0.51764 (13)	1.13666 (16)	0.68744 (10)	0.0237 (4)
O4	0.52714 (17)	0.94950 (19)	0.66243 (18)	0.0537 (8)
O5	0.5623 (2)	1.0768 (2)	0.57469 (13)	0.0745 (11)
O6	0.65599 (14)	1.05191 (19)	0.69196 (15)	0.0437 (6)
O1W	0.65439 (14)	0.95242 (16)	0.44434 (12)	0.0222 (4)
H1WA	0.605 (3)	0.978 (4)	0.426 (3)	0.064 (14)*
H1WB	0.677 (3)	0.930 (4)	0.407 (3)	0.064 (14)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.01452 (14)	0.00776 (13)	0.01630 (14)	0.000	0.00499 (10)	0.000
O1	0.0151 (9)	0.0163 (9)	0.0192 (9)	0.0029 (7)	-0.0008 (7)	-0.0031 (7)
O2	0.0146 (8)	0.0157 (9)	0.0152 (9)	-0.0041 (7)	-0.0031 (7)	-0.0019 (7)
O2W	0.030 (3)	0.0144 (17)	0.028 (3)	-0.0005 (16)	-0.0090 (18)	0.0029 (15)
N1	0.0119 (10)	0.0087 (10)	0.0162 (10)	-0.0006 (8)	0.0024 (8)	0.0007 (8)
N2	0.0138 (10)	0.0123 (10)	0.0125 (10)	-0.0024 (8)	0.0008 (8)	-0.0017 (8)
N3	0.0136 (10)	0.0181 (11)	0.0115 (10)	0.0034 (8)	0.0030 (8)	0.0028 (9)
N4	0.0181 (11)	0.0121 (10)	0.0113 (10)	-0.0042 (8)	-0.0010 (8)	0.0012 (8)
N5	0.0166 (11)	0.0134 (10)	0.0109 (10)	-0.0032 (8)	-0.0047 (8)	0.0009 (8)
N6	0.0148 (10)	0.0137 (11)	0.0124 (10)	0.0044 (8)	-0.0032 (8)	0.0037 (9)
C1	0.0080 (11)	0.0126 (11)	0.0107 (11)	-0.0024 (9)	-0.0014 (9)	-0.0007 (9)
C2	0.0154 (12)	0.0112 (12)	0.0207 (13)	-0.0013 (10)	0.0036 (10)	0.0059 (10)
C3	0.0137 (12)	0.0193 (13)	0.0109 (12)	-0.0034 (10)	0.0017 (9)	-0.0033 (10)
C4	0.0090 (11)	0.0106 (11)	0.0130 (11)	-0.0015 (9)	0.0001 (9)	0.0013 (9)
C5	0.0148 (12)	0.0090 (11)	0.0145 (12)	-0.0003 (9)	-0.0013 (9)	-0.0036 (9)
C6	0.0125 (11)	0.0117 (12)	0.0100 (11)	0.0001 (9)	-0.0013 (9)	-0.0007 (9)
C7	0.0124 (11)	0.0129 (12)	0.0111 (11)	-0.0013 (9)	-0.0003 (9)	0.0000 (9)
C8	0.0181 (12)	0.0191 (13)	0.0116 (12)	-0.0042 (10)	-0.0010 (10)	0.0008 (10)
C9	0.0146 (12)	0.0163 (13)	0.0166 (12)	-0.0009 (10)	0.0024 (10)	0.0054 (10)
C10	0.0169 (12)	0.0097 (12)	0.0135 (12)	0.0043 (9)	0.0016 (10)	-0.0009 (9)
C11	0.0087 (11)	0.0129 (12)	0.0127 (12)	0.0001 (9)	-0.0016 (9)	0.0010 (9)
C12	0.0193 (13)	0.0128 (13)	0.0142 (12)	0.0001 (10)	-0.0016 (10)	0.0024 (10)
C13	0.0132 (12)	0.0164 (12)	0.0130 (12)	-0.0014 (10)	0.0026 (9)	-0.0020 (10)
C14	0.0127 (12)	0.0112 (12)	0.0127 (11)	0.0004 (9)	-0.0012 (9)	0.0020 (9)
Cl1	0.0200 (3)	0.0188 (3)	0.0134 (3)	0.0048 (2)	0.0001 (2)	-0.0002 (2)
O3	0.0316 (11)	0.0204 (10)	0.0198 (10)	0.0068 (8)	0.0065 (8)	-0.0031 (8)
O4	0.0507 (15)	0.0245 (12)	0.094 (2)	-0.0173 (11)	0.0379 (15)	-0.0302 (13)
O5	0.141 (3)	0.072 (2)	0.0133 (11)	0.076 (2)	0.0223 (14)	0.0138 (12)
O6	0.0219 (11)	0.0406 (14)	0.0635 (16)	0.0056 (10)	-0.0095 (10)	-0.0041 (12)
O1W	0.0199 (10)	0.0218 (10)	0.0241 (11)	0.0022 (8)	0.0009 (9)	-0.0043 (8)

Geometric parameters (Å, º)

Cd1—O1^{i}	2.5585 (17)	N6—C5	1.356 (3)
Cd1—O1^{ii}	2.5585 (17)	N6—C14	1.450 (3)
Cd1—O2W	2.176 (3)	C1—C4	1.483 (3)
Cd1—O2W^{iii}	2.176 (3)	C1—C7	1.390 (3)
Cd1—N1^{iii}	2.318 (2)	C2—H2	0.97 (3)
Cd1—N1	2.318 (2)	C2—C9	1.383 (4)
Cd1—N2^{iii}	2.460 (2)	C3—H3A	0.96 (3)
Cd1—N2	2.460 (2)	C3—C8	1.384 (4)
O1—C5	1.238 (3)	C4—C11	1.385 (3)
O2—C10	1.238 (3)	C6—C11	1.520 (3)
O2W—H2WA	0.8668	C6—C14	1.577 (3)
O2W—H2WB	0.8675	C7—C12	1.393 (3)
O2W—H2WB^{iii}	0.874 (9)	C7—C14	1.514 (3)
N1—C2	1.338 (3)	C8—H8	1.05 (3)
N1—C4	1.354 (3)	C8—C12	1.380 (4)
N2—C1	1.344 (3)	C9—H9	1.08 (3)
N2—C3	1.338 (3)	C9—C13	1.384 (4)
N3—H3	0.79 (3)	C11—C13	1.387 (3)
N3—C5	1.351 (3)	C12—H12	0.92 (3)
N3—C6	1.439 (3)	C13—H13	0.90 (3)
N4—H4	0.86 (3)	Cl1—O3	1.4529 (19)
N4—C10	1.355 (3)	Cl1—O4	1.422 (2)
N4—C14	1.456 (3)	Cl1—O5	1.418 (2)
N5—H5	0.86 (4)	Cl1—O6	1.404 (2)
N5—C6	1.451 (3)	O1W—H1WA	0.83 (5)
N5—C10	1.355 (3)	O1W—H1WB	0.84 (5)
N6—H6	0.78 (3)		

O1^{ii}—Cd1—O1^{i}	139.80 (8)	N2—C1—C7	121.9 (2)
O2W^{iii}—Cd1—O1^{i}	71.77 (12)	C7—C1—C4	121.6 (2)
O2W—Cd1—O1^{i}	68.89 (12)	N1—C2—H2	115.4 (16)
O2W—Cd1—O1^{ii}	71.77 (12)	N1—C2—C9	122.8 (2)
O2W^{iii}—Cd1—O1^{ii}	68.89 (12)	C9—C2—H2	121.8 (16)
O2W^{iii}—Cd1—O2W	23.6 (2)	N2—C3—H3A	114.8 (16)
O2W^{iii}—Cd1—N1^{iii}	98.07 (12)	N2—C3—C8	123.0 (2)
O2W^{iii}—Cd1—N1	121.62 (12)	C8—C3—H3A	122.2 (16)
O2W—Cd1—N1	98.07 (12)	N1—C4—C1	117.5 (2)
O2W—Cd1—N1^{iii}	121.63 (12)	N1—C4—C11	121.4 (2)
O2W—Cd1—N2	138.60 (13)	C11—C4—C1	121.1 (2)
O2W—Cd1—N2^{iii}	141.68 (13)	O1—C5—N3	125.8 (2)

O2W^{iii}—Cd1—N2	141.68 (13)	O1—C5—N6	125.8 (2)
O2W^{iii}—Cd1—N2^{iii}	138.60 (13)	N3—C5—N6	108.4 (2)
N1—Cd1—O1^{i}	91.56 (6)	N3—C6—N5	113.7 (2)
N1^{iii}—Cd1—O1^{i}	101.90 (6)	N3—C6—C11	112.4 (2)
N1^{iii}—Cd1—O1^{ii}	91.56 (6)	N3—C6—C14	102.28 (18)
N1—Cd1—O1^{ii}	101.90 (6)	N5—C6—C11	108.63 (19)
N1^{iii}—Cd1—N1	140.31 (10)	N5—C6—C14	102.51 (19)
N1—Cd1—N2	69.01 (7)	C11—C6—C14	117.06 (19)
N1—Cd1—N2^{iii}	79.98 (7)	C1—C7—C12	118.4 (2)
N1^{iii}—Cd1—N2	79.98 (7)	C1—C7—C14	122.0 (2)
N1^{iii}—Cd1—N2^{iii}	69.01 (7)	C12—C7—C14	119.6 (2)
N2—Cd1—O1^{ii}	72.89 (6)	C3—C8—H8	120.5 (16)
N2^{iii}—Cd1—O1^{ii}	146.41 (6)	C12—C8—C3	118.1 (2)
N2^{iii}—Cd1—O1^{i}	72.89 (6)	C12—C8—H8	121.3 (16)
N2—Cd1—O1^{i}	146.41 (6)	C2—C9—H9	122.2 (15)
N2^{iii}—Cd1—N2	76.78 (9)	C2—C9—C13	118.2 (2)
C5—O1—Cd1^{ii}	116.47 (15)	C13—C9—H9	119.5 (15)
Cd1—O2W—H2WA	110.2	O2—C10—N4	126.1 (2)
Cd1—O2W—H2WB	110.9	O2—C10—N5	125.1 (2)
Cd1—O2W—H2WB^{iii}	110.5 (12)	N4—C10—N5	108.8 (2)
H2WA—O2W—H2WB^{iii}	126.8	C4—C11—C6	121.4 (2)
H2WA—O2W—H2WB	103.4	C4—C11—C13	119.0 (2)
H2WB—O2W—H2WB^{iii}	92.4	C13—C11—C6	119.4 (2)
C2—N1—Cd1	121.40 (16)	C7—C12—H12	119.7 (18)
C2—N1—C4	119.0 (2)	C8—C12—C7	119.7 (2)
C4—N1—Cd1	117.03 (15)	C8—C12—H12	120.6 (18)
C1—N2—Cd1	113.20 (15)	C9—C13—C11	119.7 (2)
C3—N2—Cd1	126.14 (16)	C9—C13—H13	118.7 (18)
C3—N2—C1	118.8 (2)	C11—C13—H13	121.6 (18)
C5—N3—H3	123 (2)	N4—C14—C6	102.39 (18)
C5—N3—C6	113.8 (2)	N4—C14—C7	109.7 (2)
C6—N3—H3	123 (2)	N6—C14—N4	115.0 (2)
C10—N4—H4	125 (2)	N6—C14—C6	102.38 (19)
C10—N4—C14	113.0 (2)	N6—C14—C7	111.26 (19)
C14—N4—H4	122 (2)	C7—C14—C6	115.77 (19)
C6—N5—H5	122 (2)	O4—Cl1—O3	109.07 (13)
C10—N5—H5	123 (2)	O5—Cl1—O3	107.81 (13)
C10—N5—C6	113.2 (2)	O5—Cl1—O4	109.4 (2)
C5—N6—H6	121 (2)	O6—Cl1—O3	109.15 (13)
C5—N6—C14	112.9 (2)	O6—Cl1—O4	109.55 (16)
C14—N6—H6	124 (2)	O6—Cl1—O5	111.8 (2)
N2—C1—C4	116.6 (2)	H1WA—O1W—H1WB	106 (4)

Cd1^{ii}—O1—C5—N3	-120.1 (2)	C3—C8—C12—C7	-1.6 (4)
Cd1^{ii}—O1—C5—N6	56.0 (3)	C4—N1—C2—C9	0.9 (4)
Cd1—N1—C2—C9	162.07 (19)	C4—C1—C7—C12	-174.8 (2)
Cd1—N1—C4—C1	20.3 (3)	C4—C1—C7—C14	8.3 (3)
Cd1—N1—C4—C11	-160.37 (17)	C4—C11—C13—C9	0.9 (3)
Cd1—N2—C1—C4	-19.1 (2)	C5—N3—C6—N5	110.2 (2)
Cd1—N2—C1—C7	162.06 (17)	C5—N3—C6—C11	-125.9 (2)
Cd1—N2—C3—C8	-163.14 (18)	C5—N3—C6—C14	0.5 (3)
N1—C2—C9—C13	-2.4 (4)	C5—N6—C14—N4	-105.2 (2)
N1—C4—C11—C6	172.0 (2)	C5—N6—C14—C6	4.9 (3)
N1—C4—C11—C13	-2.5 (3)	C5—N6—C14—C7	129.2 (2)
N2—C1—C4—N1	0.4 (3)	C6—N3—C5—O1	179.2 (2)
N2—C1—C4—C11	-178.9 (2)	C6—N3—C5—N6	2.5 (3)
N2—C1—C7—C12	3.9 (3)	C6—N5—C10—O2	-175.8 (2)
N2—C1—C7—C14	-172.9 (2)	C6—N5—C10—N4	2.6 (3)
N2—C3—C8—C12	2.2 (4)	C6—C11—C13—C9	-173.7 (2)
N3—C6—C11—C4	126.9 (2)	C7—C1—C4—N1	179.3 (2)
N3—C6—C11—C13	-58.7 (3)	C7—C1—C4—C11	0.0 (3)
N3—C6—C14—N4	116.4 (2)	C10—N4—C14—N6	113.5 (2)
N3—C6—C14—N6	-3.1 (2)	C10—N4—C14—C6	3.3 (3)
N3—C6—C14—C7	-124.3 (2)	C10—N4—C14—C7	-120.1 (2)
N5—C6—C11—C4	-106.5 (2)	C10—N5—C6—N3	-110.0 (2)
N5—C6—C11—C13	68.0 (3)	C10—N5—C6—C11	124.1 (2)
N5—C6—C14—N4	-1.6 (2)	C10—N5—C6—C14	-0.4 (3)
N5—C6—C14—N6	-121.08 (19)	C11—C6—C14—N4	-120.4 (2)
N5—C6—C14—C7	117.7 (2)	C11—C6—C14—N6	120.2 (2)
C1—N2—C3—C8	0.3 (3)	C11—C6—C14—C7	-1.0 (3)
C1—C4—C11—C6	-8.7 (3)	C12—C7—C14—N4	-68.9 (3)
C1—C4—C11—C13	176.8 (2)	C12—C7—C14—N6	59.5 (3)
C1—C7—C12—C8	-1.3 (4)	C12—C7—C14—C6	175.9 (2)
C1—C7—C14—N4	107.9 (2)	C14—N4—C10—O2	174.5 (2)
C1—C7—C14—N6	-123.6 (2)	C14—N4—C10—N5	-3.8 (3)
C1—C7—C14—C6	-7.3 (3)	C14—N6—C5—O1	178.5 (2)
C2—N1—C4—C1	-177.7 (2)	C14—N6—C5—N3	-4.9 (3)
C2—N1—C4—C11	1.6 (3)	C14—C6—C11—C4	8.9 (3)
C2—C9—C13—C11	1.4 (4)	C14—C6—C11—C13	-176.6 (2)
C3—N2—C1—C4	175.4 (2)	C14—C7—C12—C8	175.6 (2)
C3—N2—C1—C7	-3.4 (3)		

Symmetry codes: (i) *x*+1/2, -*y*+1, *z*; (ii) -*x*+1, -*y*+1, -*z*+1; (iii) -*x*+3/2, *y*, -*z*+1.

poly[[bis(4b,5,7,7a-tetrahydro-4b,7a-epiminomethanoimino-6H-imidazo[4,5-f] [1,10]-phenanthroline-6,13-dione)]-lead(II) diperchlorate dihydrate (CP 1)

Crystal data

$C_{28}H_{20}N_{12}O_4Pb\cdot 2(ClO_4)\cdot 2(H_2O)$	$F(000)$ = 2016
M_r = 1030.68	D_x = 2.038 Mg m^{-3}
Monoclinic, *I*2/*a*	Mo *K*α radiation, λ = 0.71073 Å
a = 15.2909 (3) Å	Cell parameters from 3673 reflections
b = 14.2702 (3) Å	θ = 3.3–27.1°
c = 15.4064 (4) Å	μ = 5.27 mm^{-1}
β = 92.174 (2)°	*T* = 293 K
V = 3359.32 (13) Å^3	Block, colorless
Z = 4	0.2 × 0.15 × 0.15 mm

Data collection

Goniometer KM4/Xcalibur, detector: Sapphire3 diffractometer	3692 reflections with $I > 2\sigma(I)$
Detector resolution: 16.1048 pixels mm^{-1}	R_{int} = 0.019
ϕ and ω scans	θ_{max} = 29.2°, θ_{min} = 3.3°
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2013)	*h* = -19→20
T_{min} = 0.419, T_{max} = 0.505	*k* = -13→19
13500 measured reflections	*l* = -17→20
4008 independent reflections	

Refinement

Refinement on F^2	Primary atom site location: dual
Least-squares matrix: full	Hydrogen site location: mixed
$R[F^2 > 2\sigma(F^2)]$ = 0.026	H-atom parameters constrained
$wR(F^2)$ = 0.071	$w = 1/[\sigma^2(F_o^2) + (0.0427P)^2 + 7.4648P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.06	$(\Delta/\sigma)_{max}$ = 0.002
4008 reflections	$\Delta\rho_{max}$ = 1.23 e Å^{-3}
261 parameters	$\Delta\rho_{min}$ = -0.68 e Å^{-3}
0 restraints	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used

when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*Z*	U_{iso}*/U_{eq}
Pb1	0.250000	1.17680 (2)	0.500000	0.02815 (7)
O1	0.64130 (15)	0.77739 (18)	0.36773 (18)	0.0372 (6)
O2	0.26959 (19)	0.66658 (18)	0.33525 (19)	0.0404 (6)
N1	0.33977 (17)	1.02768 (19)	0.54831 (17)	0.0277 (5)
N2	0.34276 (18)	1.09595 (19)	0.38429 (19)	0.0307 (6)
N3	0.5092 (2)	0.8301 (2)	0.3118 (2)	0.0347 (7)
H3	0.524609	0.838666	0.259275	0.042*
N4	0.51911 (19)	0.7901 (2)	0.4497 (2)	0.0348 (6)
H4	0.542975	0.774416	0.499006	0.042*
N5	0.3547 (2)	0.7922 (2)	0.30041 (19)	0.0335 (6)
H5	0.334880	0.799381	0.247860	0.040*
N6	0.3708 (2)	0.7319 (2)	0.4313 (2)	0.0359 (7)
H6	0.365616	0.692282	0.472893	0.043*
C1	0.3433 (2)	0.9985 (2)	0.6304 (2)	0.0312 (7)
H1	0.323791	1.038775	0.673020	0.037*
C2	0.3744 (3)	0.9116 (3)	0.6554 (2)	0.0392 (8)
H2	0.377395	0.894472	0.713684	0.047*
C3	0.4008 (3)	0.8511 (3)	0.5927 (2)	0.0391 (8)
H3A	0.419915	0.791192	0.607692	0.047*
C4	0.3988 (2)	0.8798 (2)	0.5061 (2)	0.0264 (6)
C5	0.36904 (19)	0.9698 (2)	0.48686 (19)	0.0239 (6)
C6	0.4275 (2)	0.8128 (2)	0.4369 (2)	0.0255 (6)
C7	0.4220 (2)	0.8507 (2)	0.3411 (2)	0.0248 (6)
C8	0.37027 (19)	1.0061 (2)	0.3969 (2)	0.0238 (6)
C9	0.3990 (2)	0.9525 (2)	0.3293 (2)	0.0261 (6)
C10	0.4021 (2)	0.9922 (3)	0.2469 (2)	0.0362 (8)
H10	0.423001	0.957859	0.200775	0.043*
C11	0.3738 (3)	1.0830 (3)	0.2348 (2)	0.0407 (8)
H11	0.374725	1.110825	0.180262	0.049*
C12	0.3443 (3)	1.1318 (2)	0.3045 (2)	0.0364 (8)
H12	0.324491	1.192765	0.295703	0.044*
C13	0.5634 (2)	0.7964 (2)	0.3752 (2)	0.0302 (7)
C14	0.3269 (2)	0.7251 (2)	0.3545 (2)	0.0296 (7)
Cl1	0.38295 (7)	0.39334 (7)	0.39974 (7)	0.0464 (2)
O3	0.3955 (6)	0.4128 (6)	0.4862 (4)	0.172 (4)

O4	0.4482 (4)	0.3231 (3)	0.3789 (4)	0.1053 (19)
O5	0.3011 (5)	0.3618 (8)	0.3815 (9)	0.239 (6)
O6	0.3992 (6)	0.4650 (5)	0.3503 (6)	0.189 (4)
O1W	0.3527 (3)	0.5970 (3)	0.5563 (2)	0.0685 (10)
H1WA	0.305881	0.580653	0.528893	0.103*
H1WB	0.364616	0.551137	0.590015	0.103*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pb1	0.02771 (9)	0.02163 (9)	0.03463 (11)	0.000	-0.00537 (6)	0.000
O1	0.0263 (11)	0.0365 (14)	0.0483 (15)	0.0066 (10)	-0.0055 (10)	-0.0135 (11)
O2	0.0422 (14)	0.0376 (14)	0.0404 (15)	-0.0128 (11)	-0.0105 (12)	0.0041 (11)
N1	0.0308 (13)	0.0266 (13)	0.0253 (13)	0.0024 (11)	-0.0024 (10)	0.0009 (11)
N2	0.0339 (14)	0.0248 (13)	0.0330 (15)	0.0020 (11)	-0.0032 (11)	0.0065 (11)
N3	0.0292 (14)	0.0449 (18)	0.0301 (15)	0.0090 (12)	0.0009 (12)	0.0019 (12)
N4	0.0314 (14)	0.0424 (16)	0.0300 (15)	0.0096 (13)	-0.0082 (11)	0.0023 (13)
N5	0.0383 (15)	0.0345 (15)	0.0267 (14)	-0.0085 (13)	-0.0129 (12)	0.0042 (12)
N6	0.0498 (17)	0.0285 (14)	0.0287 (15)	-0.0082 (13)	-0.0087 (12)	0.0049 (12)
C1	0.0369 (16)	0.0312 (16)	0.0254 (16)	0.0019 (14)	-0.0004 (13)	-0.0013 (13)
C2	0.056 (2)	0.0384 (19)	0.0228 (16)	0.0062 (17)	0.0002 (15)	0.0053 (14)
C3	0.058 (2)	0.0311 (17)	0.0285 (18)	0.0098 (17)	-0.0008 (16)	0.0079 (14)
C4	0.0288 (14)	0.0270 (15)	0.0231 (15)	0.0026 (12)	-0.0037 (12)	0.0029 (12)
C5	0.0237 (13)	0.0245 (14)	0.0230 (14)	0.0004 (12)	-0.0047 (11)	0.0012 (11)
C6	0.0287 (15)	0.0231 (14)	0.0242 (15)	0.0024 (12)	-0.0051 (12)	0.0022 (11)
C7	0.0260 (14)	0.0263 (14)	0.0217 (14)	0.0004 (12)	-0.0033 (11)	0.0014 (11)
C8	0.0243 (13)	0.0231 (14)	0.0239 (15)	-0.0021 (11)	-0.0016 (11)	0.0038 (11)
C9	0.0254 (14)	0.0266 (15)	0.0258 (15)	-0.0007 (12)	-0.0044 (11)	0.0048 (12)
C10	0.0440 (19)	0.0387 (19)	0.0257 (17)	0.0021 (15)	0.0015 (14)	0.0037 (14)
C11	0.058 (2)	0.0376 (19)	0.0262 (17)	-0.0049 (17)	-0.0031 (16)	0.0116 (14)
C12	0.0446 (19)	0.0270 (17)	0.0372 (19)	0.0011 (15)	-0.0039 (15)	0.0113 (14)
C13	0.0305 (15)	0.0244 (14)	0.0351 (18)	0.0028 (13)	-0.0069 (13)	-0.0082 (13)
C14	0.0294 (15)	0.0268 (16)	0.0322 (17)	0.0002 (13)	-0.0026 (13)	-0.0001 (13)
Cl1	0.0514 (5)	0.0424 (5)	0.0454 (5)	0.0022 (4)	-0.0004 (4)	0.0062 (4)
O3	0.262 (9)	0.190 (7)	0.065 (3)	0.125 (7)	0.010 (4)	-0.013 (4)
O4	0.124 (4)	0.100 (4)	0.090 (4)	0.058 (3)	-0.019 (3)	-0.022 (3)
O5	0.070 (4)	0.236 (10)	0.407 (18)	-0.022 (6)	-0.059 (7)	-0.014 (12)
O6	0.211 (8)	0.141 (6)	0.220 (8)	0.040 (6)	0.083 (7)	0.126 (6)
O1W	0.097 (3)	0.059 (2)	0.050 (2)	0.020 (2)	0.0141 (19)	0.0186 (17)

Geometric parameters (Å, º)

Pb1—O1^{i}	2.662 (2)	C1—H1	0.9300
Pb1—O1^{ii}	2.662 (2)	C1—C2	1.378 (5)
Pb1—N1	2.625 (3)	C2—H2	0.9300
Pb1—N1^{iii}	2.625 (3)	C2—C3	1.368 (5)
Pb1—N2^{iii}	2.591 (3)	C3—H3A	0.9300
Pb1—N2	2.591 (3)	C3—C4	1.395 (5)
O1—C13	1.231 (4)	C4—C5	1.390 (4)
O2—C14	1.238 (4)	C4—C6	1.510 (4)
N1—C1	1.331 (4)	C5—C8	1.480 (4)
N1—C5	1.346 (4)	C6—C7	1.572 (4)
N2—C8	1.361 (4)	C7—C9	1.503 (4)
N2—C12	1.332 (4)	C8—C9	1.378 (5)
N3—H3	0.8600	C9—C10	1.392 (5)
N3—C7	1.454 (4)	C10—H10	0.9300
N3—C13	1.345 (5)	C10—C11	1.377 (5)
N4—H4	0.8600	C11—H11	0.9300
N4—C6	1.443 (4)	C11—C12	1.370 (6)
N4—C13	1.358 (5)	C12—H12	0.9300
N5—H5	0.8600	Cl1—O3	1.368 (6)
N5—C7	1.449 (4)	Cl1—O4	1.458 (5)
N5—C14	1.349 (4)	Cl1—O5	1.350 (7)
N6—H6	0.8600	Cl1—O6	1.305 (6)
N6—C6	1.445 (4)	O1W—H1WA	0.8498
N6—C14	1.342 (4)	O1W—H1WB	0.8505
O1^{i}—Pb1—O1^{ii}	151.57 (12)	C5—C4—C6	122.4 (3)
N1—Pb1—O1^{ii}	136.12 (9)	N1—C5—C4	122.1 (3)
N1^{iii}—Pb1—O1^{i}	136.12 (9)	N1—C5—C8	117.4 (3)
N1^{iii}—Pb1—O1^{ii}	71.18 (8)	C4—C5—C8	120.5 (3)
N1—Pb1—O1^{i}	71.17 (8)	N4—C6—N6	114.0 (3)
N1^{iii}—Pb1—N1	71.66 (12)	N4—C6—C4	110.7 (3)
N2—Pb1—O1^{ii}	85.69 (9)	N4—C6—C7	102.8 (3)
N2—Pb1—O1^{i}	107.09 (8)	N6—C6—C4	111.0 (3)
N2^{iii}—Pb1—O1^{ii}	107.09 (8)	N6—C6—C7	102.0 (2)
N2^{iii}—Pb1—O1^{i}	85.69 (9)	C4—C6—C7	116.0 (3)
N2^{iii}—Pb1—N1^{iii}	62.61 (8)	N3—C7—C6	101.8 (2)
N2—Pb1—N1	62.61 (8)	N3—C7—C9	111.8 (3)
N2—Pb1—N1^{iii}	74.80 (9)	N5—C7—N3	113.2 (3)
N2^{iii}—Pb1—N1	74.80 (9)	N5—C7—C6	102.7 (3)
N2^{iii}—Pb1—N2	127.11 (12)	N5—C7—C9	110.2 (3)
C13—O1—Pb1^{i}	116.9 (2)	C9—C7—C6	116.7 (3)
C1—N1—Pb1	121.7 (2)	N2—C8—C5	116.7 (3)

C1—N1—C5	118.3 (3)	N2—C8—C9	121.4 (3)
C5—N1—Pb1	118.8 (2)	C9—C8—C5	121.9 (3)
C8—N2—Pb1	119.7 (2)	C8—C9—C7	121.7 (3)
C12—N2—Pb1	119.6 (2)	C8—C9—C10	119.1 (3)
C12—N2—C8	118.5 (3)	C10—C9—C7	119.2 (3)
C7—N3—H3	123.4	C9—C10—H10	120.5
C13—N3—H3	123.4	C11—C10—C9	119.0 (3)
C13—N3—C7	113.2 (3)	C11—C10—H10	120.5
C6—N4—H4	123.8	C10—C11—H11	120.6
C13—N4—H4	123.8	C12—C11—C10	118.9 (3)
C13—N4—C6	112.5 (3)	C12—C11—H11	120.6
C7—N5—H5	123.9	N2—C12—C11	123.1 (3)
C14—N5—H5	123.9	N2—C12—H12	118.4
C14—N5—C7	112.2 (3)	C11—C12—H12	118.4
C6—N6—H6	123.5	O1—C13—N3	125.6 (4)
C14—N6—H6	123.5	O1—C13—N4	125.4 (3)
C14—N6—C6	112.9 (3)	N3—C13—N4	108.9 (3)
N1—C1—H1	118.4	O2—C14—N5	124.6 (3)
N1—C1—C2	123.3 (3)	O2—C14—N6	125.8 (3)
C2—C1—H1	118.4	N6—C14—N5	109.5 (3)
C1—C2—H2	120.7	O3—Cl1—O4	106.4 (4)
C3—C2—C1	118.6 (3)	O5—Cl1—O3	111.5 (7)
C3—C2—H2	120.7	O5—Cl1—O4	111.2 (6)
C2—C3—H3A	120.2	O6—Cl1—O3	112.8 (6)
C2—C3—C4	119.6 (3)	O6—Cl1—O4	105.3 (5)
C4—C3—H3A	120.2	O6—Cl1—O5	109.5 (7)
C3—C4—C6	119.5 (3)	H1WA—O1W—H1WB	104.5
C5—C4—C3	118.1 (3)		

Pb1^{i}—O1—C13—N3	139.8 (3)	C5—N1—C1—C2	-0.8 (5)
Pb1^{i}—O1—C13—N4	-37.5 (4)	C5—C4—C6—N4	116.7 (3)
Pb1—N1—C1—C2	166.6 (3)	C5—C4—C6—N6	-115.7 (3)
Pb1—N1—C5—C4	-164.8 (2)	C5—C4—C6—C7	0.0 (4)
Pb1—N1—C5—C8	16.4 (4)	C5—C8—C9—C7	6.5 (5)
Pb1—N2—C8—C5	-18.2 (4)	C5—C8—C9—C10	-177.2 (3)
Pb1—N2—C8—C9	162.7 (2)	C6—N4—C13—O1	-177.1 (3)
Pb1—N2—C12—C11	-164.2 (3)	C6—N4—C13—N3	5.2 (4)
N1—C1—C2—C3	-1.9 (6)	C6—N6—C14—O2	-174.4 (3)
N1—C5—C8—N2	1.0 (4)	C6—N6—C14—N5	5.7 (4)
N1—C5—C8—C9	180.0 (3)	C6—C4—C5—N1	176.9 (3)
N2—C8—C9—C7	-174.5 (3)	C6—C4—C5—C8	-4.3 (5)
N2—C8—C9—C10	1.8 (5)	C6—C7—C9—C8	-10.3 (4)

N3—C7—C9—C8	-126.9 (3)	C6—C7—C9—C10	173.4 (3)
N3—C7—C9—C10	56.8 (4)	C7—N3—C13—O1	-176.8 (3)
N4—C6—C7—N3	8.0 (3)	C7—N3—C13—N4	0.8 (4)
N4—C6—C7—N5	125.3 (3)	C7—N5—C14—O2	179.7 (3)
N4—C6—C7—C9	-114.0 (3)	C7—N5—C14—N6	-0.4 (4)
N5—C7—C9—C8	106.3 (3)	C7—C9—C10—C11	174.4 (3)
N5—C7—C9—C10	-70.0 (4)	C8—N2—C12—C11	-1.2 (5)
N6—C6—C7—N3	-110.4 (3)	C8—C9—C10—C11	-2.0 (5)
N6—C6—C7—N5	7.0 (3)	C9—C10—C11—C12	0.7 (6)
N6—C6—C7—C9	127.7 (3)	C10—C11—C12—N2	1.0 (6)
C1—N1—C5—C4	3.0 (5)	C12—N2—C8—C5	178.8 (3)
C1—N1—C5—C8	-175.8 (3)	C12—N2—C8—C9	-0.2 (5)
C1—C2—C3—C4	2.5 (6)	C13—N3—C7—N5	-115.2 (3)
C2—C3—C4—C5	-0.5 (6)	C13—N3—C7—C6	-5.7 (4)
C2—C3—C4—C6	-179.7 (4)	C13—N3—C7—C9	119.6 (3)
C3—C4—C5—N1	-2.3 (5)	C13—N4—C6—N6	101.2 (3)
C3—C4—C5—C8	176.4 (3)	C13—N4—C6—C4	-132.9 (3)
C3—C4—C6—N4	-64.1 (4)	C13—N4—C6—C7	-8.4 (4)
C3—C4—C6—N6	63.5 (4)	C14—N5—C7—N3	104.6 (3)
C3—C4—C6—C7	179.3 (3)	C14—N5—C7—C6	-4.4 (4)
C4—C5—C8—N2	-177.9 (3)	C14—N5—C7—C9	-129.4 (3)
C4—C5—C8—C9	1.2 (5)	C14—N6—C6—N4	-118.0 (3)
C4—C6—C7—N3	128.9 (3)	C14—N6—C6—C4	116.2 (3)
C4—C6—C7—N5	-113.7 (3)	C14—N6—C6—C7	-7.9 (4)
C4—C6—C7—C9	7.0 (4)		

Symmetry codes: (i) -*x*+1, -*y*+2, -*z*+1; (ii) *x*-1/2, -*y*+2, *z*; (iii) -*x*+1/2, *y*, -*z*+1.