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Syntheses and crystal structures of bis(2,3-dimethylpyrazine-κN)diiodidocadmium(II) and *catena*-poly[[diiodidocadmium(II)]-μ-2,3-dimethylpyrazine-$\kappa^2 N^1:N^4$]

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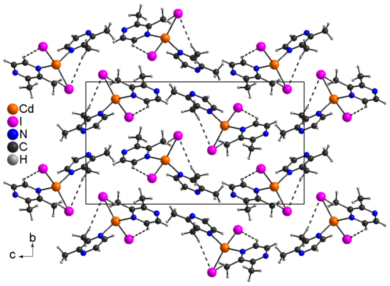
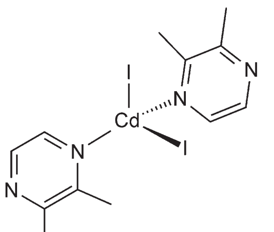
The reaction of cadmium iodide with 2,3-dimethylpyrazine leads to the formation of two compounds with the compositions [$CdI_2(C_6H_8N_2)_2$] or [CdI_2(2,3-dimethylpyrazine)$_2$] (**1**) and [$CdI_2(C_6H_8N_2)$]$_n$ or [CdI_2(2,3-dimethylpyrazine)]$_n$ (**2**). The asymmetric unit of **1** is built up of one Cd^{II} cation as well as two iodide anions and two 2,3-dimethylpyrazine ligands representing complete molecules. The Cd^{II} cations are tetrahedrally coordinated, forming discrete complexes that are connected *via* weak C—H$\cdots$I interactions. The asymmetric unit of **2** consists of one Cd^{II} cation and two crystallographically independent iodide anions that are located on a crystallographic mirror plane, as well as one 2,3-dimethylpyrazine ligand that is located on a twofold rotation axis. The Cd^{II} cations are tetrahedrally coordinated by two iodide anions and two 2,3-dimethylpyrazine ligands into corrugated chains. As in **1**, intermolecular C—H$\cdots$I interactions are observed. Comparison of the experimental powder patterns with those calculated from single-crystal data proves that pure compounds have been obtained. The crystal structures are compared with those of related MX_2 (M = Zn, Cd, X = Cl, Br, I) coordination compounds with pyrazine and 2,3-dimethylpyrazine, that are reported in the literature.

1. Chemical context

For many years we and others have been interested in the synthesis, crystal structures and thermal properties of transition metal halide compounds with one- and twofold positively charged cations and N-donor coligands (Kromp & Sheldrick, 1999; Peng *et al.*, 2010; Li *et al.*, 2005; Näther & Jess, 2002). For one definite N-donor ligand and one definite halide anion, compounds with a different ratio between the metal halide and the coligand are usually observed. Many years ago, we found that many coligand-rich Cu^I compounds lose their coligands in different steps upon heating, leading to the formation of coligand-deficient phases as intermediates (Näther & Jess, 2001; Näther *et al.*, 2001, 2002). Later we also observed that some metal halide compounds with Zn^{II} or Cd^{II} show a similar thermal reactivity, even if it is not as pronounced as for the Cu^I compounds (Neumann *et al.*, 2018*a*, *b*). This can be traced back to the fact that in copper(I) compounds, a number of different CuX substructures such as rings or layers are observed, which are not observed for Zn^{II} compounds and only rarely for Cd^{II} compounds. However, some examples exist where the metal cations in ZnX_2 or CdX_2 compounds are linked by bridging halide anions into, for example, dinuclear units (Geringer *et al.*, 2020; Panda *et al.*, 2024; Rogers, 2020; Pickardt & Staub, 1997).





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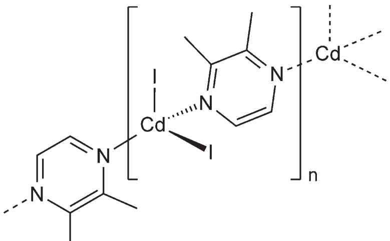

2

However, compounds with a different ratio between the metal halide and the N-donor ligands can also be obtained if bridging, instead of monocoordinating coligands, are used. This is the case, for example, for compounds with pyrazine as coligand, for which ligand-rich and ligand-deficient compounds with the composition ZnX_2(pyrazine)$_2$ [X = Cl (refcode REMPAB; Bhosekar *et al.*, 2006) and X = Br (EBOLAI; Bourne *et al.*, 2001)] and ZnX_2(pyrazine) (X = Cl, Br, I) [X = Cl (refcode TISTAQ; Pickardt & Staub, 1997), X = Br (EBOKUB; Bourne *et al.*, 2001), X = I (ISOPOV; Song *et al.*, 2004 and ISOPOV01; Bhosekar *et al.*, 2006)] are reported. Surprisingly, with Cd^{II} only the pyrazine-deficient compounds with the composition CdX_2(pyrazine) are listed in the Cambridge Structural Database (CSD Version 5.43, 2025; Groom *et al.*, 2016) [X = Cl (refcode TISSUJ; Pickardt & Staub, 1996, TISSUJ01; Bailey & Pennington, 1997, Lusi *et al.*, 2011), X = Br (RINSIQ; Bailey & Pennington, 1997, RINSIQ01, Pickardt & Staub, 1996), X = I (RINSOW; Bailey & Pennington, 1997, Pickardt & Staub, 1997)].

In the course of our systematic project, we became interested in ZnX_2 and CdX_2 compounds with 2,3-dimethylpyrazine, in which the metal coordination is more difficult, because of the methyl groups that are adjacent to the coordinating N atom. With ZnX_2 (X = Cl, Br, I) chloride-bearing compounds with the composition [ZnCl$_2$(2,3-dimethylpyrazine)$_2$] and [ZnCl$_2$(2,3-dimethylpyrazine)]$_n$ were characterized (Näther & Bhosekar, 2025*a*). The former compound consists of discrete tetrahedral complexes, whereas in the second compound the tetrahedra are linked into chains *via* the 2,3-dimethylpyrazine ligands. [ZnBr$_2$(2,3-Dimethylpyrazine)$_2$] is isotypic with the corresponding ZnCl$_2$ compound (Yang *et al.*, 2025) and in [ZnBr$_2$(2,3-dimethylpyrazine)]$_n$ the metal cations are linked into chains (Näther & Bhosekar, 2025*b*). Finally, [ZnI$_2$(2,3-dimethylpyrazine)] is also reported and is isotypic to its bromide analog (Näther & Bhosekar, 2026). Compounds based on CdX_2 (X = Cl, Br, I) are not reported and therefore, in our initial experiments we tried to prepare such compounds. Here we report on our investigations.

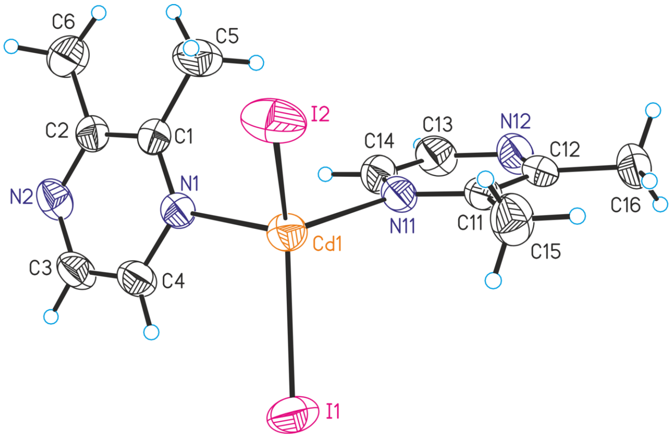

Figure 1
Crystal structure of **1** with labeling and displacement ellipsoids drawn at the 50% probability level.

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

Cd1—N1	2.329 (3)	Cd1—I2	2.7084 (4)
Cd1—N11	2.331 (3)	Cd1—I1	2.7309 (4)
N1—Cd1—N11	97.83 (10)	N1—Cd1—I1	102.85 (7)
N1—Cd1—I2	113.60 (7)	N11—Cd1—I1	106.28 (7)
N11—Cd1—I2	113.12 (7)	I2—Cd1—I1	120.373 (14)

2. Structural commentary

The asymmetric unit of the 2,3-dimethylpyrazine-rich compound [CdI$_2$(2,3-dimethylpyrazine)$_2$] (**1**) consists of one Cd^{II} cation, as well as two crystallographically independent iodide anions and 2,3-dimethylpyrazine ligands (Fig. 1). In the crystal structure, the Cd^{II} cations are surrounded by two iodide anions and two 2,3-dimethylpyrazine ligands, forming discrete tetrahedral complexes. The bond angles deviate from the ideal geometry, which shows that the tetrahedra are strongly distorted (Table 1). The largest value of 120.373 (14) ° is observed for the I—Cd—I angle, which can be traced back to steric repulsion between the large halide anions.

It is noted that [ZnCl$_2$(2,3-dimethylpyrazine)$_2$] and [ZnBr$_2$(2,3-dimethylpyrazine)$_2$] also form discrete tetrahedral complexes but they are not isotypic to **1** (Näther & Bhosekar, 2025*a*,*b*). It is also noted that a 2,3-dimethylpyrazine-rich compound with ZnI$_2$ is unknown. However, similar compounds with pyrazine are reported. This includes [ZnCl$_2$(pyrazine)$_2$]$_n$ (refcode REMPAB; Bhosekar *et al.*, 2006) and [ZnBr$_2$(pyrazine)$_2$]$_n$ (EBOLAI; Bourne *et al.*, 2001 and EBOLAI01; Bhosekar *et al.*, 2006), in which the Zn^{II} cations are tetrahedrally coordinated and linked into layers by the pyrazine ligands. ZnI$_2$(pyrazine)$_2$ as well as pyrazine-rich compounds with the composition CdX_2(pyrazine)$_2$ (X = Cl, Br, I) are unknown. Finally, the reason why compound **1** as well as [ZnCl$_2$(2,3-dimethylpyrazine)$_2$] and [ZnBr$_2$(2,3-dimethylpyrazine)$_2$] form discrete complexes whereas the corresponding compounds with pyrazine form layers might originate from steric repulsion between the cation and the methyl group adjacent to the N atom, which makes a metal coordination more difficult.

The asymmetric unit of [CdI$_2$(2,3-dimethylpyrazine)] (**2**) is built up of one Cd^{II} cation and two crystallographically independent iodide anions that are located on a crystallographic mirror plane, as well as one 2,3-dimethylpyrazine ligand that is located on a twofold rotation axis (Fig. 2). The

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

Cd1—N1^{i}	2.354 (3)	Cd1—I2	2.6941 (6)
Cd1—N1	2.354 (3)	Cd1—I1	2.7170 (7)
N1^{i}—Cd1—N1	94.00 (17)	N1—Cd1—I1	105.18 (8)
N1—Cd1—I2	116.09 (8)	I2—Cd1—I1	117.27 (2)
N1^{i}—Cd1—I1	105.18 (8)		

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

Cd^{II} cations are fourfold coordinated by two iodide anions and two bridging 2,3-dimethylpyrazine ligands and are linked into corrugated chains by the coligands (Fig. 3). The bond angles deviate from the ideal values, which shows that the tetrahedra are slightly distorted (Table 2). In contrast to **1**, the largest deviation is found for the N—Cd—N angles (Table 2).

Comparison of the structure of **2** with that of the isotypic Zn^{II} compounds ZnCl$_2$(2,3-dimethylpyrazine) (Näther & Bhosekar, 2025*a*) and ZnBr$_2$(2,3-dimethylpyrazine) (Näther & Bhosekar, 2025*b*) shows that neither is isotypic to compound **2**. In this context, it is noted that the corresponding compounds with pyrazine show different structures in which the Zn^{II} cations are linked into layers by the pyrazine ligands (REMPAB; Bhosekar *et al.*, 2006 and EBOLAI; Bourne *et al.*, 2001). This might also originate from the fact that the coordination to the N atom in the 2,3-dimethylpyrazine compounds is sterically hindered, which is not the case in the pyrazine compounds.

Table 3
Hydrogen-bond geometry (Å, °) for **1**.

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···I1	0.93	3.13	3.848 (4)	136
C5—H5A···I2^{i}	0.96	3.26	4.151 (5)	156
C15—H15C···I2	0.96	3.28	4.186 (5)	158

Symmetry code: (i) $x - 1, y, z$.

Table 4
Hydrogen-bond geometry (Å, °) for **2**.

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···I1	0.93	3.19	3.915 (5)	136
C3—H3A···I2	0.96	3.08	4.036 (5)	175
C3—H3C···I2^{ii}	0.96	3.14	4.081 (5)	167

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

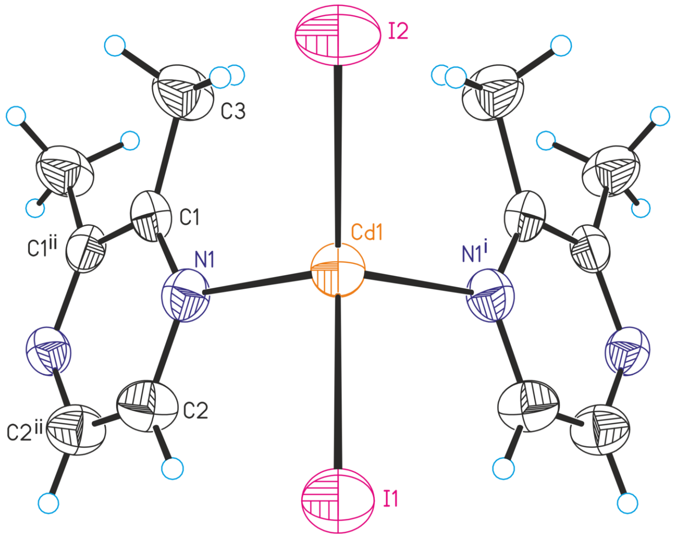

Figure 2
Crystal structure of **2** with labeling and displacement ellipsoids drawn at the 50% probability level. Symmetry codes for the generation of equivalent atoms: (i) $x, y, -z + \frac{1}{2}$; (ii) $x, -y + \frac{1}{2}, -z + 1$.

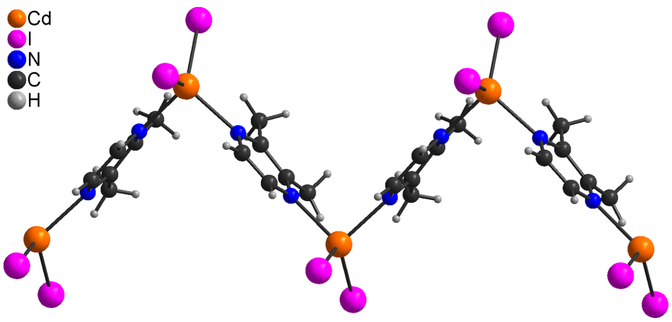

Figure 3
Crystal structure of **2** with view of a part of a chain.

3. Supramolecular features

In compound **1**, C—H···I interactions, especially between two of the methyl H atoms and both iodide anions, are observed within each complex (Fig. 4 and Table 3). The C—H···I angle is close to linear, indicating that this is a significant interaction (Table 3). No such interactions are observed between the complexes.

In the 2,3-dimethylpyrazine-deficient compound **2**, the complexes are arranged into columns that elongate in the *c*-axis direction and are linked by intermolecular C—H···I interactions (Table 4). The strongest C—H···I interactions are also observed between the methyl H atoms and the iodide anions (Fig. 5 and Table 4). In contrast to **1**, the H···I distances are shortened and both C—H···I angles are very

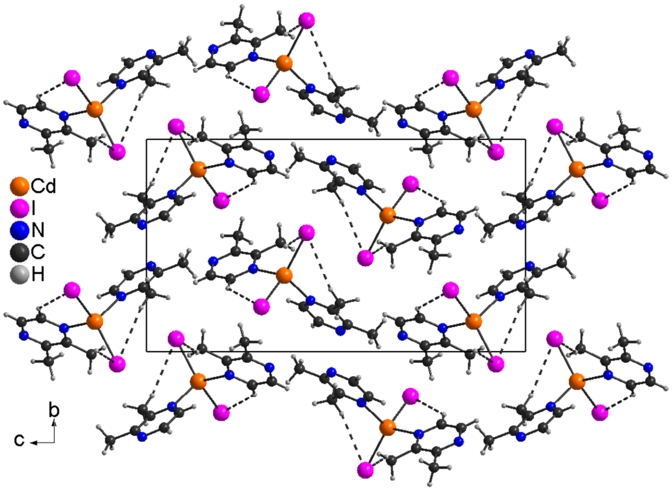

Figure 4
Crystal structure of **1** with intramolecular C—H···I interactions shown as dashed lines.

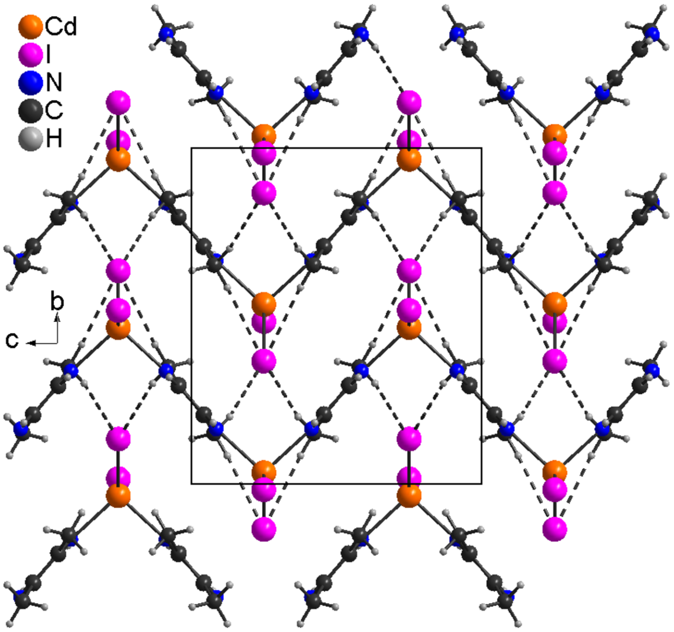

Figure 5
Crystal structure of **2** with intermolecular C—H· · ·I interactions shown as dashed lines.

close to linear, which indicate that these interactions are stronger than in **1**. These interactions lead to the formation of a three-dimensional network (Fig. 5).

4. Database survey

A search in the Cambridge Structural Database (CSD Version 5.43, 2025; Groom *et al.*, 2016) using CONQUEST (Bruno *et al.*, 2002) reveals that no coordination compounds with cadmium halides and 2,3-dimethylpyrazine as ligands are reported. However, some compounds with zinc halides are reported, as already mentioned in the *Chemical context* section. These include $ZnCl_2$(2,3-dimethylpyrazine), $ZnBr_2$(2,3-dimethylpyrazine) and ZnI_2(2,3-dimethylpyrazine) (Näther & Bhosekar, 2025*a*,*b*, 2026), as well as $ZnCl_2$(2,3-dimethylpyrazine)$_2$ (Näther & Bhosekar, 2025*a*) and $ZnBr_2$(2,3-dimethylpyrazine)$_2$ (Yang *et al.*, 2025). Finally, a compound with the composition $[ZnI_2(C_6H_8N_2)(H_2O)]$-$(H_2O)_{0.5}(C_6H_8N_2)_{0.5}$ is also known (Näther & Bhosekar, 2026).

With the related ligand pyrazine, some compounds with CdI_2 are also listed in the CSD. These include $CdCl_2$(pyrazine) (refcode TISSUJ; Pickardt & Staub, 1996, TISSUJ01, Bailey & Pennington, 1997, Lusi *et al.*, 2011), $CdBr_2$(pyrazine) (RINSIQ; Bailey & Pennington, 1997, RINSIQ01; Pickardt & Staub, 1996) and CdI_2(pyrazine) (RINSOW; Bailey & Pennington, 1997; Pickardt & Staub, 1997).

5. Powder X-ray diffraction and thermoanalytical measurements

Both compounds were additionally investigated by powder X-ray diffraction (PXRD). Comparison of the experimental patterns with those calculated from single crystal data proves, that pure phases were obtained (Figs. 6 and 7). In the pattern of compound **1** there is one peak of very low intensity at a Bragg angle of 10.2°, indicating traces of a second crystalline phase.

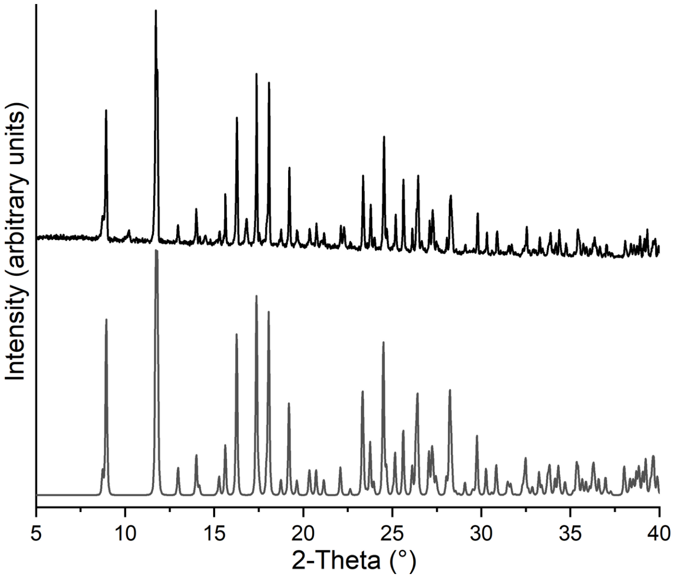

Figure 6
Experimental (top) and calculated (bottom) X-ray powder pattern of **1**.

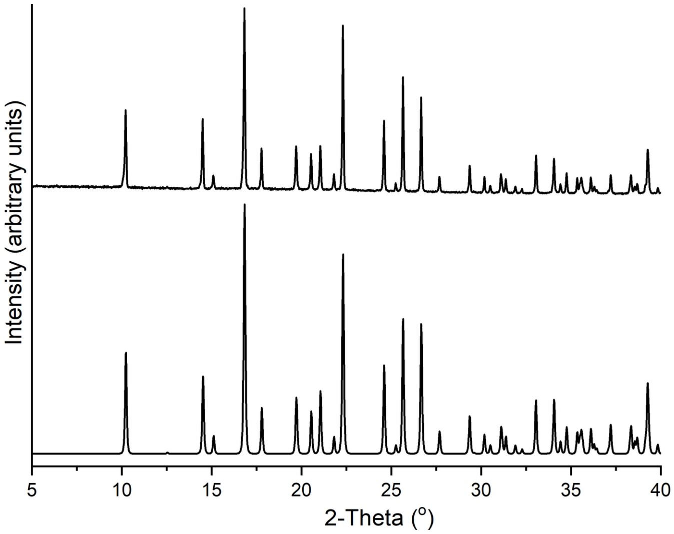

Figure 7
Experimental (top) and calculated (bottom) X-ray powder pattern of **2**.

Measurements using thermogravimetry and differential thermoanalysis on compound **1** show that two mass losses are observed, which are accompanied by endothermic events in the DTA curve and are perfectly resolved as obvious from the DTG curve (Fig. S1). The experimental mass losses of 17.8 and 18.6% are in reasonable agreement with those calculated for the removal of each one 2,3-dimethylpyrazine ligand in each step ($\Delta m_{calc.}$ = 18.6%). Therefore, it can be assumed that compound **2** has formed in the first mass loss and that the remaining ligands are emitted in the second mass loss.

Table 5
Experimental details.

	1	**2**
Crystal data		
Chemical formula	$[CdI_2(C_6H_8N_2)_2]$	$[CdI_2(C_6H_8N_2)]$
M_r	582.49	474.34
Crystal system, space group	Monoclinic, $P2_1/n$	Orthorhombic, *Pbcm*
Temperature (K)	293	293
a, b, c (Å)	7.6955 (4), 11.3271 (7), 20.4421 (13)	8.639 (1), 12.183 (1), 10.519 (1)
α, β, γ (°)	90, 98.112 (7), 90	90, 90, 90
V (Å^3)	1764.06 (18)	1107.11 (19)
Z	4	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	4.73	7.50
Crystal size (mm)	0.15 × 0.12 × 0.10	0.12 × 0.10 × 0.08
Data collection		
Diffractometer	Stoe *IPDS1*	Stoe Stadi-4
Absorption correction	Numerical (*X-RED* and *X-SHAPE*; Stoe, 2008)	ψ scan (*REDU*; Stoe 1990)
$T_{\min}$, $T_{\max}$	0.468, 0.549	0.300, 0.372
No. of measured, independent and observed $[I > 2\sigma(I)]$ reflections	12802, 4166, 3277	1623, 1273, 1022
$R_{\rm int}$	0.034	0.018
$(\sin \theta/\lambda)_{\max}$ (Å^{-1})	0.660	0.639
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.028, 0.071, 1.01	0.023, 0.056, 1.04
No. of reflections	4166	1273
No. of parameters	177	57
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å^{-3})	0.48, −0.68	0.65, −0.61

Computer programs: *X-AREA* (Stoe, 2008), *DIF4* and *REDU* (Stoe 1990), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg, 1999), *XP* in *SHELXTL-PC* (Sheldrick, 2008) and *publCIF* (Westrip, 2010).

TG-DTA measurements on **2** show only one mass loss at 471 K, which corresponds to the temperature where the second mass loss is observed for compound **1** (Fig. S2). The experimental mass loss of 22.8% is in perfect agreement with that calculated for the removal of one 2,3-dimethylpyrazine ligand ($\Delta m_{\rm calc.}$ = 22.8%).

6. Synthesis and crystallization

General

Cadmium iodide and 2,3-dimethylpyrazine were purchased from Sigma-Aldrich. The purity of both compounds was proven by powder X-ray diffraction.

Synthesis of 1

0.5 mmol (183.1 mg) of cadmium iodide and 1.0 mmol (108.1 mg) of 2,3-dimethylpyrazine were stirred in 4 mL of acetonitrile for 2 d. The precipitate was filtered off and dried. Single crystals were obtained using the same ratio of reactants without stirring.

Synthesis of 2

0.5 mmol (183.1 mg) of cadmium iodide and 0.5 mmol (54.1 mg) of 2,3-dimethylpyrazine were stirred in 3 mL of acetonitrile for 2 d. The precipitate was filtered off and dried. Single crystals were obtained using the same ratio of reactands without stirring.

Experimental details

The PXRD measurements were performed with a Stoe Transmission Powder Diffraction System (STADI P) with Cu $K\alpha_1$ radiation (λ = 1.540598 Å) equipped with a MYTHEN 1K detector and a Johansson-type Ge(111) monochromator.

The TG-DTA measurements were performed using a Linseis thermobalance in Al_2O_3 crucibles with 4°C/min in a flowing nitrogen atmosphere.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 5. 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 $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$ (1.5 for methyl H atoms).

Acknowledgements

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supporting information

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Syntheses and crystal structures of bis(2,3-dimethylpyrazine-*κN*)diiodidocadmium(II) and *catena*-poly[[diiodidocadmium(II)]-*μ*-2,3-dimethylpyrazine-κ^2N^1:N^4]

Christian Näther

Computing details

Bis(2,3-dimethylpyrazine-*κN*)diiodidocadmium(II) (1)

Crystal data

$[CdI_2(C_6H_8N_2)_2]$
$M_r = 582.49$
Monoclinic, $P2_1/n$
$a = 7.6955$ (4) Å
$b = 11.3271$ (7) Å
$c = 20.4421$ (13) Å
$\beta = 98.112$ (7)°
$V = 1764.06$ (18) Å^3
$Z = 4$
$F(000) = 1080$
$D_x = 2.193$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8000 reflections
$\theta = 11–27°$
$\mu = 4.73$ mm^{-1}
$T = 293$ K
Block, colorless
0.15 × 0.12 × 0.10 mm

Data collection

Stoe IPDS-1
diffractometer
Phi scans
Absorption correction: numerical
(X-Red and X-Shape; Stoe, 2008)
$T_{min} = 0.468$, $T_{max} = 0.549$
12802 measured reflections
4166 independent reflections
3277 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 28.0°$, $\theta_{min} = 3.0°$
$h = -10\rightarrow9$
$k = -14\rightarrow14$
$l = -26\rightarrow22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.071$
$S = 1.01$
4166 reflections
177 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0405P)^2 + 0.5502P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.48$ e Å^{-3}
$\Delta\rho_{min} = -0.68$ e Å^{-3}
Extinction correction: SHELXL-2016/6 (Sheldrick 2015b), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0063 (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	0.66284 (4)	0.35851 (2)	0.63661 (2)	0.03811 (9)
I1	0.91725 (4)	0.21125 (2)	0.69702 (2)	0.05213 (10)
I2	0.75133 (4)	0.55962 (3)	0.57769 (2)	0.06045 (12)
N1	0.4860 (4)	0.3899 (2)	0.71854 (14)	0.0341 (6)
C1	0.3409 (5)	0.4564 (3)	0.71153 (18)	0.0349 (7)
C2	0.2466 (5)	0.4720 (3)	0.76515 (18)	0.0374 (8)
N2	0.2996 (4)	0.4245 (3)	0.82422 (16)	0.0445 (7)
C3	0.4466 (5)	0.3601 (4)	0.83032 (19)	0.0456 (9)
H3	0.487150	0.325882	0.870983	0.055*
C4	0.5395 (5)	0.3427 (3)	0.77855 (19)	0.0420 (8)
H4	0.641429	0.297510	0.784996	0.050*
C5	0.2810 (6)	0.5132 (5)	0.6460 (2)	0.0582 (12)
H5A	0.158870	0.496394	0.632675	0.087*
H5B	0.348121	0.482539	0.613616	0.087*
H5C	0.297712	0.597047	0.649698	0.087*
C6	0.0828 (6)	0.5459 (4)	0.7586 (2)	0.0560 (11)
H6A	−0.002863	0.513566	0.724627	0.084*
H6B	0.110167	0.625297	0.747174	0.084*
H6C	0.036455	0.546043	0.799809	0.084*
N11	0.4689 (4)	0.2402 (3)	0.56727 (14)	0.0364 (6)
C11	0.5070 (5)	0.1972 (3)	0.50933 (17)	0.0361 (7)
C12	0.3836 (5)	0.1269 (3)	0.46968 (18)	0.0398 (8)
N12	0.2297 (5)	0.0979 (3)	0.48809 (17)	0.0483 (8)
C13	0.1962 (5)	0.1411 (4)	0.5464 (2)	0.0475 (9)
H13	0.090245	0.122120	0.560718	0.057*
C14	0.3124 (5)	0.2120 (3)	0.58549 (19)	0.0419 (8)
H14	0.282776	0.241054	0.625020	0.050*
C15	0.6814 (6)	0.2263 (4)	0.4894 (2)	0.0531 (10)
H15A	0.666872	0.245297	0.443174	0.080*
H15B	0.758338	0.159609	0.497679	0.080*
H15C	0.731196	0.292773	0.514520	0.080*
C16	0.4179 (6)	0.0813 (4)	0.4037 (2)	0.0536 (11)
H16A	0.532148	0.045737	0.408124	0.080*
H16B	0.412715	0.145589	0.372821	0.080*
H16C	0.330658	0.023588	0.387850	0.080*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.03579 (15)	0.04114 (15)	0.03721 (15)	0.00477 (10)	0.00448 (11)	0.00103 (10)
I1	0.04418 (16)	0.05245 (16)	0.05978 (19)	0.01851 (11)	0.00745 (12)	0.00847 (12)
I2	0.05478 (19)	0.05355 (18)	0.0691 (2)	−0.00347 (12)	−0.00479 (15)	0.02270 (14)
N1	0.0339 (15)	0.0374 (14)	0.0308 (15)	0.0023 (11)	0.0032 (12)	−0.0016 (11)
C1	0.0365 (18)	0.0338 (16)	0.0343 (18)	0.0034 (13)	0.0044 (15)	−0.0041 (13)
C2	0.0377 (18)	0.0375 (17)	0.0361 (19)	0.0008 (14)	0.0022 (15)	−0.0045 (14)
N2	0.0422 (18)	0.0588 (19)	0.0328 (17)	−0.0024 (14)	0.0058 (14)	−0.0035 (14)
C3	0.046 (2)	0.060 (2)	0.0289 (18)	0.0045 (18)	0.0005 (16)	0.0044 (16)
C4	0.038 (2)	0.050 (2)	0.0359 (19)	0.0062 (16)	−0.0010 (16)	0.0008 (16)
C5	0.054 (3)	0.077 (3)	0.045 (2)	0.029 (2)	0.013 (2)	0.015 (2)
C6	0.052 (3)	0.066 (3)	0.053 (3)	0.019 (2)	0.016 (2)	−0.003 (2)
N11	0.0345 (15)	0.0451 (15)	0.0293 (15)	0.0042 (12)	0.0033 (12)	0.0009 (12)
C11	0.0341 (18)	0.0445 (18)	0.0298 (17)	0.0089 (14)	0.0050 (14)	0.0055 (14)
C12	0.042 (2)	0.0453 (19)	0.0303 (17)	0.0128 (15)	−0.0006 (15)	0.0045 (14)
N12	0.0419 (19)	0.063 (2)	0.0390 (18)	0.0025 (15)	0.0012 (15)	−0.0026 (15)
C13	0.034 (2)	0.065 (2)	0.044 (2)	0.0023 (17)	0.0066 (17)	0.0017 (18)
C14	0.039 (2)	0.051 (2)	0.0365 (19)	0.0053 (16)	0.0091 (16)	−0.0019 (16)
C15	0.046 (2)	0.070 (3)	0.046 (2)	−0.003 (2)	0.0157 (19)	−0.006 (2)
C16	0.056 (3)	0.070 (3)	0.034 (2)	0.011 (2)	0.0022 (18)	−0.0124 (19)

Geometric parameters (Å, º)

Cd1—N1	2.329 (3)	C6—H6B	0.9600
Cd1—N11	2.331 (3)	C6—H6C	0.9600
Cd1—I2	2.7084 (4)	N11—C14	1.349 (5)
Cd1—I1	2.7309 (4)	N11—C11	1.350 (5)
N1—C1	1.338 (4)	C11—C12	1.405 (5)
N1—C4	1.348 (5)	C11—C15	1.494 (6)
C1—C2	1.408 (5)	C12—N12	1.334 (5)
C1—C5	1.499 (5)	C12—C16	1.503 (5)
C2—N2	1.332 (5)	N12—C13	1.346 (5)
C2—C6	1.504 (6)	C13—C14	1.372 (6)
N2—C3	1.337 (5)	C13—H13	0.9300
C3—C4	1.373 (6)	C14—H14	0.9300
C3—H3	0.9300	C15—H15A	0.9600
C4—H4	0.9300	C15—H15B	0.9600
C5—H5A	0.9600	C15—H15C	0.9600
C5—H5B	0.9600	C16—H16A	0.9600
C5—H5C	0.9600	C16—H16B	0.9600
C6—H6A	0.9600	C16—H16C	0.9600
N1—Cd1—N11	97.83 (10)	C2—C6—H6C	109.5
N1—Cd1—I2	113.60 (7)	H6A—C6—H6C	109.5
N11—Cd1—I2	113.12 (7)	H6B—C6—H6C	109.5
N1—Cd1—I1	102.85 (7)	C14—N11—C11	118.0 (3)

N11—Cd1—I1	106.28 (7)	C14—N11—Cd1	119.2 (2)
I2—Cd1—I1	120.373 (14)	C11—N11—Cd1	122.8 (2)
C1—N1—C4	117.6 (3)	N11—C11—C12	119.9 (3)
C1—N1—Cd1	124.9 (2)	N11—C11—C15	118.3 (3)
C4—N1—Cd1	117.3 (2)	C12—C11—C15	121.9 (3)
N1—C1—C2	120.1 (3)	N12—C12—C11	122.1 (4)
N1—C1—C5	118.9 (3)	N12—C12—C16	116.4 (4)
C2—C1—C5	121.0 (3)	C11—C12—C16	121.5 (4)
N2—C2—C1	122.0 (3)	C12—N12—C13	116.6 (3)
N2—C2—C6	116.8 (4)	N12—C13—C14	122.6 (4)
C1—C2—C6	121.2 (3)	N12—C13—H13	118.7
C2—N2—C3	116.8 (3)	C14—C13—H13	118.7
N2—C3—C4	122.2 (4)	N11—C14—C13	120.8 (4)
N2—C3—H3	118.9	N11—C14—H14	119.6
C4—C3—H3	118.9	C13—C14—H14	119.6
N1—C4—C3	121.3 (4)	C11—C15—H15A	109.5
N1—C4—H4	119.4	C11—C15—H15B	109.5
C3—C4—H4	119.4	H15A—C15—H15B	109.5
C1—C5—H5A	109.5	C11—C15—H15C	109.5
C1—C5—H5B	109.5	H15A—C15—H15C	109.5
H5A—C5—H5B	109.5	H15B—C15—H15C	109.5
C1—C5—H5C	109.5	C12—C16—H16A	109.5
H5A—C5—H5C	109.5	C12—C16—H16B	109.5
H5B—C5—H5C	109.5	H16A—C16—H16B	109.5
C2—C6—H6A	109.5	C12—C16—H16C	109.5
C2—C6—H6B	109.5	H16A—C16—H16C	109.5
H6A—C6—H6B	109.5	H16B—C16—H16C	109.5

C4—N1—C1—C2	−2.0 (5)	C14—N11—C11—C12	0.9 (5)
Cd1—N1—C1—C2	−178.2 (2)	Cd1—N11—C11—C12	−179.6 (2)
C4—N1—C1—C5	178.1 (4)	C14—N11—C11—C15	−179.0 (3)
Cd1—N1—C1—C5	1.9 (5)	Cd1—N11—C11—C15	0.5 (4)
N1—C1—C2—N2	1.6 (5)	N11—C11—C12—N12	−1.8 (5)
C5—C1—C2—N2	−178.5 (4)	C15—C11—C12—N12	178.1 (4)
N1—C1—C2—C6	−179.8 (4)	N11—C11—C12—C16	177.5 (3)
C5—C1—C2—C6	0.1 (6)	C15—C11—C12—C16	−2.6 (6)
C1—C2—N2—C3	−0.5 (5)	C11—C12—N12—C13	1.1 (5)
C6—C2—N2—C3	−179.1 (4)	C16—C12—N12—C13	−178.2 (4)
C2—N2—C3—C4	−0.2 (6)	C12—N12—C13—C14	0.3 (6)
C1—N1—C4—C3	1.3 (5)	C11—N11—C14—C13	0.5 (5)
Cd1—N1—C4—C3	177.8 (3)	Cd1—N11—C14—C13	−179.0 (3)
N2—C3—C4—N1	−0.3 (6)	N12—C13—C14—N11	−1.2 (6)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···I1	0.93	3.13	3.848 (4)	136

C5—H5*A*···I2^i	0.96	3.26	4.151 (5)	156
C15—H15*C*···I2	0.96	3.28	4.186 (5)	158

Symmetry code: (i) $x-1, y, z$.

catena-Poly[[diiodidocadmium(II)]-*μ*-2,3-dimethylpyrazine-$\kappa^2N^1:N^4$] (2)

Crystal data

$[CdI_2(C_6H_8N_2)]$
$M_r = 474.34$
Orthorhombic, *Pbcm*
$a = 8.639$ (1) Å
$b = 12.183$ (1) Å
$c = 10.519$ (1) Å
$V = 1107.11$ (19) Å^3
$Z = 4$
$F(000) = 848$
$D_x = 2.846$ Mg m^{-3}
Mo *Kα* radiation, $\lambda = 0.71073$ Å
Cell parameters from 120 reflections
$\theta = 10.0$–15.0°
$\mu = 7.50$ mm^{-1}
$T = 293$ K
Block, colorless
0.12 × 0.10 × 0.08 mm

Data collection

Stoe Stadi-4 diffractometer
Phi scans
Absorption correction: ψ scan (REDU; Stoe 1990)
$T_{min} = 0.300$, $T_{max} = 0.372$
1623 measured reflections
1273 independent reflections
1022 reflections with $I > 2\sigma(I)$
$R_{int} = 0.018$
$\theta_{max} = 27.0°$, $\theta_{min} = 2.4°$
$h = -11 \rightarrow 1$
$k = -1 \rightarrow 15$
$l = -13 \rightarrow 1$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.023$
$wR(F^2) = 0.056$
$S = 1.04$
1273 reflections
57 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0229P)^2 + 1.2591P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.65$ e Å^{-3}
$\Delta\rho_{min} = -0.61$ e Å^{-3}
Extinction correction: SHELXL-2016/6 (Sheldrick 2015b), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00184 (13)

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}
Cd1	0.40619 (5)	0.46580 (4)	0.250000	0.03304 (13)
I1	0.71252 (5)	0.51634 (4)	0.250000	0.04672 (14)
I2	0.20422 (5)	0.63429 (4)	0.250000	0.05234 (16)
N1	0.3756 (4)	0.3358 (3)	0.4137 (3)	0.0340 (7)
C1	0.2422 (5)	0.2952 (3)	0.4580 (4)	0.0324 (9)

C2	0.5081 (5)	0.2913 (3)	0.4560 (5)	0.0422 (10)
H2	0.601953	0.317212	0.424685	0.051*
C3	0.0932 (5)	0.3485 (4)	0.4212 (5)	0.0508 (12)
H3A	0.114314	0.415217	0.375865	0.076*
H3B	0.034355	0.364828	0.496250	0.076*
H3C	0.035105	0.299658	0.367747	0.076*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0352 (2)	0.0294 (2)	0.0346 (2)	−0.00002 (17)	0.000	0.000
I1	0.0378 (2)	0.0481 (3)	0.0543 (3)	−0.01019 (19)	0.000	0.000
I2	0.0471 (3)	0.0339 (2)	0.0760 (4)	0.00816 (18)	0.000	0.000
N1	0.0378 (17)	0.0334 (17)	0.0306 (17)	−0.0009 (15)	0.0023 (15)	0.0022 (15)
C1	0.037 (2)	0.036 (2)	0.025 (2)	−0.0011 (17)	−0.0039 (16)	−0.0021 (18)
C2	0.036 (2)	0.040 (2)	0.051 (3)	0.0012 (18)	0.000 (2)	0.005 (2)
C3	0.041 (2)	0.061 (3)	0.050 (3)	0.000 (2)	0.001 (2)	0.023 (3)

Geometric parameters (Å, º)

Cd1—N1^{i}	2.354 (3)	C1—C3	1.493 (6)
Cd1—N1	2.354 (3)	C2—C2^{ii}	1.368 (9)
Cd1—I2	2.6941 (6)	C2—H2	0.9300
Cd1—I1	2.7170 (7)	C3—H3A	0.9600
N1—C1	1.338 (5)	C3—H3B	0.9600
N1—C2	1.343 (5)	C3—H3C	0.9600
C1—C1^{ii}	1.412 (8)		
N1^{i}—Cd1—N1	94.00 (17)	C1^{ii}—C1—C3	120.1 (2)
N1^{i}—Cd1—I2	116.09 (8)	N1—C2—C2^{ii}	121.4 (2)
N1—Cd1—I2	116.09 (8)	N1—C2—H2	119.3
N1^{i}—Cd1—I1	105.18 (8)	C2^{ii}—C2—H2	119.3
N1—Cd1—I1	105.18 (8)	C1—C3—H3A	109.5
I2—Cd1—I1	117.27 (2)	C1—C3—H3B	109.5
C1—N1—C2	118.0 (4)	H3A—C3—H3B	109.5
C1—N1—Cd1	126.9 (3)	C1—C3—H3C	109.5
C2—N1—Cd1	114.7 (3)	H3A—C3—H3C	109.5
N1—C1—C1^{ii}	120.4 (2)	H3B—C3—H3C	109.5
N1—C1—C3	119.4 (4)		
C2—N1—C1—C1^{ii}	−3.0 (7)	Cd1—N1—C1—C3	−12.3 (6)
Cd1—N1—C1—C1^{ii}	169.6 (4)	C1—N1—C2—C2^{ii}	−1.6 (8)
C2—N1—C1—C3	175.1 (4)	Cd1—N1—C2—C2^{ii}	−175.0 (5)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···I1	0.93	3.19	3.915 (5)	136
C3—H3*A*···I2	0.96	3.08	4.036 (5)	175
C3—H3*C*···I2^{iii}	0.96	3.14	4.081 (5)	167

Symmetry code: (iii) −*x*, *y*−1/2, −*z*+1/2.