Two cadmium coordination polymers with bridging acetate and phenylenediamine ligands that exhibit two-dimensional layered structures

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Poly[tetra-μ_2-acetato-$\kappa^8 O$:O'-bis(μ_2-benzene-1,2-diamine-$\kappa^2 N$:N')dicadmium], [Cd$_2$(CH$_3$COO)$_4$(C$_6$H$_8$N$_2$)$_2$]$_n$, (I), and poly[[(μ_2-acetato-$\kappa^2 O$:O')(acetato-$\kappa^2 O$,O')(μ_2-benzene-1,3-diamine-$\kappa^2 N$:N')cadmium] hemihydrate], {[Cd(CH$_3$COO)$_2$(C$_6$H$_8$N$_2$)]·0.5H$_2$O}$_n$, (II), have two-dimensional polymeric structures in which monomeric units are joined by bridging acetate and benzenediamine ligands. Each of the Cd^{II} ions has an O$_4$N$_2$ coordination environment. The coordination geometries of the symmetry-independent Cd^{II} ions are distorted octahedral and distorted trigonal antiprismatic in (I) and distorted antiprismatic in (II). Both compounds exhibit an intralayer hydrogen-bonding network. In addition, the water of hydration in (II) is involved in interlayer hydrogen bonding.

1. Chemical context

Cd^{II} is able to substitute for Zn^{II} in the active sites of zinc-containing enzymes and to interfere with the metabolism of Ca^{II}, which are the primary reasons for its toxicity (Borsari, 2014). In addition, the substitution of Cd^{II} for spectroscopically silent Zn^{II} provides a means of exploring zinc-containing biomolecules using ^{111}Cd and ^{113}Cd NMR spectroscopies (Kimblin & Parkin, 1996; Henehan et al., 1993; Jalilehvand et al., 2009, 2012). Thus, the coordination chemistry of cadmium is of interest.

Metal–organic frameworks (MOFs) have received much attention because of their many potential applications including gas storage, catalysis, chemical sensors and molecular separation (Dey et al., 2014; Kreno et al., 2012; Farha & Hupp, 2010). Our previous efforts in the area of coordination polymers have focused on compounds based on phenylenediamine and acetate ligands incorporating Zn^{II} (Geiger & Parsons, 2014) and Pb^{II} (Geiger et al., 2014). We have extended this work to include Cd and report the structural analyses of two Cd compounds herein. Although acetate ligands adopt a myriad of different metal-binding modes, only the μ_2-acetato-$\kappa^2 O$:O' mode is observed in (I). Both acetato-$\kappa^2 O$,O' and μ_2-acetato-$\kappa^2 O$:O' modes are found in (II).

Numerous examples of structures with benzene-1,2-diamines exhibiting monodentate and/or bidentate coordination modes have been reported (Narayanan & Bhadbhade, 1996; Ovalle-Marroquín et al., 2002; Ariyananda & Norman, 2005; Chen et al., 2006; Maxcy et al., 2000; Qian et al., 2007; Dickman, 2000; Mei et al., 2009; Djebli et al., 2012; Zick & Geiger, 2016; Geiger et al., 2014; Geiger & Parsons, 2014; Geiger, 2012). Examples of benzene-1,4-diamine metal-complex structures
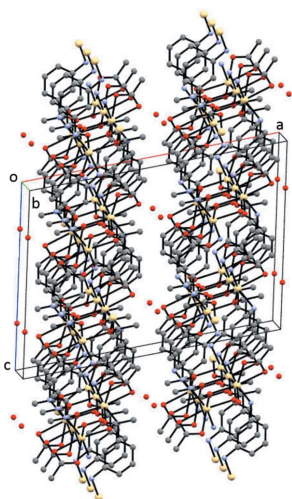
have also been reported (Batten *et al.*, 2001; Faizi & Prisyazhnaya, 2015). Few examples of bridging benzene-1,2-diamine-$\kappa^2 N$:N' (Liang & Qu, 2008; Duff, 1968), 1,3-diamine-$\kappa^2 N$:N' (Chemli *et al.*, 2013), or benzene-1,4-diamine-$\kappa^2 N$:N' (Liu *et al.*, 2012) ligands have been reported. Compounds (I) and (II) are two new examples of coordination polymers in which benzenediamine ligands bridge two metal atoms.

(I)

(II)
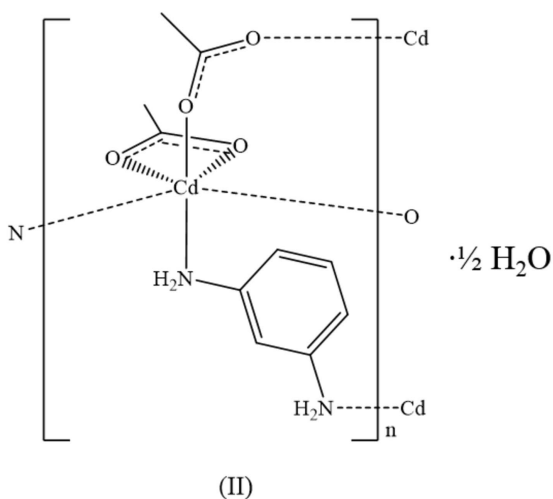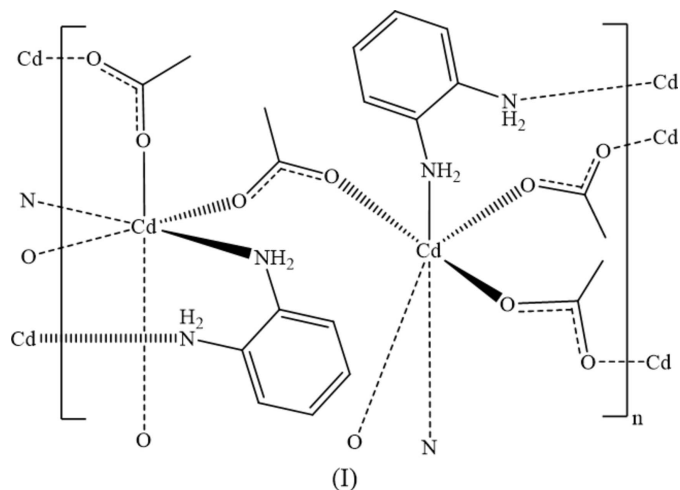
2. Structural commentary

As shown in Fig. 1, (I) has two symmetry-independent Cd$^{\mathrm{II}}$ ions. Cd1 sits on a crystallographically imposed inversion center and Cd2 resides on a crystallographically imposed twofold rotation axis. Each of the Cd$^{\mathrm{II}}$ ions exhibits an O$_4$N$_2$ coordination sphere composed of four bridging $\kappa^2 O$:O' acetate ligands and two bridging $\kappa^2 N$:N' benzene-1,2-diamine ligands. For the coordination sphere of Cd1, the twist angles (Muetterties & Guggenberger, 1974; Dymock & Palenik, 1975) defined employing the triangular face centroids N1O1O3 and N1$^{\mathrm{iii}}$O3$^{\mathrm{iii}}$O1$^{\mathrm{iii}}$ (see Fig. 2) are 52.26 (12), 66.27 (15) and 56.47 (9)°, giving an average value of 60 (5)°. Perfect O$_{\mathrm{h}}$ or D$_{3\mathrm{d}}$ trigonal antiprismatic structures have a twist angle of 60°, whereas a D$_{3\mathrm{h}}$ trigonal prismatic structure has a twist angle of 0°. The coordination sphere of Cd2 exhibits twist angles of

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

|			
Cd1—O3	2.323 (3)	Cd2—O4$^{\mathrm{i}}$	2.365 (3)
Cd1—O1	2.332 (3)	Cd2—O2	2.260 (3)
Cd1—N1	2.325 (4)	Cd2—N2$^{\mathrm{ii}}$	2.416 (4)
O3—Cd1—N1	84.79 (12)	O4$^{\mathrm{i}}$—Cd2—O4$^{\mathrm{iv}}$	80.73 (15)
O3—Cd1—O1	82.98 (11)	O2$^{\mathrm{iii}}$—Cd2—N2$^{\mathrm{ii}}$	79.40 (12)
N1—Cd1—O1	84.38 (12)	O2—Cd2—N2$^{\mathrm{ii}}$	115.81 (12)
O2$^{\mathrm{iii}}$—Cd2—O2	99.65 (17)	O4$^{\mathrm{i}}$—Cd2—N2$^{\mathrm{ii}}$	76.91 (12)
O2$^{\mathrm{iii}}$—Cd2—O4$^{\mathrm{i}}$	156.01 (10)	O4$^{\mathrm{iv}}$—Cd2—N2$^{\mathrm{ii}}$	85.97 (11)
O2—Cd2—O4$^{\mathrm{i}}$	93.98 (12)	N2$^{\mathrm{ii}}$—Cd2—N2$^{\mathrm{v}}$	157.5 (2)

Symmetry codes: (i) $-x+1, -y+3, -z+2$; (ii) $x, y+1, z$; (iii) $-x+1, y, -z+\frac{3}{2}$; (iv) $x, -y+3, z-\frac{1}{2}$; (v) $-x+1, y+1, -z+\frac{3}{2}$.

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

|			
Cd1—O3	2.275 (3)	Cd1—O1	2.374 (4)
Cd1—O4$^{\mathrm{i}}$	2.301 (3)	Cd1—N2$^{\mathrm{ii}}$	2.388 (4)
Cd1—N1	2.324 (4)	Cd1—O2	2.443 (4)
O3—Cd1—O4$^{\mathrm{i}}$	79.37 (11)	N1—Cd1—N2$^{\mathrm{ii}}$	101.86 (14)
O3—Cd1—N1	107.45 (13)	O1—Cd1—N2$^{\mathrm{ii}}$	84.00 (13)
O4$^{\mathrm{i}}$—Cd1—N1	99.25 (13)	O3—Cd1—O2	168.71 (11)
O3—Cd1—O1	114.63 (11)	O4$^{\mathrm{i}}$—Cd1—O2	98.78 (12)
O4$^{\mathrm{i}}$—Cd1—O1	85.82 (12)	N1—Cd1—O2	83.83 (13)
N1—Cd1—O1	137.80 (13)	O1—Cd1—O2	54.09 (11)
O3—Cd1—N2$^{\mathrm{ii}}$	86.63 (14)	N2$^{\mathrm{ii}}$—Cd1—O2	91.49 (13)
O4$^{\mathrm{i}}$—Cd1—N2$^{\mathrm{ii}}$	157.39 (13)		

Symmetry codes: (i) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (ii) $x, -y+1, z+\frac{1}{2}$.

35.49 (8), 45.92 (17) and 45.92 (17)° [average 42 (6)°] using opposite triangular faces O2O4$^{\mathrm{i}}$N2$^{\mathrm{iv}}$ and N2$^{\mathrm{ii}}$O4$^{\mathrm{iv}}$O2$^{\mathrm{vii}}$ (see Fig. 2). The coordination geometry is best described as distorted octahedral with the two nitrogen donor atoms *trans* for Cd1 and distorted trigonal antiprismatic for Cd2 with O$_2$N trigonal faces. Selected geometrical parameters are given in Table 1.
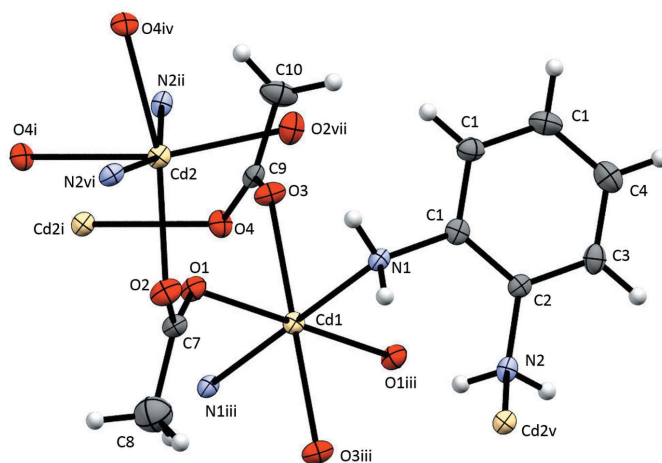
Figure 1
The atom-labeling scheme for (I). Anisotropic displacement parameters for non-H atoms are drawn at the 30% probability level. [Symmetry codes: (i) $-x+1, -y+3, -z+2$; (ii) $x, y+1, z$; (iii) $-x+1, -y+2, -z+2$; (iv) $x, -y+3, z-\frac{1}{2}$; (v) $x, y-1, z$; (vi) $-x+1, y+1, -z+\frac{3}{2}$; (vii) $-x+1, y, -z+\frac{3}{2}$.]
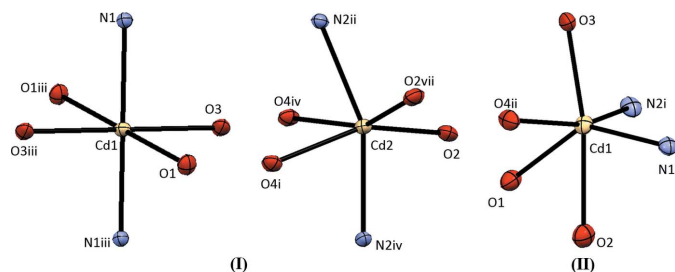
Figure 2
Representations of the Cd^{II} coordination environments observed in (I) and (II). Symmetry identifiers are those used in Figs. 1 and 3.

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1A⋯O2^{iii}	0.86 (2)	2.34 (2)	3.175 (5)	163 (4)
N1—H1B⋯O4^{vi}	0.91 (2)	2.21 (3)	3.003 (5)	146 (4)
N1—H1B⋯O4^{vii}	0.91 (2)	2.38 (4)	3.029 (5)	128 (4)
N2—H2A⋯O3^{viii}	0.86 (2)	2.30 (2)	3.111 (5)	158 (4)
N2—H2B⋯O3^{vi}	0.86 (2)	2.64 (2)	3.458 (5)	161 (4)
N2—H2B⋯O4^{vi}	0.86 (2)	2.55 (4)	2.973 (5)	111 (3)

Symmetry codes: (iii) $-x+1, y, -z+\frac{3}{2}$; (vi) $-x+1, -y+2, -z+2$; (vii) $x, -y+2, z-\frac{1}{2}$; (viii) $x, y-1, z$.

The N$_2$O$_4$ coordination geometry of (II) can be described as severely distorted trigonal antiprismatic with bidentate acetate oxygen atoms and a $\kappa^2 N{:}N'$ benzene-1,3-diamine nitrogen atom (O1O2N2^i) forming one of the trigonal faces and two $\kappa^2 O{:}O'$ acetate ligand oxygen atoms and a nitrogen atom from a $\kappa^2 N{:}N'$ benzene-1,3-diamine (O3O4^{ii}N1) forming the other trigonal face (see Fig. 2). The atom-labeling scheme is shown in Fig. 3. The twist angles are 53.71 (11), 22.56 (8) and 45.38 (13)° [average = 41 (16)°]. As seen in Table 2, the Cd—O bond lengths associated with the bidentate acetate ligand are shorter than those of the bridging, monodentate acetate ligands, as has been observed in other cadmium complexes (Wang *et al.*, 2011, 2013).

3. Supramolecular features

As seen in Fig. 4, the supramolecular architecture of (I) exhibits independent layers in the *bc* plane, which are repeated in the [100] direction. Extensive N—H⋯O hydrogen-bonding interactions exist (see Table 3), but none of them extend between the layers. Based on an analysis of the extended structure using the *SOLV* routine of *PLATON* (Spek, 2009), the unit cell contains no solvent-accessible voids.

Compound (II) also exhibits a two-dimensional extended structure. Layers parallel to the *bc* plane and repeated in the [100] direction are observed as seen in Fig. 5. N—H⋯O(acetate) hydrogen bonds (Table 4) are present within the layers. The water of hydration sits on a crystallographically imposed twofold rotation axis and, as seen in Fig. 6, is involved in O—H⋯O and N—H⋯O hydrogen-bonding interactions (Table 4) that link adjacent layers.
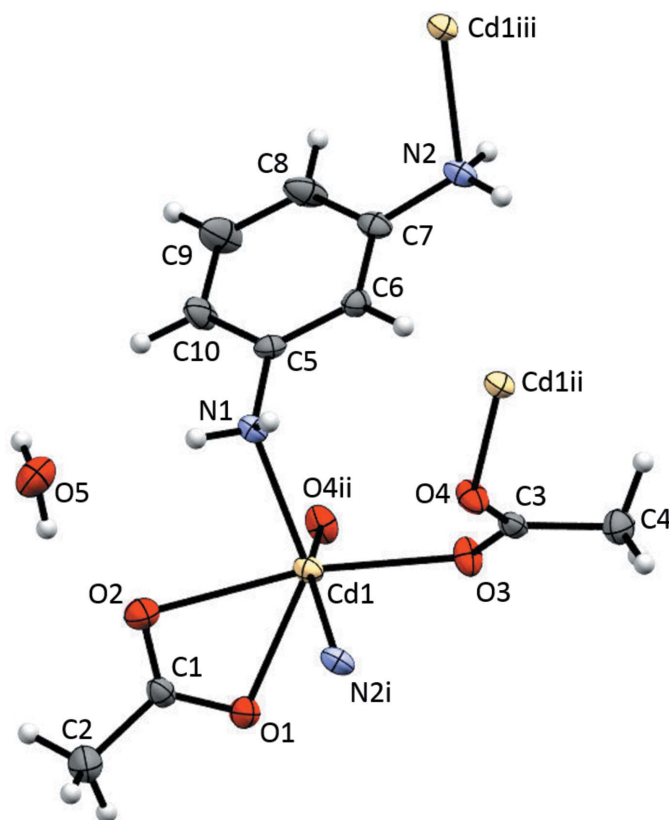

Figure 3
The atom-labeling scheme for (II). Anisotropic displacement parameters for non-H atoms are drawn at the 30% probability level. [Symmetry codes: (i) $x, -y+1, z+\frac{1}{2}$; (ii) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (iii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$.]
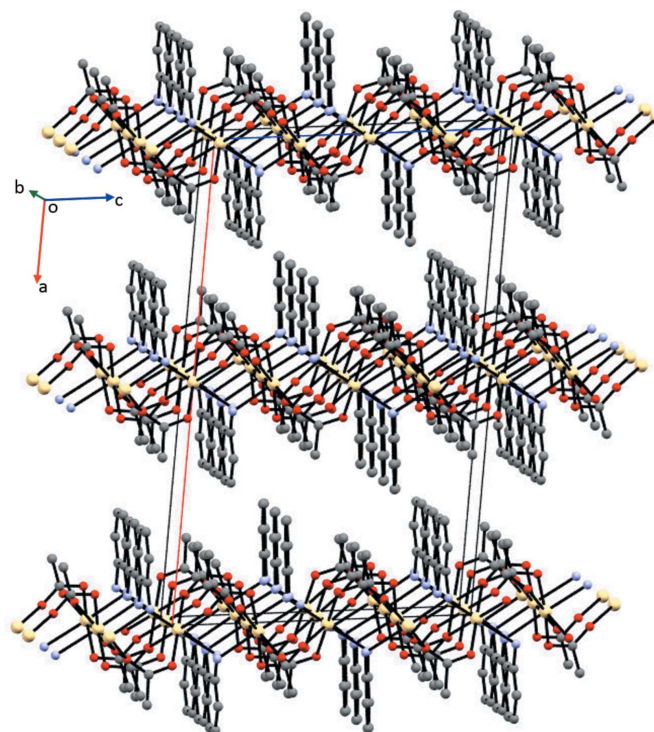
Figure 4
Packing diagram for (I) showing the two-dimensional network parallel to (100). All H atoms have been omitted for clarity.

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

| $D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O5—H5$\cdots$O2	0.81 (2)	2.06 (4)	2.788 (5)	149 (7)
N1—H$N1A\cdots$O5	0.86 (2)	2.34 (2)	3.183 (4)	166 (4)
N1—H$N1B\cdots$O3^{iii}	0.89 (2)	2.12 (2)	2.991 (5)	166 (5)
N2—H$N2A\cdots$O4^{iv}	0.87 (2)	2.32 (4)	3.012 (6)	137 (4)
N2—H$N2B\cdots$O1^{iii}	0.88 (2)	2.17 (3)	2.994 (5)	156 (5)

Symmetry codes: (iii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$; (iv) $x, -y+1, z-\frac{1}{2}$.

4. Database survey

Examples of cadmium coordination polymers with carboxylate ligands and that exhibit two-dimensional sheet structures have been reported (Li *et al.*, 2014; Gao *et al.*, 2004; Chen & Zhang, 2014; Zhang *et al.*, 2007; Liu & Xu, 2005; Song *et al.*, 2006; Kong *et al.*, 2008a,b; Xu *et al.*, 2013; Zhuo *et al.*, 2006).
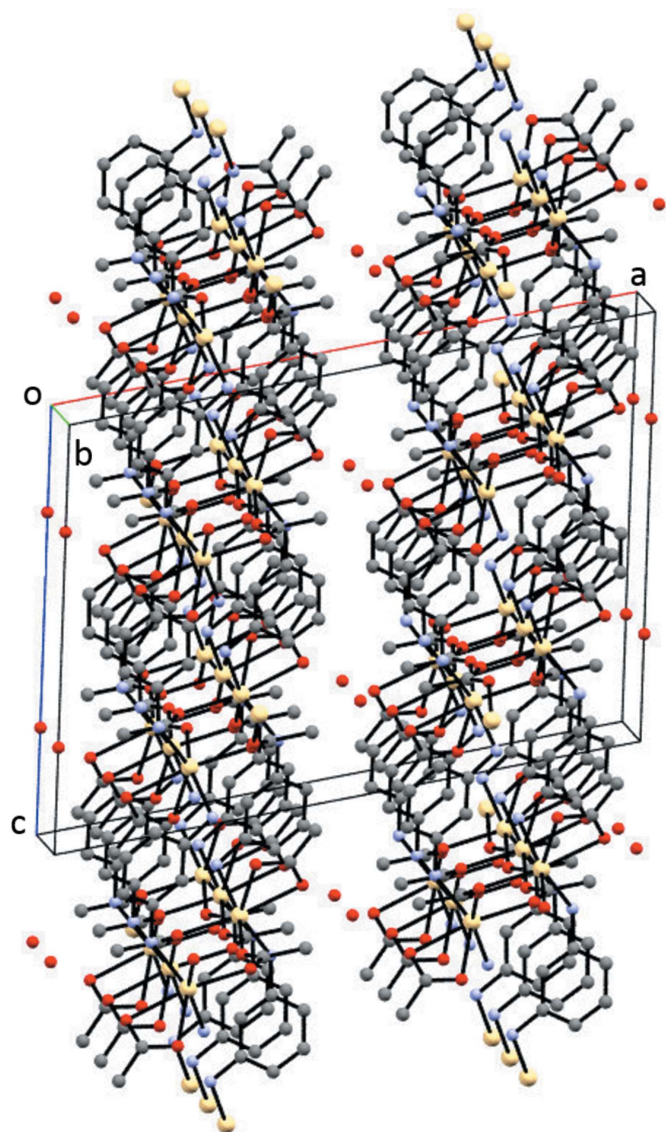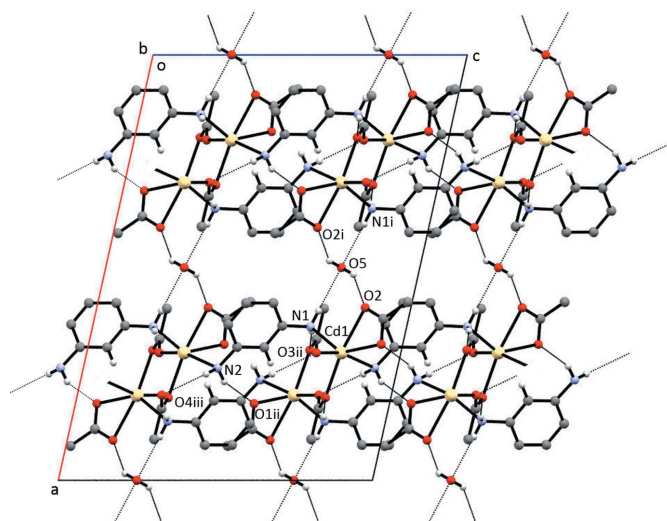
Figure 6
Partial packing diagram for (II) showing the hydrogen-bonded network. Only H atoms involved in the hydrogen-bonded network are shown. [Symmetry codes: (i) $-x+1, y, -z+\frac{3}{2}$; (ii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$; (iii) $x, -y+1, z-\frac{1}{2}$.]

Cadmium is commonly observed with a trigonal–prismatic or trigonal–antiprismatic coordination geometry, often with one or two capping ligands (Bygott *et al.*, 2007; Cherni *et al.*, 2012; Uçar *et al.*, 2004; Banerjee *et al.*, 2005; Keypour *et al.*, 2000). Coordination polymers with bridging benzene-1,2-diamine ligands (Liang & Qu, 2008; Duff, 1968), bridging benzene-1,3-diamine ligands (Chemli *et al.*, 2013), and bridging benzene-1,4-diamine ligands (Liu *et al.*, 2012) have been reported

5. Synthesis and crystallization

5.1. Preparation of (I)

213 mg (0.924 mmole) cadmium acetate hydrate were dissolved in 10 mL of ethanol. With stirring, 204 mg (1.89 mmol) of benzene-1,2-diamine were added and the resulting solution was refluxed for 2 h. A white precipitate formed, which was isolated by filtration and dried under vacuum. The yield was quantitative (310 mg). Selected IR bands (diamond anvil, cm^{-1}): 3278 (*w*), 1532 (*s*), 1504 (*s*), 1405 (*s*). ^{1}H NMR (400 MHz, dmso-d_6, p.p.m.): 1.87 (*s*, 6H), 6.35 (*m*, 2H), 6.35 (*m*, 2H).

Single crystals were obtained by heating some of the product in N,N′-dimethylformamide and allowing the solution to slowly cool to room temperature. The crystal used for data collection was obtained by cutting a piece from a larger plate.

5.2. Preparation of (II)

230 mg (1.00 mmol) cadmium acetate hydrate were dissolved in 10 mL of ethanol. 217 mg (2.01 mmol) benzene-1,3-diamine were added with stirring. The solution was gently refluxed for 2 h. After chilling the reaction mixture in an ice bath, the precipitate was filtered and dried under vacuum. A yield of 248 mg (71%) was obtained. Selected IR bands (diamond anvil, cm^{-1}): 3425 (*b*), 3329 (*s*) 3328 (*b*), 3137 (*m*),

Figure 5
Packing diagram for (II) showing the layers parallel to (100). H atoms have been omitted for clarity.

Table 5
Experimental details.

	(I)	(II)
Crystal data		
Chemical formula	$[Cd_2(C_2H_3O_2)_4(C_6H_8N_2)_2]$	$[Cd(C_2H_3O_2)_2(C_6H_8N_2)]\cdot 0.5H_2O$
M_r	338.63	695.28
Crystal system, space group	Monoclinic, $C2/c$	Monoclinic, $C2/c$
Temperature (K)	200	200
a, b, c (Å)	23.283 (3), 7.2399 (9), 14.2744 (16)	20.777 (6), 8.2374 (18), 15.002 (4)
β (°)	96.887 (4)	102.583 (9)
V (Å^3)	2388.8 (5)	2505.9 (11)
Z	8	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	1.83	1.75
Crystal size (mm)	$0.40 \times 0.40 \times 0.05$	$0.40 \times 0.08 \times 0.08$
Data collection		
Diffractometer	Bruker *SMART* X2S benchtop	Bruker *SMART* X2S benchtop
Absorption correction	Multi-scan (*SADABS*; Bruker, 2013)	Multi-scan (*SADABS*; Bruker, 2013)
T_{min}, T_{max}	0.53, 0.91	0.69, 0.87
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14588, 2263, 1633	8942, 2443, 1859
R_{int}	0.089	0.057
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.610	0.617
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.038, 0.109, 1.05	0.037, 0.095, 0.99
No. of reflections	2263	2443
No. of parameters	174	180
No. of restraints	4	6
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	1.14, −1.17	0.86, −1.02

Computer programs: *APEX2* and *SAINT* (Bruker, 2013), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *PLATON* (Spek, 2009), *Mercury* (Macrae *et al.*, 2006) and *publCIF* (Westrip, 2010).

1520 (*s*), 1505 (*s*), 1400 (*s*). ^{1}H NMR (400 MHz, dmso-d_6, p.p.m.): 1.83 (*s*, 6H), 5.78 (*m*, 3H), 6.64 (*t*, 1H). ^{13}C NMR (dmso-d_6, p.p.m.): 22.1, 100.5, 103.6, 129.6, 149.5, 178.0.

Clear, brown needles suitable for X-ray analysis were obtained upon slow evaporation of an ethanolic solution of the product. The crystals exhibit a melting range of 441–443 K with decomposition.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 5. For both (I) and (II), all hydrogen atoms were located in difference Fourier maps. The hydrogen atoms were refined using a riding model with a C—H distance of 0.98 Å for the methyl groups and 0.95 Å for the phenyl carbon atoms. The methyl hydrogen atom isotropic displacement parameters were set using the approximation $U_{iso}(H) = 1.5U_{eq}(C)$. All other C—H hydrogen atom isotropic displacement parameters were set using the approximation $U_{iso}(H) = 1.2U_{eq}(C)$. The N—H bond lengths were restrained to 0.88 Å in (I) and (II). The O—H bond length of the water of hydration in (II) was restrained to 0.84 Å and the H—O—H angle was restrained to 105°. $U_{iso}(H)$ was refined freely for the amine and water hydrogen atoms, except that for (II) the isotropic displacement parameters of the hydrogen atoms associated with N2 were restrained to be the same.

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Two cadmium coordination polymers with bridging acetate and phenylenediamine ligands that exhibit two-dimensional layered structures

David K. Geiger, Dylan E. Parsons and Bracco A. Pagano

Computing details

For both compounds, data collection: *APEX2* (Bruker, 2013); cell refinement: *APEX2* (Bruker, 2013); data reduction: *SAINT* (Bruker, 2013); 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.*, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

(I) Poly[tetra-μ_2-acetato-κ^8O:O'-bis(μ_2-benzene-1,2-diamine-κ^2N:N')dicadmium]

Crystal data

[Cd$_2$(C$_2$H$_3$O$_2$)$_4$(C$_6$H$_8$N$_2$)$_2$]	$F(000) = 1344$
$M_r = 338.63$	$D_x = 1.883$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 23.283$ (3) Å	Cell parameters from 120 reflections
$b = 7.2399$ (9) Å	$\theta = 3.5$–$24.0°$
$c = 14.2744$ (16) Å	$\mu = 1.83$ mm^{-1}
$\beta = 96.887$ (4)°	$T = 200$ K
$V = 2388.8$ (5) Å^3	Plate, clear colourless
$Z = 8$	$0.40 \times 0.40 \times 0.05$ mm

Data collection

Bruker SMART X2S benchtop diffractometer	14588 measured reflections
	2263 independent reflections
Radiation source: sealed microfocus tube	1633 reflections with $I > 2\sigma(I)$
Doubly curved silicon crystal monochromator	$R_{int} = 0.089$
Detector resolution: 8.3330 pixels mm^{-1}	$\theta_{max} = 25.7°$, $\theta_{min} = 2.9°$
ω scans	$h = -28 \rightarrow 27$
Absorption correction: multi-scan (SADABS; Bruker, 2013)	$k = -8 \rightarrow 8$
	$l = -17 \rightarrow 16$
$T_{min} = 0.53$, $T_{max} = 0.91$	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.038$	
$wR(F^2) = 0.109$	
$S = 1.05$	Hydrogen site location: mixed
2263 reflections	H atoms treated by a mixture of independent and constrained refinement
174 parameters	
4 restraints	

$w = 1/[\sigma^2(F_o^2) + (0.0496P)^2 + 0.5909P]$
  where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 1.14$ e Å^{-3}
$\Delta\rho_{min} = -1.17$ e 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.5	1.0	1.0	0.02022 (18)
Cd2	0.5	1.48311 (6)	0.75	0.02246 (18)
O1	0.53894 (13)	1.2329 (4)	0.91404 (19)	0.0280 (7)
O2	0.57421 (14)	1.2817 (4)	0.7785 (2)	0.0341 (8)
O3	0.43034 (13)	1.2226 (4)	1.01819 (19)	0.0287 (8)
O4	0.44787 (12)	1.2680 (4)	1.17354 (18)	0.0275 (7)
N1	0.44368 (16)	0.9351 (5)	0.8581 (2)	0.0220 (8)
H1A	0.4354 (19)	1.040 (4)	0.831 (3)	0.033 (14)*
H1B	0.4683 (16)	0.875 (6)	0.824 (3)	0.045 (15)*
N2	0.44711 (17)	0.5481 (6)	0.8818 (2)	0.0226 (8)
H2A	0.438 (2)	0.445 (4)	0.905 (3)	0.040 (15)*
H2B	0.4719 (16)	0.612 (6)	0.917 (3)	0.044 (15)*
C1	0.39101 (18)	0.8316 (6)	0.8544 (3)	0.0232 (10)
C2	0.39284 (18)	0.6415 (6)	0.8678 (3)	0.0213 (10)
C3	0.3425 (2)	0.5424 (7)	0.8632 (3)	0.0315 (12)
H3	0.344	0.4118	0.8697	0.038*
C4	0.2890 (2)	0.6318 (8)	0.8489 (3)	0.0409 (13)
H4	0.2541	0.5629	0.8467	0.049*
C5	0.2872 (2)	0.8209 (8)	0.8380 (3)	0.0403 (13)
H5	0.251	0.8824	0.829	0.048*
C6	0.3376 (2)	0.9219 (7)	0.8400 (3)	0.0326 (11)
H6	0.336	1.052	0.8316	0.039*
C7	0.57788 (19)	1.2169 (6)	0.8615 (3)	0.0267 (11)
C8	0.6357 (3)	1.1326 (10)	0.8978 (4)	0.0650 (18)
H8A	0.6648	1.2304	0.9089	0.098*
H8B	0.6473	1.0454	0.8511	0.098*
H8C	0.6324	1.0673	0.9571	0.098*
C9	0.41522 (19)	1.2753 (6)	1.0965 (3)	0.0248 (10)
C10	0.3540 (2)	1.3437 (8)	1.0964 (3)	0.0450 (14)
H10A	0.3441	1.3462	1.1612	0.067*
H10B	0.3274	1.2609	1.0581	0.067*
H10C	0.3507	1.4686	1.0697	0.067*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0250 (3)	0.0215 (3)	0.0140 (3)	−0.00045 (16)	0.0019 (2)	−0.00028 (16)
Cd2	0.0275 (3)	0.0228 (3)	0.0180 (3)	0	0.0066 (2)	0
O1	0.0330 (18)	0.0259 (18)	0.0270 (16)	0.0015 (14)	0.0107 (14)	0.0053 (14)
O2	0.047 (2)	0.034 (2)	0.0226 (18)	0.0065 (16)	0.0110 (14)	0.0081 (15)
O3	0.0396 (18)	0.0311 (19)	0.0166 (16)	0.0122 (15)	0.0083 (13)	0.0014 (14)
O4	0.0324 (18)	0.0324 (19)	0.0173 (16)	−0.0035 (15)	0.0010 (14)	−0.0029 (14)
N1	0.030 (2)	0.018 (2)	0.017 (2)	0.0000 (18)	0.0014 (16)	0.0001 (17)
N2	0.032 (2)	0.021 (2)	0.016 (2)	−0.0048 (19)	0.0047 (17)	0.0002 (18)
C1	0.032 (3)	0.028 (3)	0.010 (2)	−0.001 (2)	0.0050 (18)	−0.0021 (18)
C2	0.028 (2)	0.023 (2)	0.012 (2)	0.0015 (19)	0.0038 (18)	−0.0012 (18)
C3	0.039 (3)	0.030 (3)	0.026 (3)	−0.008 (2)	0.007 (2)	−0.004 (2)
C4	0.033 (3)	0.051 (4)	0.038 (3)	−0.006 (3)	0.004 (2)	−0.001 (3)
C5	0.030 (3)	0.049 (4)	0.041 (3)	0.011 (3)	0.004 (2)	0.003 (3)
C6	0.032 (3)	0.035 (3)	0.029 (3)	0.006 (2)	0.000 (2)	−0.002 (2)
C7	0.029 (3)	0.023 (3)	0.028 (3)	0.003 (2)	0.004 (2)	0.001 (2)
C8	0.065 (4)	0.066 (5)	0.065 (4)	0.004 (4)	0.013 (3)	0.002 (4)
C9	0.030 (2)	0.017 (2)	0.028 (3)	−0.0014 (19)	0.009 (2)	0.000 (2)
C10	0.036 (3)	0.063 (4)	0.036 (3)	0.016 (3)	0.006 (2)	−0.004 (3)

Geometric parameters (Å, º)

C1—C6	1.398 (6)	Cd1—O1^i	2.332 (3)
C1—C2	1.390 (6)	Cd1—N1	2.325 (4)
C10—H10C	0.98	Cd1—N1^i	2.325 (4)
C10—H10B	0.98	Cd2—O4^{ii}	2.365 (3)
C10—H10A	0.98	Cd2—O4^{iii}	2.365 (3)
C2—C3	1.369 (6)	Cd2—O2^{iv}	2.260 (3)
C3—H3	0.95	Cd2—O2	2.260 (3)
C3—C4	1.398 (7)	Cd2—N2^v	2.416 (4)
C4—H4	0.95	Cd2—N2^{vi}	2.416 (4)
C4—C5	1.378 (7)	N1—H1B	0.907 (19)
C5—H5	0.95	N1—H1A	0.864 (19)
C5—C6	1.378 (7)	N1—C1	1.432 (5)
C6—H6	0.95	N2—H2B	0.857 (19)
C7—C8	1.512 (7)	N2—H2A	0.86 (2)
C8—H8C	0.98	N2—Cd2^{vii}	2.415 (4)
C8—H8B	0.98	N2—C2	1.426 (6)
C8—H8A	0.98	O1—C7	1.250 (5)
C9—C10	1.509 (6)	O2—C7	1.267 (5)
Cd1—O3^i	2.323 (3)	O3—C9	1.270 (5)
Cd1—O3	2.323 (3)	O4—Cd2^{ii}	2.365 (3)
Cd1—O1	2.332 (3)	O4—C9	1.261 (5)
O3^i—Cd1—O3	180.00 (13)	C2—N2—H2A	102 (3)
O3^i—Cd1—N1	95.21 (12)	Cd2^{vii}—N2—H2A	108 (3)

O3—Cd1—N1	84.79 (12)	C2—N2—H2B	110 (4)
O3ⁱ—Cd1—N1ⁱ	84.79 (12)	Cd2^{vii}—N2—H2B	101 (3)
O3—Cd1—N1ⁱ	95.21 (12)	H2A—N2—H2B	115 (4)
N1—Cd1—N1ⁱ	180.0	C2—C1—C6	119.7 (4)
O3ⁱ—Cd1—O1	97.02 (11)	C2—C1—N1	120.1 (4)
O3—Cd1—O1	82.98 (11)	C6—C1—N1	120.2 (4)
N1—Cd1—O1	84.38 (12)	C3—C2—C1	120.1 (4)
N1ⁱ—Cd1—O1	95.62 (12)	C3—C2—N2	119.8 (4)
O3ⁱ—Cd1—O1ⁱ	82.98 (11)	C1—C2—N2	120.1 (4)
O3—Cd1—O1ⁱ	97.02 (11)	C2—C3—C4	120.5 (5)
N1—Cd1—O1ⁱ	95.62 (12)	C2—C3—H3	119.8
N1ⁱ—Cd1—O1ⁱ	84.38 (12)	C4—C3—H3	119.8
O1—Cd1—O1ⁱ	180.0	C5—C4—C3	119.4 (5)
O2^{iv}—Cd2—O2	99.65 (17)	C5—C4—H4	120.3
O2^{iv}—Cd2—O4ⁱⁱ	156.01 (10)	C3—C4—H4	120.3
O2—Cd2—O4ⁱⁱ	93.98 (12)	C4—C5—C6	120.7 (5)
O2^{iv}—Cd2—O4ⁱⁱⁱ	93.98 (11)	C4—C5—H5	119.6
O2—Cd2—O4ⁱⁱⁱ	156.01 (10)	C6—C5—H5	119.6
O4ⁱⁱ—Cd2—O4ⁱⁱⁱ	80.73 (15)	C5—C6—C1	119.6 (5)
O2^{iv}—Cd2—N2^v	79.40 (12)	C5—C6—H6	120.2
O2—Cd2—N2^v	115.81 (12)	C1—C6—H6	120.2
O4ⁱⁱ—Cd2—N2^v	76.91 (12)	O1—C7—O2	123.6 (4)
O4ⁱⁱⁱ—Cd2—N2^v	85.97 (11)	O1—C7—C8	120.8 (4)
O2^{iv}—Cd2—N2^{vi}	115.81 (12)	O2—C7—C8	115.3 (4)
O2—Cd2—N2^{vi}	79.40 (12)	C7—C8—H8A	109.5
O4ⁱⁱ—Cd2—N2^{vi}	85.97 (12)	C7—C8—H8B	109.5
O4ⁱⁱⁱ—Cd2—N2^{vi}	76.91 (12)	H8A—C8—H8B	109.5
N2^v—Cd2—N2^{vi}	157.5 (2)	C7—C8—H8C	109.5
C7—O1—Cd1	127.2 (3)	H8A—C8—H8C	109.5
C7—O2—Cd2	111.8 (3)	H8B—C8—H8C	109.5
C9—O3—Cd1	125.3 (3)	O4—C9—O3	123.6 (4)
C9—O4—Cd2ⁱⁱ	126.4 (3)	O4—C9—C10	119.1 (4)
C1—N1—Cd1	121.9 (2)	O3—C9—C10	117.3 (4)
C1—N1—H1A	107 (3)	C9—C10—H10A	109.5
Cd1—N1—H1A	107 (3)	C9—C10—H10B	109.5
C1—N1—H1B	109 (3)	H10A—C10—H10B	109.5
Cd1—N1—H1B	104 (3)	C9—C10—H10C	109.5
H1A—N1—H1B	107 (4)	H10A—C10—H10C	109.5
C2—N2—Cd2^{vii}	120.6 (2)	H10B—C10—H10C	109.5
Cd1—N1—C1—C2	−75.0 (4)	C4—C5—C6—C1	−0.8 (7)
Cd1—N1—C1—C6	103.1 (4)	C2—C1—C6—C5	−0.9 (6)
C6—C1—C2—C3	2.6 (6)	N1—C1—C6—C5	−179.0 (4)
N1—C1—C2—C3	−179.3 (4)	Cd1—O1—C7—O2	131.3 (4)
C6—C1—C2—N2	179.5 (4)	Cd1—O1—C7—C8	−54.7 (6)
N1—C1—C2—N2	−2.4 (6)	Cd2—O2—C7—O1	13.3 (6)
Cd2^{vii}—N2—C2—C3	99.3 (4)	Cd2—O2—C7—C8	−160.9 (4)
Cd2^{vii}—N2—C2—C1	−77.6 (5)	Cd2ⁱⁱ—O4—C9—O3	100.8 (5)

C1—C2—C3—C4	−2.7 (6)	Cd2ii—O4—C9—C10	−81.4 (5)
N2—C2—C3—C4	−179.6 (4)	Cd1—O3—C9—O4	26.7 (6)
C2—C3—C4—C5	1.0 (7)	Cd1—O3—C9—C10	−151.1 (4)
C3—C4—C5—C6	0.8 (7)		

Symmetry codes: (i) −x+1, −y+2, −z+2; (ii) −x+1, −y+3, −z+2; (iii) x, −y+3, z−1/2; (iv) −x+1, y, −z+3/2; (v) x, y+1, z; (vi) −x+1, y+1, −z+3/2; (vii) x, y−1, z.

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O2iv	0.86 (2)	2.34 (2)	3.175 (5)	163 (4)
N1—H1B···O4i	0.91 (2)	2.21 (3)	3.003 (5)	146 (4)
N1—H1B···O4viii	0.91 (2)	2.38 (4)	3.029 (5)	128 (4)
N2—H2A···O3vii	0.86 (2)	2.30 (2)	3.111 (5)	158 (4)
N2—H2B···O3i	0.86 (2)	2.64 (2)	3.458 (5)	161 (4)
N2—H2B···O4i	0.86 (2)	2.55 (4)	2.973 (5)	111 (3)
C8—H8C···O3i	0.98	2.61	3.295 (7)	127

Symmetry codes: (i) −x+1, −y+2, −z+2; (iv) −x+1, y, −z+3/2; (vii) x, y−1, z; (viii) x, −y+2, z−1/2.

(II) Poly[[(μ_2-acetato-κ^2O:O')(acetato-κ^2O,O')(μ_2-benzene-1,3-diamine-κ^2N:N')cadmium] hemihydrate]

Crystal data

[Cd(C₂H₃O₂)₂(C₆H₈N₂)]·0.5H₂O	$F(000) = 1384$
$M_r = 695.28$	$D_x = 1.843$ Mg m⁻³
Monoclinic, $C2/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 20.777$ (6) Å	Cell parameters from 2588 reflections
$b = 8.2374$ (18) Å	$\theta = 2.7$–23.5°
$c = 15.002$ (4) Å	$\mu = 1.75$ mm⁻¹
$\beta = 102.583$ (9)°	$T = 200$ K
$V = 2505.9$ (11) Å³	Needle, clear brown
$Z = 4$	0.40 × 0.08 × 0.08 mm

Data collection

Bruker SMART X2S benchtop diffractometer	8942 measured reflections
	2443 independent reflections
Radiation source: sealed microfocus tube	1859 reflections with $I > 2\sigma(I)$
Doubly curved silicon crystal monochromator	$R_{int} = 0.057$
Detector resolution: 8.3330 pixels mm⁻¹	$\theta_{max} = 26.0°$, $\theta_{min} = 2.7°$
ω scans	$h = -25 \rightarrow 25$
Absorption correction: multi-scan (SADABS; Bruker, 2013)	$k = -9 \rightarrow 10$
	$l = -18 \rightarrow 11$
$T_{min} = 0.69$, $T_{max} = 0.87$	

Refinement

Refinement on F^2	Hydrogen site location: mixed
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.037$	
$wR(F^2) = 0.095$	$w = 1/[\sigma^2(F_o^2) + (0.0489P)^2]$
$S = 0.99$	where $P = (F_o^2 + 2F_c^2)/3$
2443 reflections	$(\Delta/\sigma)_{max} = 0.001$
180 parameters	$\Delta\rho_{max} = 0.86$ e Å⁻³
6 restraints	$\Delta\rho_{min} = -1.02$ e 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.69991 (2)	0.34064 (4)	0.80989 (2)	0.02831 (14)
O1	0.68026 (16)	0.1764 (4)	0.9313 (2)	0.0381 (9)
O2	0.59435 (17)	0.3087 (4)	0.8546 (2)	0.0436 (9)
O3	0.80578 (15)	0.3370 (3)	0.7917 (3)	0.0357 (8)
O4	0.79978 (15)	0.6013 (4)	0.7691 (2)	0.0375 (8)
O5	0.5	0.5121 (7)	0.75	0.0581 (16)
H5	0.517 (3)	0.455 (4)	0.792 (2)	0.09 (2)*
N1	0.63907 (19)	0.5002 (5)	0.6938 (3)	0.0281 (9)
HN1A	0.6021 (14)	0.522 (5)	0.708 (3)	0.039 (15)*
HN1B	0.649 (2)	0.605 (3)	0.701 (3)	0.039 (14)*
N2	0.7361 (2)	0.4639 (5)	0.4277 (3)	0.0328 (9)
HN2A	0.750 (2)	0.394 (5)	0.393 (3)	0.044 (11)*
HN2B	0.7682 (17)	0.526 (5)	0.457 (3)	0.044 (11)*
C1	0.6204 (2)	0.2190 (6)	0.9196 (3)	0.0316 (11)
C2	0.5810 (3)	0.1613 (6)	0.9855 (4)	0.0553 (16)
H2A	0.5764	0.2496	1.0275	0.083*
H2B	0.6034	0.0692	1.0204	0.083*
H2C	0.5372	0.1272	0.952	0.083*
C3	0.8315 (2)	0.4712 (5)	0.7778 (3)	0.0283 (10)
C4	0.9037 (2)	0.4701 (6)	0.7760 (4)	0.0423 (13)
H4A	0.9093	0.5044	0.7156	0.064*
H4B	0.9213	0.3602	0.7888	0.064*
H4C	0.9275	0.5451	0.8224	0.064*
C5	0.6364 (2)	0.4410 (5)	0.6031 (3)	0.0276 (10)
C6	0.6875 (2)	0.4739 (5)	0.5613 (3)	0.0292 (11)
H6	0.7238	0.5375	0.5921	0.035*
C7	0.6866 (2)	0.4152 (5)	0.4748 (3)	0.0314 (11)
C8	0.6335 (3)	0.3195 (6)	0.4305 (4)	0.0463 (14)
H8	0.6327	0.2769	0.3714	0.056*
C9	0.5833 (3)	0.2881 (7)	0.4720 (4)	0.0573 (17)
H9	0.5473	0.2237	0.4413	0.069*
C10	0.5832 (3)	0.3481 (5)	0.5588 (4)	0.0436 (14)
H10	0.5475	0.3258	0.5871	0.052*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0331 (2)	0.0280 (2)	0.0254 (2)	0.00293 (14)	0.00988 (14)	−0.00140 (14)
O1	0.0347 (19)	0.045 (2)	0.036 (2)	0.0083 (15)	0.0105 (16)	0.0041 (15)

O2	0.043 (2)	0.049 (2)	0.038 (2)	0.0063 (16)	0.0066 (17)	0.0087 (16)
O3	0.0333 (17)	0.0217 (17)	0.056 (2)	−0.0019 (13)	0.0175 (17)	0.0015 (15)
O4	0.0414 (19)	0.0292 (17)	0.047 (2)	0.0059 (15)	0.0204 (17)	0.0114 (15)
O5	0.044 (3)	0.065 (4)	0.058 (4)	0	−0.004 (3)	0
N1	0.032 (2)	0.029 (2)	0.026 (2)	−0.0001 (19)	0.0113 (17)	0.0008 (17)
N2	0.041 (2)	0.036 (2)	0.024 (2)	−0.0003 (19)	0.0143 (18)	−0.0007 (18)
C1	0.033 (3)	0.035 (3)	0.028 (3)	−0.006 (2)	0.011 (2)	−0.005 (2)
C2	0.041 (3)	0.073 (4)	0.054 (4)	0.004 (3)	0.014 (3)	0.014 (3)
C3	0.033 (2)	0.033 (3)	0.021 (2)	−0.001 (2)	0.0095 (19)	−0.0018 (18)
C4	0.036 (3)	0.045 (3)	0.045 (3)	−0.006 (2)	0.007 (2)	0.004 (2)
C5	0.034 (2)	0.025 (2)	0.022 (2)	0.0006 (19)	0.002 (2)	0.0044 (17)
C6	0.029 (2)	0.030 (2)	0.027 (2)	−0.0059 (19)	0.002 (2)	0.0020 (19)
C7	0.041 (3)	0.025 (2)	0.029 (3)	0.004 (2)	0.011 (2)	0.0054 (19)
C8	0.070 (4)	0.043 (3)	0.027 (3)	−0.020 (3)	0.013 (3)	−0.008 (2)
C9	0.070 (4)	0.064 (4)	0.037 (3)	−0.041 (3)	0.009 (3)	−0.014 (3)
C10	0.044 (3)	0.052 (3)	0.035 (3)	−0.025 (2)	0.012 (2)	−0.001 (2)

Geometric parameters (Å, °)

Cd1—O3	2.275 (3)	C1—C2	1.492 (8)
Cd1—O4[i]	2.301 (3)	C2—H2A	0.98
Cd1—N1	2.324 (4)	C2—H2B	0.98
Cd1—O1	2.374 (4)	C2—H2C	0.98
Cd1—N2[ii]	2.388 (4)	C3—C4	1.506 (6)
Cd1—O2	2.443 (4)	C4—H4A	0.98
O1—C1	1.268 (5)	C4—H4B	0.98
O2—C1	1.249 (5)	C4—H4C	0.98
O3—C3	1.265 (5)	C5—C6	1.374 (6)
O4—C3	1.250 (5)	C5—C10	1.388 (6)
O4—Cd1[iii]	2.301 (3)	C6—C7	1.381 (6)
O5—H5	0.808 (18)	C6—H6	0.95
N1—C5	1.435 (6)	C7—C8	1.401 (6)
N1—HN1A	0.859 (19)	C8—C9	1.350 (8)
N1—HN1B	0.886 (19)	C8—H8	0.95
N2—C7	1.425 (6)	C9—C10	1.394 (8)
N2—Cd1[iv]	2.388 (4)	C9—H9	0.95
N2—HN2A	0.870 (19)	C10—H10	0.95
N2—HN2B	0.877 (19)		
O3—Cd1—O4[i]	79.37 (11)	C1—C2—H2A	109.5
O3—Cd1—N1	107.45 (13)	C1—C2—H2B	109.5
O4[i]—Cd1—N1	99.25 (13)	H2A—C2—H2B	109.5
O3—Cd1—O1	114.63 (11)	C1—C2—H2C	109.5
O4[i]—Cd1—O1	85.82 (12)	H2A—C2—H2C	109.5
N1—Cd1—O1	137.80 (13)	H2B—C2—H2C	109.5
O3—Cd1—N2[ii]	86.63 (14)	O4—C3—O3	122.3 (4)
O4[i]—Cd1—N2[ii]	157.39 (13)	O4—C3—C4	120.5 (4)
N1—Cd1—N2[ii]	101.86 (14)	O3—C3—C4	117.1 (4)

O1—Cd1—N2ⁱⁱ	84.00 (13)	C3—C4—H4A	109.5
O3—Cd1—O2	168.71 (11)	C3—C4—H4B	109.5
O4ⁱ—Cd1—O2	98.78 (12)	H4A—C4—H4B	109.5
N1—Cd1—O2	83.83 (13)	C3—C4—H4C	109.5
O1—Cd1—O2	54.09 (11)	H4A—C4—H4C	109.5
N2ⁱⁱ—Cd1—O2	91.49 (13)	H4B—C4—H4C	109.5
C1—O1—Cd1	93.7 (3)	C6—C5—C10	120.3 (5)
C1—O2—Cd1	91.0 (3)	C6—C5—N1	119.4 (4)
C3—O3—Cd1	117.6 (3)	C10—C5—N1	120.3 (5)
C3—O4—Cd1ⁱⁱⁱ	136.7 (3)	C5—C6—C7	120.4 (4)
C5—N1—Cd1	114.9 (3)	C5—C6—H6	119.8
C5—N1—HN1A	117 (3)	C7—C6—H6	119.8
Cd1—N1—HN1A	108 (3)	C6—C7—C8	119.4 (5)
C5—N1—HN1B	114 (3)	C6—C7—N2	120.2 (4)
Cd1—N1—HN1B	113 (3)	C8—C7—N2	120.1 (5)
HN1A—N1—HN1B	88 (4)	C9—C8—C7	119.8 (5)
C7—N2—Cd1ⁱᵛ	114.3 (3)	C9—C8—H8	120.1
C7—N2—HN2A	119 (3)	C7—C8—H8	120.1
Cd1ⁱᵛ—N2—HN2A	96 (3)	C8—C9—C10	121.4 (5)
C7—N2—HN2B	118 (4)	C8—C9—H9	119.3
Cd1ⁱᵛ—N2—HN2B	94 (3)	C10—C9—H9	119.3
HN2A—N2—HN2B	111 (5)	C5—C10—C9	118.7 (5)
O2—C1—O1	121.0 (5)	C5—C10—H10	120.6
O2—C1—C2	120.0 (4)	C9—C10—H10	120.6
O1—C1—C2	119.0 (4)		
Cd1—O2—C1—O1	−4.6 (4)	N1—C5—C6—C7	178.6 (4)
Cd1—O2—C1—C2	174.9 (4)	C5—C6—C7—C8	−1.0 (7)
Cd1—O1—C1—O2	4.8 (5)	C5—C6—C7—N2	173.2 (4)
Cd1—O1—C1—C2	−174.8 (4)	Cd1ⁱᵛ—N2—C7—C6	−103.9 (4)
Cd1ⁱⁱⁱ—O4—C3—O3	−148.4 (4)	Cd1ⁱᵛ—N2—C7—C8	70.2 (5)
Cd1ⁱⁱⁱ—O4—C3—C4	34.3 (6)	C6—C7—C8—C9	1.1 (8)
Cd1—O3—C3—O4	−3.8 (6)	N2—C7—C8—C9	−173.1 (5)
Cd1—O3—C3—C4	173.5 (3)	C7—C8—C9—C10	−0.4 (9)
Cd1—N1—C5—C6	−82.6 (4)	C6—C5—C10—C9	0.6 (7)
Cd1—N1—C5—C10	95.9 (4)	N1—C5—C10—C9	−177.9 (5)
C10—C5—C6—C7	0.1 (6)	C8—C9—C10—C5	−0.5 (9)

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

Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5···O2	0.81 (2)	2.06 (4)	2.788 (5)	149 (7)
N1—HN1A···O5	0.86 (2)	2.34 (2)	3.183 (4)	166 (4)
N1—HN1B···O3ⁱⁱⁱ	0.89 (2)	2.12 (2)	2.991 (5)	166 (5)
N2—HN2A···O4ⁱᵛ	0.87 (2)	2.32 (4)	3.012 (6)	137 (4)

N2—H*N2B*···O1ⁱⁱⁱ	0.88 (2)	2.17 (3)	2.994 (5)	156 (5)
C6—H6···O1ⁱⁱⁱ	0.95	2.39	3.195 (5)	142

Symmetry codes: (iii) −*x*+3/2, *y*+1/2, −*z*+3/2; (iv) *x*, −*y*+1, *z*−1/2.