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Isotypic one-dimensional coordination polymers: *catena*-poly[[dichloridocadmium]- μ -5,6-bis(pyridin-2-yl)pyrazine-2,3-dicarboxylato- $\kappa^2 N^5:N^6$] and *catena*-poly[[dichloridomercury(II)]- μ -5,6-bis(pyridin-2-yl)pyrazine-2,3-dicarboxylato- $\kappa^2 N^5:N^6$]

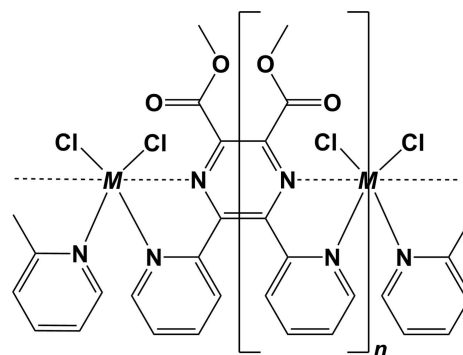
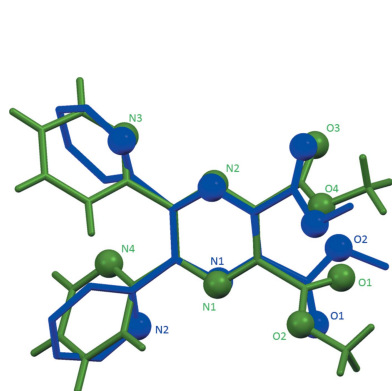
Montserrat Alfonso^a and Helen Stoeckli-Evans^{b*}

^aInstitute of Chemistry, University of Neuchâtel, Av. de Bellevaux 51, CH-2000 Neuchâtel, Switzerland, and ^bInstitute of Physics, University of Neuchâtel, rue Emile-Argand 11, CH-2000 Neuchâtel, Switzerland. *Correspondence e-mail: helen.stoeckli-evans@unine.ch

The isotypic title one-dimensional coordination polymers, $[CdCl_2(C_{18}H_{14}N_4O_4)]_n$ (I), and $[HgCl_2(C_{18}H_{14}N_4O_4)]_n$ (II), are, respectively, the cadmium(II) and mercury(II) complexes of the dimethyl ester of 5,6-bis(pyridin-2-yl)pyrazine-2,3-dicarboxylic acid. In both compounds, the metal ions are located on a twofold rotation axis and a second such axis bisects the $C_{ar}-C_{ar}$ bonds of the pyrazine ring. The metal ions are bridged by binding to the N atoms of the two pyridine rings and have an MN_2Cl_2 bisphenoidal coordination geometry. The metal– $N_{pyrazine}$ distances are much longer than the metal– $N_{pyridine}$ distances; the difference is 0.389 (2) Å for the Cd–N bonds but only 0.286 (5) Å for the Hg–N bond lengths. In the crystals of both compounds, the polymer chains are linked *via* pairs of C—H...Cl hydrogen bonds, forming corrugated slabs parallel to the *ac* plane.

1. Chemical context

The crystal structures of the dimethyl and diethyl esters of 5,6-bis(pyridin-2-yl)pyrazine-2,3-dicarboxylic acid (**LH₂**; Alfonso *et al.*, 2001) have been reported on recently (Alfonso & Stoeckli-Evans, 2016). They were originally synthesized to study the hydrolysis of these esters with first row transition metals (Alfonso, 1999). Subsequent studies of their reaction with d^{10} or post-transition metals lead to the formation of the title compounds, and we report herein on the syntheses and crystal structures of the title isotopic cadmium(II) and mercury(II) coordination polymers.



(I) $M = Cd$
(II) $M = Hg$

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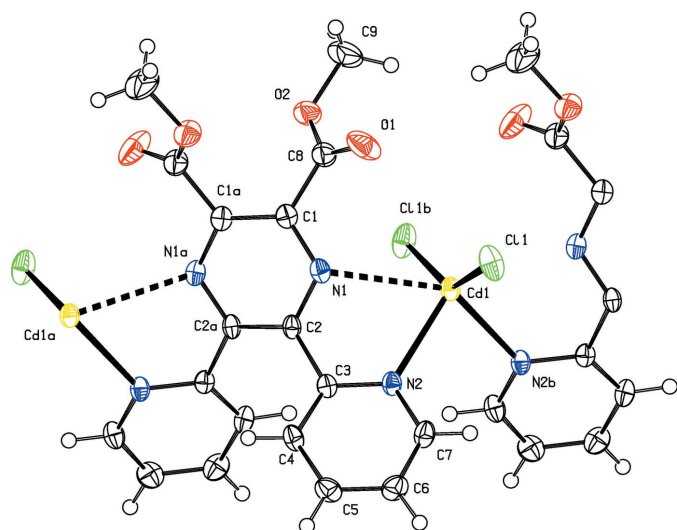


Figure 1
A view of the molecular structure of compound (I), showing the atom labelling [symmetry codes: (a) $-x + \frac{1}{2}, y, -z + \frac{3}{2}$; (b) $-x + \frac{3}{2}, y, -z + \frac{3}{2}$]. Displacement ellipsoids are drawn at the 50% probability level

2. Structural commentary

In compounds (I) and (II), the metal atom is located on a twofold rotation axis and a second such axis bisects the $C_{ar}-C_{ar}$ bonds of the pyrazine ring; as illustrated in Fig. 1 for the cadmium complex (I), and in Fig. 2 for the mercury complex (II). Details of the bond lengths and bond angles involving the metal atoms are given in Table 1 for (I), and in Table 2 for (II). The metal atoms are bridged by binding to the N atoms of the two pyridine rings, N2 and N2ⁱ; Cd1–N2 = 2.3862 (17) Å in (I) and Hg1–N2 = 2.590 (5) Å in (II). The Cd1–Cl1 bonds [2.4137 (6) Å] are longer than the Hg1–Cl1 bonds [2.3464 (16) Å], while the reverse is true for the metal–N_{pyridine}

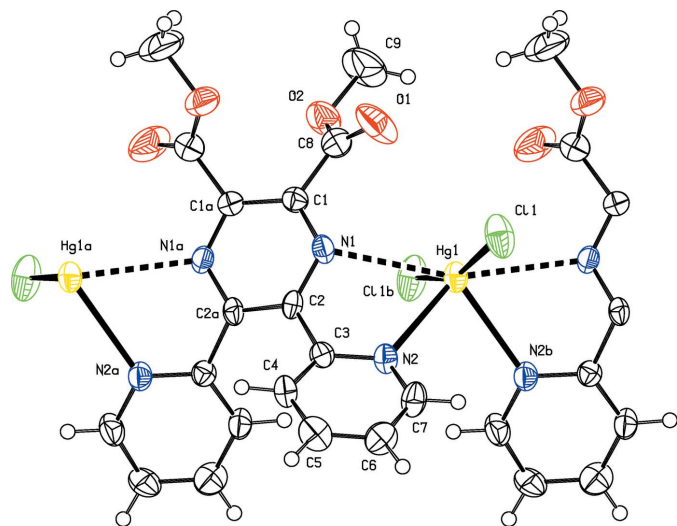


Figure 2
A view of the molecular structure of compound (II), showing the atom labelling [symmetry codes: (a) $-x + \frac{1}{2}, y, -z + \frac{3}{2}$; (b) $-x + \frac{3}{2}, y, -z + \frac{3}{2}$]. Displacement ellipsoids are drawn at the 50% probability level.

Table 1
Selected geometric parameters (Å, °) for (I).

Cd1–Cl1	2.4137 (6)	Cd1–N1	2.7757 (17)
Cd1–N2	2.3862 (17)		
Cl1 ⁱ –Cd1–Cl1	142.43 (3)	N2–Cd1–Cl1 ⁱ	110.87 (4)
N2–Cd1–N2 ⁱ	85.02 (8)	N2–Cd1–Cl1	96.81 (4)

Symmetry code: (i) $-x + \frac{3}{2}, y, -z + \frac{3}{2}$.

Table 2
Selected geometric parameters (Å, °) for (II).

Hg1–Cl1	2.3464 (16)	Hg1–N1	2.876 (5)
Hg1–N2	2.590 (5)		
Cl1 ⁱ –Hg1–Cl1	158.87 (12)	Cl1 ⁱ –Hg1–N2	102.86 (12)
N2–Hg1–N2 ⁱ	83.1 (2)	Cl1–Hg1–N2	92.97 (12)

Symmetry code: (i) $-x + \frac{3}{2}, y, -z + \frac{3}{2}$.

bonds: Cd1–N2 [2.3862 (17) Å] is shorter than Hg1–N2 [2.590 (5) Å]. The link to the pyrazine N atoms, N2 and N2ⁱ, is much weaker: Cd1···N1 = 2.7757 (17) Å and Hg1···N1 = 2.876 (5) Å. The difference in the metal–N_{pyridine} and metal–N_{pyrazine} bond lengths is 0.389 (2) Å for the Cd–N bonds but only 0.286 (5) Å for the Hg–N bonds (see Tables 1 and 2).

The fourfold coordination geometry of the metal atoms differ slightly, as illustrated in Fig. 3 a structural overlap of the two compounds. In (I) atom Cd1 has a τ_4 parameter of 0.53, while for the Hg1 atom in (II) the τ_4 parameter = 0.30 (extreme values: $\tau_4 = 0$ for square-planar, 1 for tetrahedral and 0.85 for trigonal-pyramidal geometry; Yang *et al.*, 2007). When also considering the values of the Cl–M–Cl and N–M–N bond angles in both compounds (see Tables 1 and 2), we

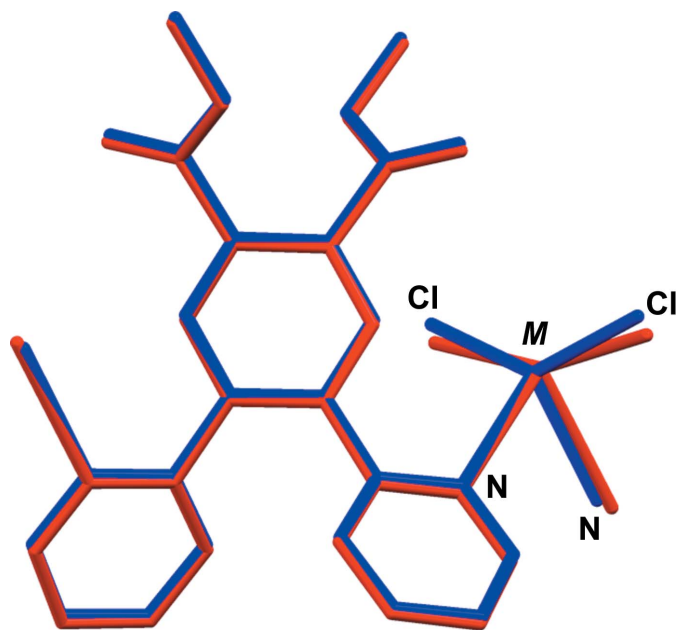


Figure 3
A view of the structural overlap of the cadmium complex (I) in blue and the mercury complex (II) in red; also illustrating the slight difference in the bisphenoidal coordination geometry of the two metal atoms (MN_2Cl_2).

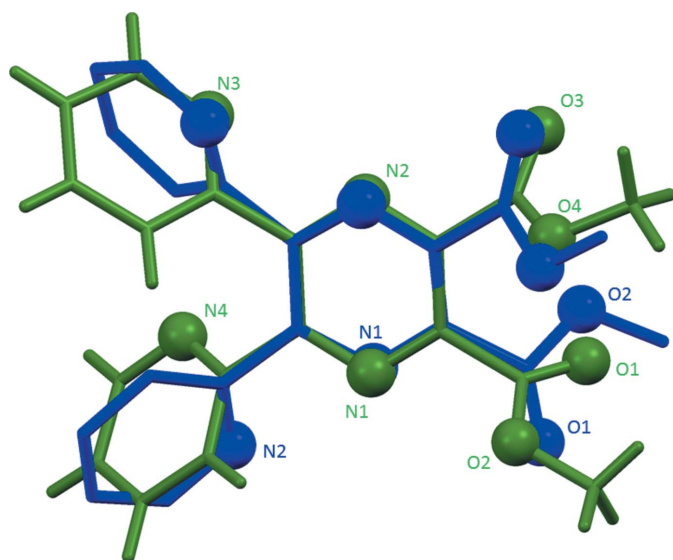


Figure 4
A view of the structural overlap of the ligand (**Me₂L**, green; Alfonso & Stoeckli-Evans, 2016) and the coordinating ligand (blue) in compound (I).

conclude that both metal atoms (*M*) have a bisphenoidal MN_2Cl_2 coordination environment.

In both compounds, the pyrazine rings (N1/C1/C2/N1ⁱ/C2ⁱ) are not ideally planar [r.m.s. deviations are 0.096 and 0.092 Å for (I) and (II), respectively] and have twist-boat-like conformations [puckering parameters: amplitude (*Q*) = 0.166 (2) Å, $\theta = 87.8$ (7)°, $\varphi = 270.0$ (7)° for (I), and amplitude (*Q*) = 0.160 (6) Å, $\theta = 90$ (2)°, $\varphi = 270$ (2)° for (II); symmetry code: (i) $-x + \frac{1}{2}, y, -z + \frac{3}{2}$].

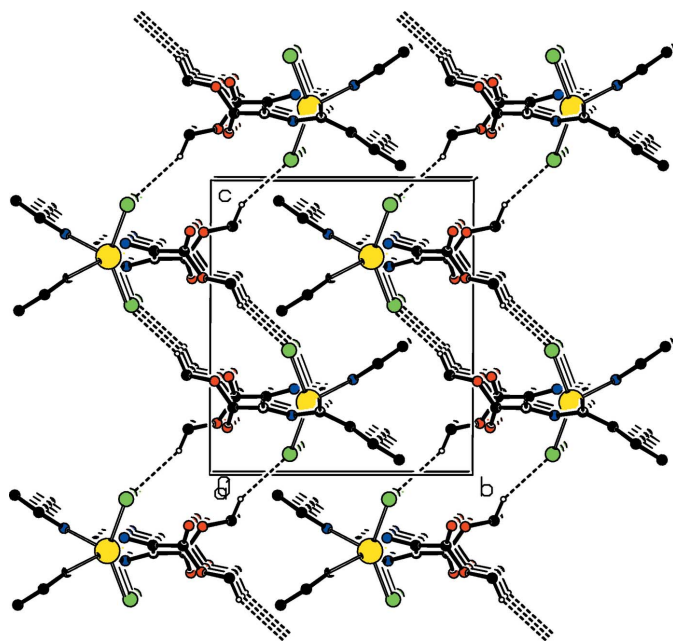


Figure 5
A view along the *a* axis of the crystal packing of compound (I). The hydrogen bonds are shown as dashed lines (see Table 3; only H atom H9A has been included).

Table 3
Hydrogen-bond geometry (Å, °) for (I).

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
C9–H9A···Cl1 ⁱⁱ	0.97	2.69	3.577 (3)	151

Symmetry code: (ii) $x - \frac{1}{2}, -y + 2, z - \frac{1}{2}$.

Table 4
Hydrogen-bond geometry (Å, °) for (II).

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
C9–H9A···Cl1 ⁱⁱ	0.96	2.81	3.647 (9)	146

Symmetry code: (ii) $x - \frac{1}{2}, -y + 2, z - \frac{1}{2}$.

The pyridine rings (N2/C3–C7), are inclined to the pyrazine ring mean planes by 40.58 (10)° in (I) and 42.1 (3)° in (II), and to one another by 67.37 (10)° in (I) and 67.3 (3)° in (II). The methylcarboxylate groups (C9/O2/C8/O1) are planar to within 0.019 (2) Å for atom O2 in (I) and 0.20 (7) Å for atom C8 in (II). Their mean planes are inclined to the mean plane of the pyrazine ring and to one another by 44.44 (16) and 68.8 (2)°, respectively, in (I), and by 43.0 (3) and 75.7 (5)°, respectively, in (II).

It can be seen from Fig. 4, a structural overlap of the ligand itself (Alfonso & Stoeckli-Evans, 2016) with the coordinating ligand in compound (I), that both the pyridine ring involving atom N4, and the carboxylate group, involving atoms O1 and O2, have been rotated by *ca* 100 and 160°, respectively, on coordination to the metal atom. While the pyrazine ring is ideally planar in the ligand (r.m.s. deviation = 0.032 Å), on coordination it is less planar with r.m.s. deviations of 0.096 and 0.092 Å for (I) and (II), respectively.

3. Supramolecular features

In the crystals of both compounds, the polymer chains are linked *via* a pair of C–H···Cl hydrogen bonds, forming corrugated slabs parallel to the *ac* plane, as illustrated in Fig. 5. Within the slabs, the hydrogen bonding forms $R_2^2(16)$ and $R_2^2(18)$ type loops, as shown in Fig. 6. Details of the hydrogen bonding are given in Table 3 for compound (I) and Table 4 for compound (II). There are no other significant intermolecular interactions present for either structure.

4. Database survey

A search of the Cambridge Structural Database (Version 5.37, update May 2016; Groom *et al.*, 2016) for MN_2Cl_2 (where *M* = Cd and Hg; N_{pyridine}) four-coordinate metal ions yielded eight hits for *M* = cadmium and 52 hits for *M* = mercury. For the cadmium complexes, the Cd–Cl bonds are consistently longer than the Cd–N_{pyridine} bonds, and the Cl–Cd–Cl bond angles are consistently larger than the N–Cd–N bond angle, as in compound (I). A good example is dichloridobis[2-[(triphenylmethyl)amino]pyridine-*κ*N]cadmium (VIWKIW; Zhang, 2008), with approximate bond lengths and bond angles

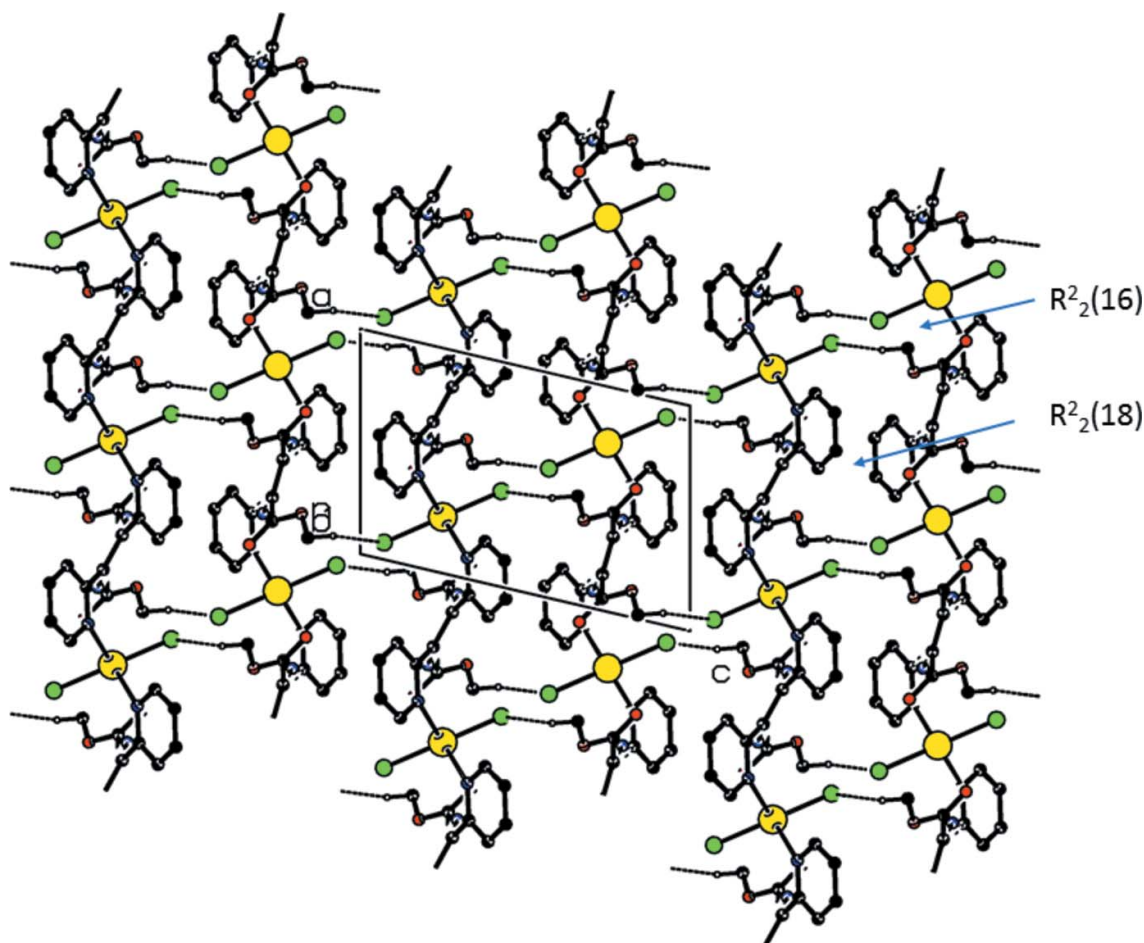


Figure 6

A projection along the b axis of the crystal packing of compound (II). The hydrogen bonds are shown as dashed lines (see Table 4; only H atom H9A has been included).

of Cd—Cl = 2.387, Cd—N = 2.285 Å, Cl—Cd—Cl = 121.2 and N—Cd—N = 95.2°.

For the mercury complexes, the Hg—Cl bond lengths are either longer or shorter than the Hg—N_{pyridine} bond lengths. For example, in bis(2-amino-3-methylpyridine)dichlorido-mercury(II) (LEHMAO; Tadjarodi *et al.*, 2012) the approximate bond lengths and angles are Hg—Cl = 2.452, Hg—N = 2.267 Å, Cl—Hg—Cl = 119.9 and N—Hg—N = 101.3°, while in dichloridobis(3,3,3',3'-tetramethyl-2,2',3,3'-tetrahydro-1,1'-spirobi[indene]6,6'-diyl diisonicotinato)mercury (HUKTAJ; Lin *et al.*, 2010) the approximate bond lengths and angles are Hg—Cl = 2.345, Hg—N = 2.593 Å, Cl—Hg—Cl = 167.5 and N—Hg—N = 104.7°. This latter example is similar to the situation in compound (II).

5. Synthesis and crystallization

The synthesis of the ligand dimethyl-5,6-bis(pyridin-2-yl)pyrazine-2,3-dicarboxylate (**Me₂L**) has been reported on recently (Alfonso & Stoeckli-Evans, 2016).

Synthesis of compound (I): CdCl₂·2H₂O (22 mg, 0.1 mmol) in 25 ml of dry MeOH was slowly added to a solution of **Me₂L** in 10 ml of dry MeOH. The colourless solution that formed was stirred at room temperature for 1 h, then filtered to

remove any impurities. The filtrate was allowed to stand over several days until colourless square rod-like crystals were obtained (yield: 40 mg, 75%). Elemental analysis for C₁₈H₁₄N₄CdCl₂O₄ (M_w = 533.63); calculated C 40.51, H 2.64, N 10.50%; found C 40.49, H 2.53, N 10.59%. Selected IR bands (KBr pellet, cm⁻¹): ν = 3066(*w*), 2997(*w*), 1751(*vs*), 1593(*m*), 1568(*w*), 1549(*w*), 1479(*m*), 1450(*m*), 1403(*m*), 1339(*s*), 1297(*m*), 1273(*m*), 1261(*m*), 1228(*s*), 1193(*m*), 1177(*m*), 1162(*m*), 1120(*m*), 1109(*w*), 1088(*s*), 1009(*m*), 974(*m*), 918(*w*), 827(*m*), 803(*m*), 789(*m*), 770(*w*), 758(*m*), 554(*m*).

Synthesis of compound (II): **Me₂L** (35 mg, 0.1 mmol) was added in solid form to a solution of HgCl₂·2H₂O (30 mg, 0.1 mmol) in 25 ml of dry MeOH. The colourless solution immediately obtained was stirred at room temperature for 2 h, filtered to remove any impurity, and the filtrate allowed to evaporate slowly. After two days colourless needle-like crystals were obtained (yield: 47 mg, 76%). Elemental analysis for C₁₈H₁₄N₄Cl₂HgO₄ (M_w = 621.82); calculated C 34.77, H 2.27, N 9.01%; found C 34.79, H 2.44, N 9.03%. Selected IR bands (KBr pellet, cm⁻¹): ν = 3065(*w*), 2997(*w*), 2951(*w*), 2882(*w*), 1747(*vs*), 1590(*m*), 1568(*m*), 1546(*w*), 1477(*m*), 1447(*m*), 1402(*m*), 1338(*s*), 1279(*m*), 1223(*s*), 1195(*m*), 1176(*s*), 1105(*w*), 1086(*s*), 1003(*m*), 973(*w*), 827(*w*), 802(*m*), 788(*m*), 769(*m*), 755(*m*), 553(*m*).

Table 5
Experimental details.

	(I)	(II)
Crystal data		
Chemical formula	[CdCl ₂ (C ₁₈ H ₁₄ N ₄ O ₄)]	[HgCl ₂ (C ₁₈ H ₁₄ N ₄ O ₄)]
M_r	533.63	621.82
Crystal system, space group	Monoclinic, $P2/n$	Monoclinic, $P2/n$
Temperature (K)	223	293
a, b, c (Å)	7.8919 (7), 10.5898 (7), 12.0875 (12)	8.1042 (6), 10.6002 (16), 12.2063 (10)
β (°)	102.061 (11)	103.158 (7)
V (Å ³)	987.90 (15)	1021.07 (19)
Z	2	2
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm ⁻¹)	1.41	7.83
Crystal size (mm)	0.40 × 0.20 × 0.10	0.49 × 0.23 × 0.04
Data collection		
Diffractometer	Stoe IPDS 1 image-plate	Stoe–Siemens AED2 four-circle
Absorption correction	Multi-scan (<i>MULABS</i> ; Spek, 2009)	ψ scan (<i>X-RED</i> ; Stoe & Cie, 1997)
T_{\min} , T_{\max}	0.938, 1.000	0.319, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7196, 1918, 1684	1855, 1855, 1723
R_{int}	0.037	0.000
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.614	0.600
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.022, 0.050, 0.95	0.032, 0.074, 1.11
No. of reflections	1918	1855
No. of parameters	133	133
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	0.34, -0.64	1.23, -1.08

Computer programs: *EXPOSE*, *CELL* and *INTEGRATE* in *IPDS-I* (Stoe & Cie, 2004), *STADIA* and *X-RED* (Stoe & Cie, 1997), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *Mercury* (Macrae *et al.*, 2008), *PLATON* (Spek, 2009) and *pubCIF* (Westrip, 2010).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 5. For both compounds the C-bound H atoms were included in calculated positions and treated as riding atoms: C–H = 0.93–0.97 Å with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C-methyl})$ and $1.2U_{\text{eq}}(\text{C})$ for other H-atoms. For the mercury complex (II), $R_{\text{int}} = 0.000$ as only one equivalent was measured.

Acknowledgements

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supporting information

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Isotypic one-dimensional coordination polymers: *catena*-poly[[dichloridocadmium]- μ -5,6-bis(pyridin-2-yl)pyrazine-2,3-dicarboxylato- $\kappa^2N^5:N^6$] and *catena*-poly[[dichloridomercury(II)]- μ -5,6-bis(pyridin-2-yl)pyrazine-2,3-dicarboxylato- $\kappa^2N^5:N^6$]

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Computing details

Data collection: *EXPOSE* in *IPDS-I* (Stoe & Cie, 2004) for (I); STADI4 Software (Stoe & Cie, 1997) for (II). Cell refinement: *CELL* in *IPDS-I* (Stoe & Cie, 2004) for (I); STADI4 Software (Stoe & Cie, 1997) for (II). Data reduction: *INTEGRATE* in *IPDS-I* (Stoe & Cie, 2004) for (I); *X-RED* Software (Stoe & Cie, 1997) for (II). For both compounds, program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *PLATON* (Spek, 2009) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL2014* (Sheldrick, 2015), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

(I) *catena*-Poly[[dichloridocadmium(II)]- μ -5,6-bis(pyridin-2-yl)pyrazine-2,3-dicarboxylato- $\kappa^2N^5:N^6$]

Crystal data

[CdCl₂(C₁₈H₁₄N₄O₄)]

$M_r = 533.63$

Monoclinic, *P2/n*

$a = 7.8919$ (7) Å

$b = 10.5898$ (7) Å

$c = 12.0875$ (12) Å

$\beta = 102.061$ (11)°

$V = 987.90$ (15) Å³

$Z = 2$

$F(000) = 528$

$D_x = 1.794$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 5000 reflections

$\theta = 2.0$ – 25.9 °

$\mu = 1.41$ mm⁻¹

$T = 223$ K

Plate, colourless

$0.40 \times 0.20 \times 0.10$ mm

Data collection

Stoe IPDS 1 image-plate diffractometer

Radiation source: fine-focus sealed tube

Plane graphite monochromator

φ rotation scans

Absorption correction: multi-scan (MULABS; Spek, 2009)

$T_{\min} = 0.938$, $T_{\max} = 1.000$

7196 measured reflections

1918 independent reflections

1684 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.037$

$\theta_{\max} = 25.9$ °, $\theta_{\min} = 2.6$ °

$h = -9 \rightarrow 8$

$k = -12 \rightarrow 12$

$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.022$
 $wR(F^2) = 0.050$
 $S = 0.95$
 1918 reflections
 133 parameters
 0 restraints
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier
 map
 Hydrogen site location: inferred from
 neighbouring sites
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0331P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.34 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.64 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cd1	0.7500	0.62102 (2)	0.7500	0.02022 (8)
Cl1	0.91939 (8)	0.69442 (6)	0.92817 (4)	0.03420 (15)
O1	0.5767 (3)	0.92856 (19)	0.83392 (17)	0.0493 (5)
O2	0.3843 (2)	0.97480 (15)	0.67432 (14)	0.0320 (4)
N1	0.4264 (2)	0.68120 (17)	0.79108 (14)	0.0207 (4)
N2	0.6038 (2)	0.45491 (16)	0.82537 (14)	0.0200 (4)
C1	0.3400 (3)	0.7889 (2)	0.76437 (17)	0.0212 (4)
C2	0.3377 (3)	0.5727 (2)	0.77768 (16)	0.0186 (4)
C3	0.4350 (3)	0.45962 (19)	0.82904 (15)	0.0183 (4)
C4	0.3567 (3)	0.3710 (2)	0.88644 (17)	0.0235 (4)
H4	0.2384	0.3774	0.8878	0.028*
C5	0.4558 (3)	0.2725 (2)	0.94191 (18)	0.0280 (5)
H5	0.4058	0.2111	0.9813	0.034*
C6	0.6287 (3)	0.2667 (2)	0.93806 (19)	0.0292 (5)
H6	0.6987	0.2007	0.9742	0.035*
C7	0.6976 (3)	0.3592 (2)	0.88040 (18)	0.0254 (5)
H7	0.8163	0.3552	0.8794	0.030*
C8	0.4490 (3)	0.9051 (2)	0.7648 (2)	0.0277 (5)
C9	0.4881 (4)	1.0825 (3)	0.6553 (3)	0.0502 (8)
H9A	0.4411	1.1183	0.5814	0.075*
H9B	0.6065	1.0555	0.6587	0.075*
H9C	0.4861	1.1456	0.7131	0.075*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.01561 (12)	0.02520 (13)	0.01861 (12)	0.000	0.00071 (8)	0.000
Cl1	0.0255 (3)	0.0559 (4)	0.0204 (3)	-0.0113 (3)	0.0031 (2)	-0.0094 (2)
O1	0.0389 (11)	0.0448 (11)	0.0538 (12)	-0.0200 (9)	-0.0140 (9)	0.0170 (9)

O2	0.0327 (9)	0.0284 (8)	0.0340 (9)	-0.0013 (7)	0.0045 (7)	0.0099 (7)
N1	0.0177 (9)	0.0279 (9)	0.0163 (8)	-0.0020 (8)	0.0032 (7)	0.0030 (7)
N2	0.0157 (9)	0.0263 (9)	0.0177 (8)	0.0006 (7)	0.0025 (7)	0.0027 (7)
C1	0.0200 (11)	0.0264 (11)	0.0165 (10)	-0.0007 (9)	0.0023 (8)	0.0011 (8)
C2	0.0152 (11)	0.0263 (10)	0.0151 (9)	0.0007 (9)	0.0052 (8)	0.0016 (8)
C3	0.0166 (11)	0.0243 (10)	0.0132 (9)	-0.0014 (8)	0.0010 (8)	-0.0014 (8)
C4	0.0172 (10)	0.0323 (11)	0.0204 (10)	-0.0041 (10)	0.0023 (8)	0.0027 (9)
C5	0.0304 (13)	0.0296 (12)	0.0232 (11)	-0.0044 (10)	0.0037 (9)	0.0076 (9)
C6	0.0297 (13)	0.0295 (12)	0.0258 (12)	0.0050 (10)	0.0000 (10)	0.0069 (9)
C7	0.0189 (11)	0.0331 (13)	0.0235 (11)	0.0046 (9)	0.0030 (9)	0.0033 (9)
C8	0.0253 (13)	0.0280 (12)	0.0295 (12)	-0.0001 (9)	0.0049 (10)	0.0069 (9)
C9	0.0538 (19)	0.0375 (15)	0.0599 (18)	-0.0097 (13)	0.0134 (15)	0.0201 (13)

Geometric parameters (Å, °)

Cd1—C11 ⁱ	2.4137 (6)	C2—C2 ⁱⁱ	1.406 (4)
Cd1—C11	2.4137 (6)	C2—C3	1.486 (3)
Cd1—N2	2.3862 (17)	C3—C4	1.387 (3)
Cd1—N2 ⁱ	2.3862 (17)	C4—C5	1.389 (3)
Cd1—N1	2.7757 (17)	C4—H4	0.9400
O1—C8	1.193 (3)	C5—C6	1.377 (4)
O2—C8	1.330 (3)	C5—H5	0.9400
O2—C9	1.450 (3)	C6—C7	1.378 (3)
N1—C1	1.333 (3)	C6—H6	0.9400
N1—C2	1.337 (3)	C7—H7	0.9400
N2—C3	1.343 (3)	C9—H9A	0.9700
N2—C7	1.346 (3)	C9—H9B	0.9700
C1—C1 ⁱⁱ	1.390 (4)	C9—H9C	0.9700
C1—C8	1.501 (3)		
C11 ⁱ —Cd1—C11	142.43 (3)	C3—C4—H4	120.5
N2—Cd1—N2 ⁱ	85.02 (8)	C5—C4—H4	120.5
N2—Cd1—C11 ⁱ	110.87 (4)	C6—C5—C4	118.7 (2)
N2 ⁱ —Cd1—C11 ⁱ	96.81 (4)	C6—C5—H5	120.7
N2—Cd1—C11	96.81 (4)	C4—C5—H5	120.7
N2 ⁱ —Cd1—C11	110.87 (4)	C5—C6—C7	118.9 (2)
C8—O2—C9	115.7 (2)	C5—C6—H6	120.5
C1—N1—C2	118.54 (18)	C7—C6—H6	120.5
C3—N2—C7	117.28 (18)	N2—C7—C6	123.4 (2)
C3—N2—Cd1	123.17 (13)	N2—C7—H7	118.3
C7—N2—Cd1	118.96 (14)	C6—C7—H7	118.3
N1—C1—C1 ⁱⁱ	120.30 (13)	O1—C8—O2	125.7 (2)
N1—C1—C8	115.93 (19)	O1—C8—C1	124.9 (2)
C1 ⁱⁱ —C1—C8	123.75 (12)	O2—C8—C1	109.33 (19)
N1—C2—C2 ⁱⁱ	119.71 (12)	O2—C9—H9A	109.5
N1—C2—C3	115.48 (17)	O2—C9—H9B	109.5
C2 ⁱⁱ —C2—C3	124.75 (12)	H9A—C9—H9B	109.5
N2—C3—C4	122.68 (18)	O2—C9—H9C	109.5

N2—C3—C2	116.45 (17)	H9A—C9—H9C	109.5
C4—C3—C2	120.60 (19)	H9B—C9—H9C	109.5
C3—C4—C5	119.0 (2)		
C2—N1—C1—C1 ⁱⁱ	7.2 (3)	C2—C3—C4—C5	-174.32 (19)
C2—N1—C1—C8	-171.29 (18)	C3—C4—C5—C6	0.1 (3)
C1—N1—C2—C2 ⁱⁱ	8.5 (3)	C4—C5—C6—C7	0.6 (3)
C1—N1—C2—C3	-168.82 (18)	C3—N2—C7—C6	0.8 (3)
C7—N2—C3—C4	0.0 (3)	Cd1—N2—C7—C6	172.27 (17)
Cd1—N2—C3—C4	-171.05 (15)	C5—C6—C7—N2	-1.2 (3)
C7—N2—C3—C2	174.10 (18)	C9—O2—C8—O1	5.2 (4)
Cd1—N2—C3—C2	3.0 (2)	C9—O2—C8—C1	-172.5 (2)
N1—C2—C3—N2	-36.1 (2)	N1—C1—C8—O1	-41.0 (3)
C2 ⁱⁱ —C2—C3—N2	146.7 (2)	C1 ⁱⁱ —C1—C8—O1	140.6 (3)
N1—C2—C3—C4	138.1 (2)	N1—C1—C8—O2	136.7 (2)
C2 ⁱⁱ —C2—C3—C4	-39.0 (3)	C1 ⁱⁱ —C1—C8—O2	-41.7 (3)
N2—C3—C4—C5	-0.5 (3)		

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C9—H9A \cdots C11 ⁱⁱⁱ	0.97	2.69	3.577 (3)	151

Symmetry code: (iii) $x-1/2, -y+2, z-1/2$.

(II) *catena*-Poly[[dichloridomercury(II)]- μ -5,6-bis(pyridin-2-yl)pyrazine-2,3-dicarboxylato- $\kappa^2N^5:N^6$]

Crystal data

$[\text{HgCl}_2(\text{C}_{18}\text{H}_{14}\text{N}_4\text{O}_4)]$

$M_r = 621.82$

Monoclinic, $P2_1/n$

$a = 8.1042$ (6) \AA

$b = 10.6002$ (16) \AA

$c = 12.2063$ (10) \AA

$\beta = 103.158$ (7) $^\circ$

$V = 1021.07$ (19) \AA^3

$Z = 2$

$F(000) = 592$

$D_x = 2.023$ Mg m^{-3}

Mo $K\alpha$ radiation, $\lambda = 0.71073$ \AA

Cell parameters from 31 reflections

$\theta = 12.5\text{--}15.9^\circ$

$\mu = 7.83$ mm^{-1}

$T = 293$ K

Plate, colourless

$0.49 \times 0.23 \times 0.04$ mm

Data collection

Stoe–Siemens AED2 four-circle diffractometer

Radiation source: fine-focus sealed tube

Plane graphite monochromator

$\omega/2\theta$ scans

Absorption correction: ψ scan

(X-RED software; Stoe & Cie, 1997)

$T_{\min} = 0.319, T_{\max} = 1.000$

1855 measured reflections

1855 independent reflections

1723 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.000$

$\theta_{\max} = 25.2^\circ, \theta_{\min} = 2.6^\circ$

$h = -9 \rightarrow 9$

$k = 0 \rightarrow 12$

$l = 0 \rightarrow 14$

2 standard reflections every 60 min

intensity decay: 2%

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.032$
 $wR(F^2) = 0.074$
 $S = 1.11$
 1855 reflections
 133 parameters
 0 restraints
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier
 map
 Hydrogen site location: inferred from
 neighbouring sites
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.028P)^2 + 4.815P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 1.23 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -1.08 \text{ e } \text{Å}^{-3}$

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	$U_{\text{iso}}^*/U_{\text{eq}}$
Hg1	0.7500	0.64352 (4)	0.7500	0.03521 (13)
Cl1	0.9248 (2)	0.6841 (2)	0.92787 (14)	0.0574 (5)
O1	0.5742 (7)	0.9336 (6)	0.8357 (5)	0.0780 (19)
O2	0.3825 (7)	0.9822 (5)	0.6779 (4)	0.0557 (13)
N1	0.4215 (6)	0.6897 (5)	0.7942 (4)	0.0319 (11)
N2	0.5940 (6)	0.4607 (5)	0.8247 (4)	0.0341 (12)
C1	0.3392 (7)	0.7964 (6)	0.7663 (5)	0.0315 (13)
C2	0.3366 (7)	0.5809 (6)	0.7789 (4)	0.0279 (12)
C3	0.4304 (7)	0.4674 (6)	0.8294 (4)	0.0289 (12)
C4	0.3561 (7)	0.3796 (6)	0.8876 (5)	0.0365 (15)
H4	0.2428	0.3874	0.8903	0.044*
C5	0.4514 (9)	0.2810 (7)	0.9412 (5)	0.0467 (17)
H5	0.4030	0.2207	0.9795	0.056*
C6	0.6207 (9)	0.2725 (7)	0.9373 (6)	0.0463 (17)
H6	0.6886	0.2070	0.9729	0.056*
C7	0.6856 (8)	0.3655 (7)	0.8783 (5)	0.0419 (16)
H7	0.7995	0.3609	0.8761	0.050*
C8	0.4467 (9)	0.9113 (7)	0.7670 (6)	0.0432 (16)
C9	0.4826 (13)	1.0900 (9)	0.6588 (9)	0.084 (3)
H9A	0.4477	1.1161	0.5817	0.126*
H9B	0.6003	1.0671	0.6752	0.126*
H9C	0.4661	1.1581	0.7070	0.126*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hg1	0.02386 (18)	0.0439 (2)	0.03582 (19)	0.000	0.00254 (12)	0.000
Cl1	0.0379 (9)	0.0962 (16)	0.0361 (8)	-0.0145 (10)	0.0041 (7)	-0.0109 (9)
O1	0.061 (4)	0.065 (4)	0.090 (4)	-0.029 (3)	-0.022 (3)	0.019 (3)

O2	0.053 (3)	0.045 (3)	0.067 (3)	-0.007 (3)	0.010 (3)	0.018 (3)
N1	0.023 (2)	0.036 (3)	0.037 (3)	-0.003 (2)	0.008 (2)	0.004 (2)
N2	0.025 (2)	0.040 (3)	0.036 (3)	0.000 (2)	0.006 (2)	0.003 (2)
C1	0.031 (3)	0.028 (3)	0.036 (3)	-0.001 (3)	0.008 (2)	0.003 (3)
C2	0.022 (3)	0.037 (3)	0.028 (3)	0.003 (3)	0.011 (2)	0.001 (3)
C3	0.027 (3)	0.031 (3)	0.027 (3)	-0.001 (2)	0.004 (2)	0.000 (2)
C4	0.024 (3)	0.046 (4)	0.039 (3)	-0.002 (3)	0.007 (2)	0.003 (3)
C5	0.048 (4)	0.053 (5)	0.036 (3)	-0.005 (4)	0.002 (3)	0.008 (3)
C6	0.044 (4)	0.044 (4)	0.045 (4)	0.011 (3)	-0.001 (3)	0.014 (3)
C7	0.028 (3)	0.054 (4)	0.042 (3)	0.009 (3)	0.005 (3)	0.010 (3)
C8	0.041 (4)	0.038 (4)	0.051 (4)	0.003 (3)	0.009 (3)	0.003 (3)
C9	0.092 (7)	0.055 (6)	0.105 (8)	-0.020 (5)	0.022 (6)	0.031 (5)

Geometric parameters (Å, °)

Hg1—C11 ⁱ	2.3464 (16)	C2—C2 ⁱⁱ	1.420 (11)
Hg1—C11	2.3464 (16)	C2—C3	1.480 (8)
Hg1—N2	2.590 (5)	C3—C4	1.389 (8)
Hg1—N2 ⁱ	2.590 (5)	C4—C5	1.373 (9)
Hg1—N1	2.876 (5)	C4—H4	0.9300
O1—C8	1.197 (8)	C5—C6	1.386 (10)
O2—C8	1.327 (8)	C5—H5	0.9300
O2—C9	1.450 (9)	C6—C7	1.393 (10)
N1—C1	1.317 (8)	C6—H6	0.9300
N1—C2	1.334 (8)	C7—H7	0.9300
N2—C7	1.333 (8)	C9—H9A	0.9600
N2—C3	1.342 (7)	C9—H9B	0.9600
C1—C1 ⁱⁱ	1.409 (12)	C9—H9C	0.9600
C1—C8	1.497 (9)		
C11 ⁱ —Hg1—C11	158.87 (12)	C5—C4—H4	120.3
N2—Hg1—N2 ⁱ	83.1 (2)	C3—C4—H4	120.3
C11 ⁱ —Hg1—N2	102.86 (12)	C4—C5—C6	119.1 (7)
C11—Hg1—N2	92.97 (12)	C4—C5—H5	120.4
C11 ⁱ —Hg1—N2 ⁱ	92.97 (12)	C6—C5—H5	120.4
C11—Hg1—N2 ⁱ	102.86 (12)	C5—C6—C7	117.7 (6)
C8—O2—C9	116.6 (6)	C5—C6—H6	121.1
C1—N1—C2	119.4 (5)	C7—C6—H6	121.1
C7—N2—C3	117.7 (5)	N2—C7—C6	123.8 (6)
C7—N2—Hg1	118.5 (4)	N2—C7—H7	118.1
C3—N2—Hg1	122.8 (4)	C6—C7—H7	118.1
N1—C1—C1 ⁱⁱ	120.0 (3)	O1—C8—O2	125.3 (7)
N1—C1—C8	115.9 (5)	O1—C8—C1	125.0 (7)
C1 ⁱⁱ —C1—C8	124.0 (4)	O2—C8—C1	109.7 (6)
N1—C2—C2 ⁱⁱ	119.3 (3)	O2—C9—H9A	109.5
N1—C2—C3	116.4 (5)	O2—C9—H9B	109.5
C2 ⁱⁱ —C2—C3	124.2 (3)	H9A—C9—H9B	109.5
N2—C3—C4	122.3 (5)	O2—C9—H9C	109.5

N2—C3—C2	116.4 (5)	H9A—C9—H9C	109.5
C4—C3—C2	121.1 (5)	H9B—C9—H9C	109.5
C5—C4—C3	119.4 (6)		
C2—N1—C1—C1 ⁱⁱ	7.6 (10)	C2—C3—C4—C5	-174.7 (6)
C2—N1—C1—C8	-169.7 (5)	C3—C4—C5—C6	1.0 (10)
C1—N1—C2—C2 ⁱⁱ	7.3 (9)	C4—C5—C6—C7	-0.2 (11)
C1—N1—C2—C3	-170.0 (5)	C3—N2—C7—C6	0.8 (10)
C7—N2—C3—C4	0.1 (9)	Hg1—N2—C7—C6	169.5 (6)
Hg1—N2—C3—C4	-168.1 (4)	C5—C6—C7—N2	-0.7 (11)
C7—N2—C3—C2	174.1 (5)	C9—O2—C8—O1	4.7 (12)
Hg1—N2—C3—C2	5.9 (7)	C9—O2—C8—C1	-173.0 (7)
N1—C2—C3—N2	-38.4 (7)	N1—C1—C8—O1	-39.6 (10)
C2 ⁱⁱ —C2—C3—N2	144.5 (7)	C1 ⁱⁱ —C1—C8—O1	143.2 (9)
N1—C2—C3—C4	135.7 (6)	N1—C1—C8—O2	138.2 (6)
C2 ⁱⁱ —C2—C3—C4	-41.5 (9)	C1 ⁱⁱ —C1—C8—O2	-39.0 (10)
N2—C3—C4—C5	-1.0 (9)		

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

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C9—H9A...C11 ⁱⁱⁱ	0.96	2.81	3.647 (9)	146

Symmetry code: (iii) $x-1/2, -y+2, z-1/2$.