Acta Cryst E
CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

Synthesis and crystal structure of *catena*-poly-[[[aqua(2,3-dimethylpyrazine-κ*N*)cadmium(II)]-di-*μ*-bromido] 2,3-dimethylpyrazine monosolvate hemihydrate]

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Received 27 April 2026
Accepted 21 May 2026

Edited by S. P. Kelley, University of Missouri-Columbia, USA

Keywords: coordination polymer; synthesis; cadmium bromide; 2,3-dimethylpyrazine; crystal structure.

CCDC reference: 2555772

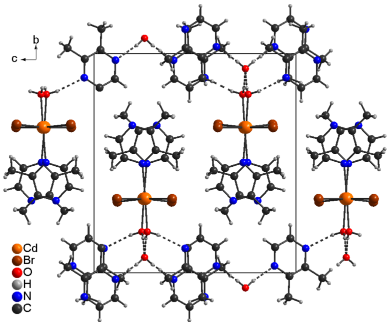
Supporting information: this article has supporting information at journals.iucr.org/e

Crystals of the title compound, $\{[CdBr_2(C_6H_8N_2)(H_2O)]\cdot C_6H_8N_2\cdot 0.5H_2O\}_n$ ($C_6H_8N_2$ = 2,3-dimethylpyrazine), were obtained accidentally by the reaction of cadmium bromide with 2,3-dimethylpyrazine in water. The asymmetric unit consists of one Cd cation, two bromide anions, one 2,3-dimethylpyrazine ligand, one non-coordinating 2,3-dimethylpyrazine molecule, and one water molecule in general positions as well as an additional water molecule that is located on a twofold rotation axis. The cadmium cations are octahedrally coordinated by four bromide anions, one 2,3-dimethylpyrazine ligand and one water molecule, and are linked by pairs of *μ*-1,1-bridging bromide anions into chains that propagate in the *a*-axis direction. These chains are further connected into layers by intermolecular hydrogen bonding. The coordinated water ligand is hydrogen bonded to the 2,3-dimethylpyrazine, and the water solvate molecule and the 2,3-dimethylpyrazine molecules of crystallization are linked by O—H⋯N hydrogen bonding *via* the water solvate molecules into chains along the *c*-axis direction. The water solvate molecule therefore acts as donor for two O—H⋯N and as acceptor for two O—H⋯O hydrogen bonds.

1. Chemical context

In recent years, numerous transition-metal halide and pseudohalide coordination compounds have been reported. In particular, those with copper(I) show a large structural variability, which can partly be traced back to the fact that these anions can act as bridging anionic ligands, leading to the formation of different metal-halide substructures (Kromp & Sheldrick, 1999; Peng *et al.*, 2010; Li *et al.*, 2005, Näther *et al.*, 2002). This variability frequently leads to the formation of compounds of different stoichiometry in which the ratio between the metal halide or metal pseudohalide is different. Whether this is the case for a given metal halide or pseudohalide and a given ligand can easily be checked by thermal treatment of coligand-rich compounds because in many cases they lose the neutral ligands in separate steps, leading to the formation of coligand-deficient compounds as intermediates (Näther *et al.*, 2001; Näther & Jess, 2001).

In the beginning, we focused on compounds based on Cu^I but later we also became interested in coordination compounds based on twofold positively charged metal cations such as zinc or cadmium. These compounds are of interest, for example, because of their luminescence properties (Mautner *et al.*, 2016; Jess *et al.*, 2020). In contrast to copper(I), such compounds do not show a comparable structural variability. However, the structural variability can be enhanced if ligands



are used that can act not only as monocoordinating but also as bridging ligands.

In this context, we recently reported on Zn and Cd halide compounds with 2,3-dimethylpyrazine as coligand. In contrast to Cd, which frequently exhibits an octahedral coordination, Zn cations usually prefer a tetrahedral coordination, even if compounds with an octahedral coordination are known. Compounds of different stoichiometry have been reported with Zn halides and 2,3-dimethylpyrazine, including $ZnCl_2$(2,3-dimethylpyrazine) (Näther & Bhosekar, 2025*a*), $ZnBr_2$(2,3-dimethylpyrazine) (Näther & Bhosekar, 2025*b*) and ZnI_2(2,3-dimethylpyrazine) (Näther & Bhosekar, 2026), with a ratio between ZnX_2 and coordinating coligands of 1:1. All of these compounds are isotypic and consist of tetrahedrally coordinated Zn cations that are linked by the 2,3-dimethylpyrazine ligands into chains.

2,3-Dimethylpyrazine-rich compounds with a ratio of 1:2 between ZnX_2 and coordinating coligands are also known. These are the isotypic compounds $ZnCl_2$(2,3-dimethylpyrazine)$_2$ (Näther & Bhosekar, 2025*a*) and $ZnBr_2$(2,3-dimethylpyrazine)$_2$ (Yang *et al.*, 2025), which consist of discrete complexes in which the Zn cations are tetrahedrally coordinated by two halide anions and two only terminally coordinated 2,3-dimethylpyrazine ligands. An additional compound with a ratio of 1:2 is the heteroleptic tetrahedral discrete complex [ZnI_2(2,3-dimethylpyrazine)(H_2O)](H_2O)$_{0.5}$(2,3-dimethylpyrazine)$_{0.5}$ that crystallizes with additional water and 2,3-dimethylpyrazine as solvate molecules (Näther & Bhosekar, 2026).

Within this project, we also reported the first compounds with cadmium halides and 2,3-dimethylpyrazine, including CdI_2(2,3-dimethylpyrazine)$_2$ and CdI_2(2,3-dimethylpyrazine) with a ratio of 1:2 or 1:1 between CdI_2 and coligands (Näther, 2026). The former consists of discrete complexes with only terminal coligands, whereas in the latter the 2,3-dimethylpyrazine ligands link the Cd cations into chains. These structures are therefore comparable to those with Zn halides and 2,3-dimethylpyrazine mentioned above. However, in none of these compounds are condensed metal halide substructures found in which the metal cations are linked by bridging halide anions. Therefore, in the course of our systematic investigations we decided to prepare compounds with cadmium and the remaining halide anions and within these investigations we accidentally obtained crystals from the reaction of $CdBr_2$ with 2,3-dimethylpyrazine in water that were characterized by single crystal X-ray diffraction.

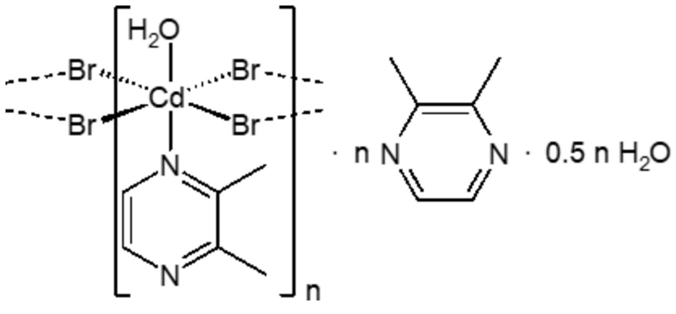


Table 1
Selected geometric parameters (Å, °).

Cd1—O1	2.346 (2)	Cd1—Br2	2.7255 (4)
Cd1—N1	2.484 (3)	Cd1—Br2^{i}	2.7450 (4)
Cd1—Br1	2.7245 (4)	Cd1—Br1^{ii}	2.7497 (4)
O1—Cd1—N1	176.18 (8)	Br2—Cd1—Br2^{i}	90.562 (11)
O1—Cd1—Br1	87.46 (6)	O1—Cd1—Br1^{ii}	91.94 (6)
N1—Cd1—Br1	96.11 (6)	N1—Cd1—Br1^{ii}	89.49 (6)
O1—Cd1—Br2	83.45 (6)	Br1—Cd1—Br1^{ii}	88.437 (11)
N1—Cd1—Br2	95.00 (6)	Br2—Cd1—Br1^{ii}	175.052 (12)
Br1—Cd1—Br2	93.156 (11)	Br2^{i}—Cd1—Br1^{ii}	87.487 (11)
O1—Cd1—Br2^{i}	88.39 (6)	Cd1—Br1—Cd1^{ii}	90.863 (11)
N1—Cd1—Br2^{i}	88.14 (6)	Cd1—Br2—Cd1^{i}	89.438 (11)
Br1—Cd1—Br2^{i}	174.086 (12)		

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

2. Structural commentary

The asymmetric unit of the title compound, [$CdBr_2(C_6H_8N_2)(H_2O)$]·$C_6H_8N_2$·$0.5H_2O$ ($C_6H_8N_2$ = 2,3-dimethylpyrazine), is built up of a half water molecule that is located on a twofold rotation axis, as well as one cadmium cation, one water molecule, one coordinating and one non-coordinating 2,3-dimethylpyrazine molecules that occupy general positions (Fig. 1). The cadmium cations are sixfold coordinated by four μ-1,1 bridging bromide anions as well as one 2,3-dimethylpyrazine ligand and one aqua ligand that occupy the apical positions. The bond lengths deviate only slightly from the ideal values, which shows that the octahedra are slightly distorted (Table 1). Because of steric repulsion, the Br—Cd—Br angles of the bromide atoms in the *cis*-position are larger than 90° (Table 1).

The Cd cations are linked by pairs of μ-1,1-bromide anions into chains along the *a*-axis direction (Fig. 2). These chains consist of octahedra that share common Br edges and the resulting Cd_2Br_2 rings are located around a twofold rotation axis. This chain motif is also observed in *catena*-[hexakis-(μ_2-bromo)diaquabis(2-hydroxyethylsulfide-*O*,*S*)tricadmium] (Refcode HAXGUI; Rogers *et al.*, 1993) and additional examples are given in the *Database survey*.

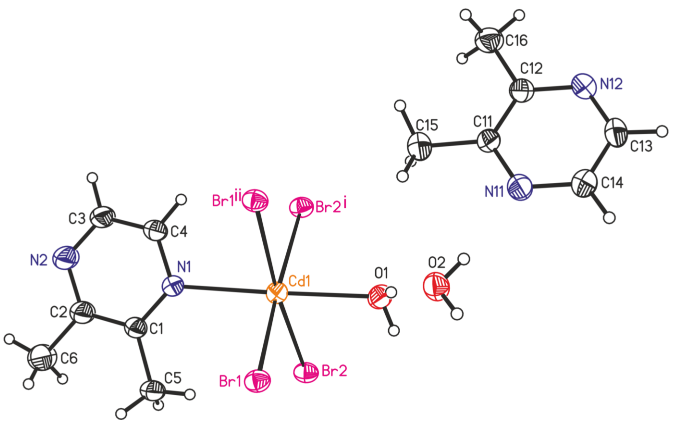


Figure 1
Crystal structure of the title compound with labeling and displacement ellipsoids drawn at the 50% probability level. [Symmetry codes: (i) $-x, y, -z + \frac{3}{2}$; (ii) $-x + 1, y, -z + \frac{3}{2}$.]

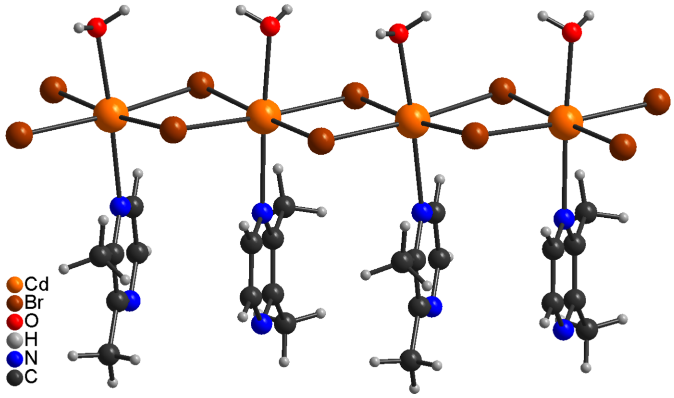


Figure 2
View of part of a chain in the crystal structure of the title compound.

3. Supramolecular features

In the crystal structure of the title compound, the H atoms of the coordinated water molecule are involved in intermolecular O—H⋯O and O—H⋯N hydrogen bonding to the solvate water molecule and the solvate 2,3-dimethylpyrazine molecule (Fig. 3). The latter is also connected to the solvate water molecule by intermolecular O—H⋯N hydrogen bonding. The uncoordinated water molecule is involved in four hydrogen bonds. First of all it acts as donor for two O—H⋯N hydrogen bonds to the 2,3-dimethylpyrazine molecules (O2—H1*O*2⋯N11) and secondly as acceptor for two O—H⋯O hydrogen bonds to the coordinated water molecules (O1—H1*O*1⋯O2, Fig. 3). This leads to the formation of hydrogen-bonded chains built up of water and 2,3-dimethylpyrazine molecules that propagate in the *c*-axis direction (Fig. 3). The O—H⋯N and O—H⋯O angles are close to linear, which suggests strong hydrogen-bonding interactions (Table 2). The $CdBr_2$ chains and the hydrogen-bonded network condense into layers that are parallel to the *a*/*c*-plane (Fig. 4). There are additional C—H⋯Br contacts but from the distances and angles they only correspond to weak interactions (Table 2).

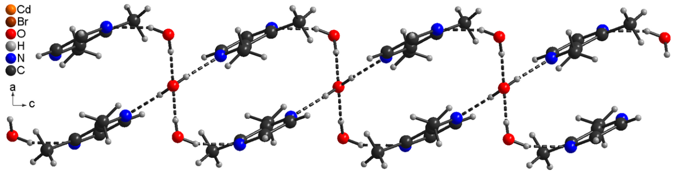


Figure 3
View of the hydrogen-bonded chains in the crystal structure of the title compound with intermolecular O—H⋯O and O—H⋯N hydrogen bonding shown as dashed lines.

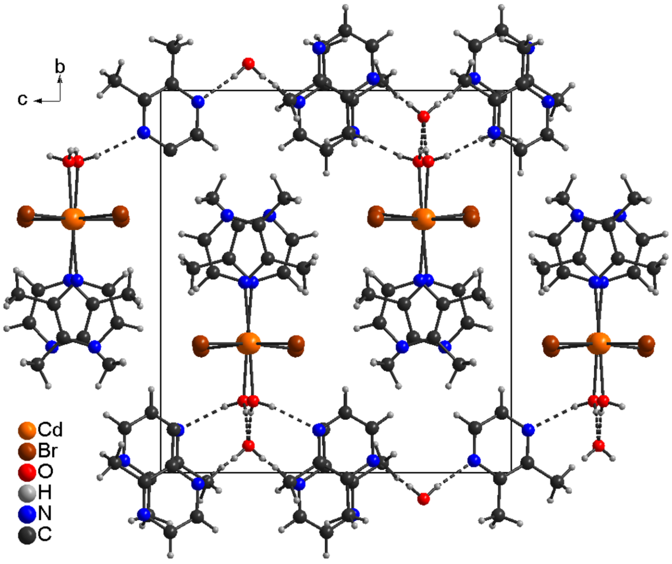


Figure 4
Crystal structure of the title compound in a view along the *a*-axis direction and intermolecular O—H⋯O and O—H⋯N hydrogen bonding shown as dashed lines.

Table 2
Hydrogen-bond geometry (Å, °).

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
O1—H1*O*1⋯O2	0.84	2.01	2.839 (3)	169
O1—H2*O*1⋯N12^{iii}	0.84	2.13	2.926 (4)	158
C4—H4⋯Br1^{ii}	0.95	3.00	3.592 (3)	122
C4—H4⋯Br2^{i}	0.95	3.01	3.545 (3)	117
C5—H5*A*⋯Br1	0.98	2.94	3.804 (3)	147
C5—H5*A*⋯Br2	0.98	3.01	3.657 (4)	125
C15—H15*C*⋯O2	0.98	2.65	3.449 (4)	139
O2—H1*O*2⋯N11	0.84	2.02	2.861 (3)	174

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

4. Database survey

As already mentioned in the *Chemical context* section, some compounds with zinc halides and 2,3-dimethylpyrazine have already been reported. In contrast, only two cadmium compounds with the composition CdI_2(2,3-dimethylpyrazine)$_2$ and CdI_2(2,3-dimethylpyrazine) are known (Näther, 2026). In both of these compounds the metal cations are in a tetrahedral coordination and are not connected *via* the halide anions, which, especially for cadmium, is somehow surprising.

However, a search in the CSD (CSD Version 5.43, 2025; Groom *et al.*, 2016) using CONQUEST (Bruno *et al.*, 2002) revealed that many compounds with cadmium halides and other pyrazine derivatives as coligands have been reported that also incorporate CdX_2 chains. These include CdX_2(pyrazine) [X = Cl, Br, I; CSD refcodes TISSUJ (Pickardt & Staub, 1996), RINSIQ and RINSOW (Bailey & Pennington, 1997), RINSOW01 and RINSIQ01 (Pickardt & Staub, 1997)] in which the Cd cations are linked by pairs of bridging halide anions into chains, which are further connected into layers by the pyrazine coligands. Similar CdX_2 chains are also found in compounds with 2-chloro and 2-methylpyrazine (Näther *et al.*, 2017), including $CdX_2(L)_2$ (X = Cl, Br, I, L = 2-chloro and methylpyrazine: QAWHOO, QAWGON, QAWGUT, QAWHAA, QAWHEE and QAWHII). Therefore, in the majority of cases the cadmium cations are linked into chains like those observed in the crystal structure of the title compound.

5. Synthesis and crystallization

General

Cadmium bromide and 2,3-dimethylpyrazine were purchased from Sigma-Aldrich.

Synthesis of the title compound

1 mmol (272.2 mg) of $CdBr_2$ and 2.0 mmol (216.3 mg) of 2,3-dimethylpyrazine were reacted in 3 mL of water for 3 d at room temperature, which led to the formation of crystals suitable for single-crystal X-ray diffraction analysis.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The C—H hydrogen atoms were positioned with idealized geometry (methyl H atoms allowed to rotate but not to tip) and were refined isotropically with $U_{iso}(H) = 1.2\ U_{eq}(C)$ (1.5 for methyl H atoms). The O—H hydrogen atoms were located in difference maps, their bond lengths were set to ideal values and finally they were refined isotropically with $U_{iso}(H) = 1.5\ U_{eq}(O)$ using a riding model.

Table 3
Experimental details.

Crystal data	
Chemical formula	$[CdBr_2(C_6H_8N_2)(H_2O)]\cdot C_6H_8N_2\cdot 0.5H_2O$
M_r	515.53
Crystal system, space group	Monoclinic, *P*2/*c*
Temperature (K)	170
a, *b*, *c* (Å)	7.7459 (4), 15.4368 (5), 14.1867 (7)
β (°)	90.621 (4)
V (Å^3)	1696.23 (13)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	6.00
Crystal size (mm)	0.13 × 0.11 × 0.09
Data collection	
Diffractometer	Stoe IPDS2
Absorption correction	Numerical (*X-RED* and *X-SHAPE*; Stoe, 2002)
T_{min}, T_{max}	0.338, 0.482
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13656, 4097, 3340
R_{int}	0.031
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.661
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.033, 0.089, 1.04
No. of reflections	4097
No. of parameters	191
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.74, −0.63

Computer programs: *X-AREA* (Stoe, 2002), *SHELXT2014/4* (Sheldrick, 2015*b*), *SHELXL2016/6* (Sheldrick, 2015*a*), *DIAMOND* (Brandenburg, 1999), *XP* in *SHELXTL-PC* (Sheldrick, 2008) and *publCIF* (Westrip, 2010).

Acknowledgements

Financial support by the State of Schleswig-Holstein is gratefully acknowledged.

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supporting information

Acta Cryst. (2026). E**82**, 743-746 [https://doi.org/10.1107/S2056989026005372]

Synthesis and crystal structure of *catena*-poly[[[aqua(2,3-dimethylpyrazine-κ*N*)cadmium(II)]-di-*µ*-bromido] 2,3-dimethylpyrazine monosolvate hemihydrate]

Christian Näther

Computing details

catena-Poly[[[aqua(2,3-dimethylpyrazine-κ*N*)cadmium(II)]-di-*µ*-bromido] 2,3-dimethylpyrazine monosolvate hemihydrate]

Crystal data

$[CdBr_2(C_6H_8N_2)(H_2O)]\cdot C_6H_8N_2\cdot 0.5H_2O$
$M_r = 515.53$
Monoclinic, $P2/c$
$a = 7.7459$ (4) Å
$b = 15.4368$ (5) Å
$c = 14.1867$ (7) Å
$\beta = 90.621$ (4)°
$V = 1696.23$ (13) Å^3
$Z = 4$

$F(000) = 996$
$D_x = 2.019$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 12616 reflections
$\theta = 2.5$–$27.3°$
$\mu = 6.00$ mm^{-1}
$T = 170$ K
Block, colorless
0.13 × 0.11 × 0.09 mm

Data collection

Stoe IPDS-2
diffractometer
ω scans
Absorption correction: numerical
(X-Red and X-Shape; Stoe, 2002)
$T_{min} = 0.338$, $T_{max} = 0.482$
13656 measured reflections

4097 independent reflections
3340 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 28.0°$, $\theta_{min} = 2.0°$
$h = -10 \rightarrow 9$
$k = -20 \rightarrow 20$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.089$
$S = 1.04$
4097 reflections
191 parameters
0 restraints
Hydrogen site location: mixed
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0537P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.74$ e Å^{-3}
$\Delta\rho_{min} = -0.63$ e Å^{-3}
Extinction correction: SHELXL-2016/6
(Sheldrick 2016),
$Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0028 (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*	$U_{\rm iso}$*/$U_{\rm eq}$
Cd1	0.24844 (3)	0.33730 (2)	0.75394 (2)	0.02363 (9)
Br1	0.50745 (4)	0.32344 (2)	0.88453 (2)	0.02634 (10)
Br2	−0.00279 (4)	0.33703 (2)	0.88698 (2)	0.02708 (10)
O1	0.2182 (3)	0.18633 (15)	0.76353 (15)	0.0309 (5)
H1O1	0.309445	0.157649	0.756830	0.046*
H2O1	0.181245	0.172289	0.816830	0.046*
N1	0.2606 (3)	0.49752 (17)	0.73937 (17)	0.0261 (5)
C1	0.2571 (4)	0.5595 (2)	0.8054 (2)	0.0275 (6)
C2	0.2539 (5)	0.6471 (2)	0.7793 (3)	0.0388 (8)
N2	0.2579 (6)	0.67206 (19)	0.6891 (2)	0.0483 (9)
C3	0.2627 (5)	0.6087 (2)	0.6244 (2)	0.0389 (8)
H3	0.265776	0.623769	0.559538	0.047*
C4	0.2633 (4)	0.5231 (2)	0.6493 (2)	0.0309 (7)
H4	0.265691	0.480448	0.601080	0.037*
C5	0.2568 (5)	0.5342 (2)	0.9072 (2)	0.0331 (7)
H5A	0.274417	0.471500	0.912769	0.050*
H5B	0.145650	0.549789	0.934936	0.050*
H5C	0.349968	0.564623	0.940715	0.050*
C6	0.2480 (8)	0.7174 (3)	0.8526 (3)	0.0617 (13)
H6A	0.243977	0.774031	0.821427	0.093*
H6B	0.351389	0.713953	0.892862	0.093*
H6C	0.144923	0.710028	0.891199	0.093*
N11	0.3329 (4)	−0.03052 (18)	0.60583 (19)	0.0325 (6)
C11	0.2779 (4)	0.0162 (2)	0.5316 (2)	0.0273 (6)
C12	0.2007 (4)	−0.0250 (2)	0.4535 (2)	0.0288 (6)
N12	0.1791 (4)	−0.11062 (19)	0.4512 (2)	0.0331 (6)
C13	0.2314 (5)	−0.1561 (2)	0.5267 (2)	0.0345 (7)
H13	0.215947	−0.217148	0.527435	0.041*
C14	0.3067 (5)	−0.1161 (2)	0.6029 (2)	0.0357 (7)
H14	0.341562	−0.150324	0.655451	0.043*
C15	0.3008 (5)	0.1122 (2)	0.5364 (3)	0.0384 (8)
H15A	0.191047	0.139386	0.553252	0.058*
H15B	0.337665	0.133830	0.474869	0.058*
H15C	0.388631	0.126313	0.584184	0.058*
C16	0.1419 (5)	0.0250 (2)	0.3681 (2)	0.0393 (8)
H16A	0.242693	0.047585	0.334999	0.059*
H16B	0.068520	0.073317	0.387805	0.059*
H16C	0.076088	−0.013282	0.325975	0.059*
O2	0.500000	0.0696 (2)	0.750000	0.0333 (7)

H1O2	0.450360	0.037064	0.710700	0.050*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.02233 (14)	0.02422 (14)	0.02434 (14)	0.00021 (7)	−0.00011 (9)	0.00123 (7)
Br1	0.02315 (16)	0.03242 (17)	0.02344 (16)	−0.00015 (12)	0.00002 (11)	0.00176 (11)
Br2	0.02306 (17)	0.03493 (19)	0.02322 (16)	0.00152 (11)	−0.00020 (11)	−0.00067 (11)
O1	0.0348 (11)	0.0290 (11)	0.0290 (10)	0.0023 (10)	0.0047 (9)	0.0027 (9)
N1	0.0307 (13)	0.0250 (13)	0.0228 (12)	−0.0010 (10)	−0.0005 (10)	0.0017 (9)
C1	0.0331 (16)	0.0260 (15)	0.0234 (14)	0.0010 (12)	0.0013 (12)	−0.0024 (11)
C2	0.060 (2)	0.0293 (17)	0.0274 (15)	0.0017 (17)	0.0016 (14)	−0.0009 (13)
N2	0.088 (3)	0.0268 (16)	0.0302 (15)	0.0007 (16)	0.0021 (16)	0.0029 (11)
C3	0.064 (2)	0.0276 (17)	0.0247 (16)	0.0019 (16)	0.0002 (15)	0.0026 (12)
C4	0.0394 (17)	0.0300 (16)	0.0231 (14)	0.0001 (13)	−0.0009 (12)	−0.0023 (12)
C5	0.0446 (19)	0.0325 (17)	0.0221 (14)	0.0006 (15)	0.0002 (13)	−0.0016 (12)
C6	0.120 (4)	0.0265 (18)	0.038 (2)	0.004 (2)	0.006 (2)	−0.0026 (15)
N11	0.0389 (15)	0.0280 (14)	0.0306 (13)	0.0007 (12)	−0.0047 (11)	−0.0005 (10)
C11	0.0308 (16)	0.0254 (14)	0.0257 (14)	−0.0002 (12)	0.0034 (12)	0.0008 (11)
C12	0.0298 (15)	0.0297 (16)	0.0267 (14)	−0.0004 (12)	0.0007 (12)	−0.0003 (12)
N12	0.0388 (15)	0.0295 (14)	0.0311 (14)	−0.0016 (12)	0.0014 (12)	−0.0039 (11)
C13	0.0411 (19)	0.0232 (15)	0.0393 (17)	0.0004 (13)	0.0001 (14)	−0.0024 (13)
C14	0.0426 (19)	0.0299 (17)	0.0345 (17)	0.0011 (15)	−0.0012 (14)	0.0030 (13)
C15	0.048 (2)	0.0286 (17)	0.0382 (18)	−0.0039 (15)	−0.0019 (16)	−0.0008 (13)
C16	0.049 (2)	0.0388 (19)	0.0304 (16)	0.0063 (16)	−0.0018 (15)	0.0012 (14)
O2	0.0354 (17)	0.0290 (17)	0.0353 (17)	0.000	−0.0078 (14)	0.000

Geometric parameters (Å, º)

Cd1—O1	2.346 (2)	C6—H6A	0.9800
Cd1—N1	2.484 (3)	C6—H6B	0.9800
Cd1—Br1	2.7245 (4)	C6—H6C	0.9800
Cd1—Br2	2.7255 (4)	N11—C14	1.337 (4)
Cd1—Br2^{i}	2.7450 (4)	N11—C11	1.342 (4)
Cd1—Br1^{ii}	2.7497 (4)	C11—C12	1.406 (5)
O1—H1O1	0.8400	C11—C15	1.493 (5)
O1—H2O1	0.8400	C12—N12	1.332 (4)
N1—C4	1.338 (4)	C12—C16	1.503 (5)
N1—C1	1.339 (4)	N12—C13	1.340 (5)
C1—C2	1.402 (5)	C13—C14	1.370 (5)
C1—C5	1.497 (4)	C13—H13	0.9500
C2—N2	1.337 (4)	C14—H14	0.9500
C2—C6	1.504 (5)	C15—H15A	0.9800
N2—C3	1.342 (4)	C15—H15B	0.9800
C3—C4	1.368 (5)	C15—H15C	0.9800
C3—H3	0.9500	C16—H16A	0.9800
C4—H4	0.9500	C16—H16B	0.9800
C5—H5A	0.9800	C16—H16C	0.9800

C5—H5B	0.9800	O2—H1O2	0.8400
C5—H5C	0.9800	O2—H1O2^{ii}	0.8400

O1—Cd1—N1	176.18 (8)	H5A—C5—H5B	109.5
O1—Cd1—Br1	87.46 (6)	C1—C5—H5C	109.5
N1—Cd1—Br1	96.11 (6)	H5A—C5—H5C	109.5
O1—Cd1—Br2	83.45 (6)	H5B—C5—H5C	109.5
N1—Cd1—Br2	95.00 (6)	C2—C6—H6A	109.5
Br1—Cd1—Br2	93.156 (11)	C2—C6—H6B	109.5
O1—Cd1—Br2^{i}	88.39 (6)	H6A—C6—H6B	109.5
N1—Cd1—Br2^{i}	88.14 (6)	C2—C6—H6C	109.5
Br1—Cd1—Br2^{i}	174.086 (12)	H6A—C6—H6C	109.5
Br2—Cd1—Br2^{i}	90.562 (11)	H6B—C6—H6C	109.5
O1—Cd1—Br1^{ii}	91.94 (6)	C14—N11—C11	117.4 (3)
N1—Cd1—Br1^{ii}	89.49 (6)	N11—C11—C12	120.2 (3)
Br1—Cd1—Br1^{ii}	88.437 (11)	N11—C11—C15	117.5 (3)
Br2—Cd1—Br1^{ii}	175.052 (12)	C12—C11—C15	122.3 (3)
Br2^{i}—Cd1—Br1^{ii}	87.487 (11)	N12—C12—C11	121.4 (3)
Cd1—Br1—Cd1^{ii}	90.863 (11)	N12—C12—C16	116.9 (3)
Cd1—Br2—Cd1^{i}	89.438 (11)	C11—C12—C16	121.7 (3)
Cd1—O1—H1O1	115.6	C12—N12—C13	117.6 (3)
Cd1—O1—H2O1	110.1	N12—C13—C14	121.2 (3)
H1O1—O1—H2O1	105.2	N12—C13—H13	119.4
C4—N1—C1	117.2 (3)	C14—C13—H13	119.4
C4—N1—Cd1	112.0 (2)	N11—C14—C13	122.2 (3)
C1—N1—Cd1	130.7 (2)	N11—C14—H14	118.9
N1—C1—C2	120.3 (3)	C13—C14—H14	118.9
N1—C1—C5	119.3 (3)	C11—C15—H15A	109.5
C2—C1—C5	120.4 (3)	C11—C15—H15B	109.5
N2—C2—C1	122.0 (3)	H15A—C15—H15B	109.5
N2—C2—C6	117.0 (3)	C11—C15—H15C	109.5
C1—C2—C6	120.9 (3)	H15A—C15—H15C	109.5
C2—N2—C3	116.5 (3)	H15B—C15—H15C	109.5
N2—C3—C4	121.8 (3)	C12—C16—H16A	109.5
N2—C3—H3	119.1	C12—C16—H16B	109.5
C4—C3—H3	119.1	H16A—C16—H16B	109.5
N1—C4—C3	122.1 (3)	C12—C16—H16C	109.5
N1—C4—H4	118.9	H16A—C16—H16C	109.5
C3—C4—H4	118.9	H16B—C16—H16C	109.5
C1—C5—H5A	109.5	H1O2—O2—H1O2^{ii}	106.7
C1—C5—H5B	109.5		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*1···O2	0.84	2.01	2.839 (3)	169

O1—H2*O*1···N12^{iii}	0.84	2.13	2.926 (4)	158
C4—H4···Br1^{ii}	0.95	3.00	3.592 (3)	122
C4—H4···Br2^{i}	0.95	3.01	3.545 (3)	117
C5—H5*A*···Br1	0.98	2.94	3.804 (3)	147
C5—H5*A*···Br2	0.98	3.01	3.657 (4)	125
C15—H15*C*···O2	0.98	2.65	3.449 (4)	139
O2—H1*O*2···N11	0.84	2.02	2.861 (3)	174

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