Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

Synthesis, crystal structure and thermal properties of poly[di-μ-bromido-(μ-2,5-dimethylpyrazine)-cadmium(II)]

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Received 2 December 2024
Accepted 4 December 2024

Edited by W. T. A. Harrison, University of Aberdeen, United Kingdom

Keywords: synthesis; thermal properties; cadmium bromide; coordination polymer; 2,5-dimethylpyrazine; crystal structure.

CCDC reference: 2407788

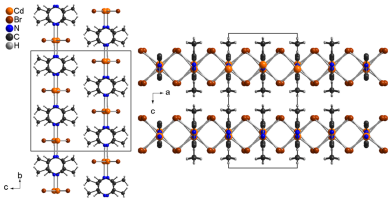
Supporting information: this article has supporting information at journals.iucr.org/e

The title compound, $[CdBr_2(C_6H_8N_2)]_n$, was prepared by the reaction of cadmium bromide with 2,5-dimethylpyrazine in water. Its asymmetric unit consists of one Cd cation and one 2,5-dimethylpyrazine ligand that are located on a crystallographic mirror plane as well as one bromide anion that occupies a general position. The Cd cations are sixfold coordinated by four bromide anions and two 2,5-dimethylpyrazine ligands within slightly distorted *trans*-$CdBr_4N_2$ octahedra. The cations are linked into [100] chains *via* pairs of bridging bromide anions that are further connected into (001) layers by the bridging 2,5-dimethylpyrazine ligands. Powder X-ray diffraction (PXRD) shows that a pure crystalline phase has been obtained. Thermogravimetry coupled to differential thermoanalysis (TG-TDA) reveal that the 2,5-dimethylpyrazine ligands are removed in two separate steps leading to the formation of a compound with the composition $(CdBr_2)_2$(2,5-dimethylpyrazine) that decomposes into $CdBr_2$ upon further heating. PXRD measurements of the residue obtained after the first mass loss show that a new crystalline phase has been formed.

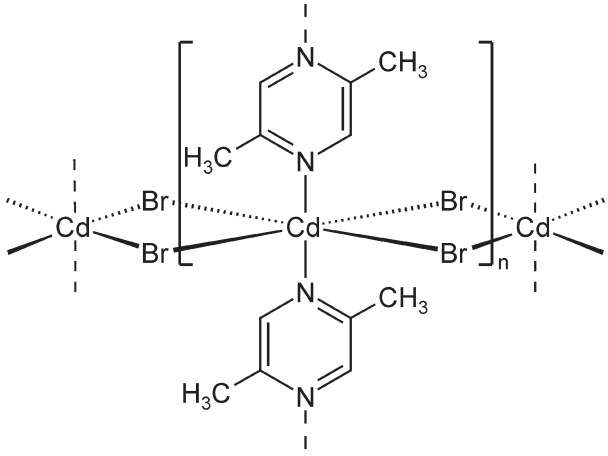
1. Chemical context

For several years, we and others have been interested in the synthesis and crystal structures of coordination compounds based on transition metal halides and neutral organic coligands. In the beginning, we focused on compounds based on Cu^I, because they show an extremely versatile structural behavior (Kromp & Sheldrick, 1999; Peng *et al.*, 2010; Näther & Jess, 2002, 2004; Li *et al.*, 2005). Such compounds usually consist of CuX subunits that can comprise monomeric and dimeric units but also different kinds of chains that are further linked into more condensed networks when bridging coligands are used in the synthesis. In the course of our systematic work we found that upon heating, such compounds frequently lose their coligands in a stepwise manner, which leads to the formation of new copper halide compounds as intermediates that consist of condensed CuX networks (Näther *et al.*, 2001, 2002). More recently, we have shown that this synthetic route can also be expanded to coordination compounds with, *e.g.* ZnX_2 and CdX_2 (X = Cl, Br, I), even if they, with few exceptions (Näther *et al.*, 2007), do not show the same structural variability as the Cu compounds.

In the course of our project we especially used bridging coligands such as pyrazine derivatives to prepare compounds with more condensed networks. Some compounds with CdX_2 (X = Cl, Br, I) and pyrazine ($C_4H_4N_2$) have already been reported, including CdX_2(pyrazine) [X = Cl, Br, I, Cambridge Structural Database 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. In this context we have reported on CdX_2 compounds with 2-chloro and 2-methylpyrazine, for which a different thermal reactivity was observed (Näther *et al.*, 2017). In the coligand-rich compounds $CdX_2(L)_2$ (X = Cl, Br, I, L = 2-chloro and methylpyrazine: QAWHOO, QAWGON, QAWGUT, QAWHAA, QAWHEE and QAWHII; Näther *et al.*, 2017), the Cd cations are octahedrally coordinated and linked into chains by pairs of bridging halide anions. If the 2-methylpyrazine compounds are heated, a transformation into 2-methylpyrazine-deficient compounds with the composition CdX_2(2-methylpyrazine) (X = Cl, Br, I) is observed, in which the CdX_2 chains are further linked into layers as with the pyrazine compounds mentioned above. In contrast, for the 2-chloropyrazine compounds, no 2-chloropyrazine-deficient compounds can be obtained and they can also not be prepared from solution (Näther *et al.*, 2017).



In a continuation of this work we became interested in compounds with 2,5-dimethylpyrazine ($C_6H_8N_2$) in which the coordination to each of the N atoms is sterically hindered because of the bulky methyl groups. A compound with the composition CdI_2(2,5-dimethylpyrazine) is already reported in the CSD (EHEQUG; Rogers, 2020). Surprisingly, the structure of this compound is completely different from that of the 2-methyl and 2-chloropyrazine compounds mentioned above. In EHEQUG, the Cd cations are tetrahedrally coordinated by two iodide anions and two 2,5-dimethylpyrazine coligands and linked into chains by the coligands. Compounds with $CdCl_2$ or $CdBr_2$ and 2,5-dimethylpyrazine have not been reported. In the course of our investigations, we obtained crystals of the title compound, (**I**), by the reaction of $CdBr_2$ and 2,5-dimethylpyrazine, which were characterized by single crystal X-ray diffraction.

2. Structural commentary

The asymmetric unit of (**I**) consists of one Cd cation and one 2,5-dimethylpyrazine ligand that are located on a crystallographic mirror plane as well as one bromide anion that occupies a general position (Fig. 1). The Cd cations are octahedrally coordinated by four bromide anions that are located in the basal plane and two N-bonded 2,5-dimethylpyrazine ligands in the axial positions. The N—Cd—N and N—Cd—Br angles are close to the ideal values,whereas the Br—Cd—Br angles are significantly different from 90°, which shows that the octahedra are significantly distorted (Table 1). The cadmium cations are linked into chains *via* pairs of μ-1,1-bridging bromide anions that propagate in the crystallographic *a*-axis direction, which means that neighboring octahedra share common edges (Fig. 2). These chains are further linked into layers lying parallel to (001) by the bridging 2,5-dimethylpyrazine ligands (Fig. 3). It is noted that this topology is well known from CdX_2 compounds with pyrazine derivatives

Table 1
Selected geometric parameters (Å, °).

Cd1—Br1	2.6869 (4)	Cd1—N1	2.482 (5)
Cd1—Br1^{i}	2.7893 (4)	Cd1—N2^{ii}	2.494 (5)
Br1—Cd1—Br1^{iii}	106.18 (2)	N1—Cd1—Br1	91.20 (6)
Br1—Cd1—Br1^{iv}	86.222 (11)	N1—Cd1—N2^{ii}	178.93 (15)
Br1^{i}—Cd1—Br1^{iv}	81.37 (2)	N2^{ii}—Cd1—Br1^{iii}	89.45 (6)
Br1^{iii}—Cd1—Br1^{iv}	167.574 (18)	N2^{ii}—Cd1—Br1^{iv}	89.94 (8)
N1—Cd1—Br1^{iv}	89.25 (8)	Cd1—Br1—Cd1^{v}	93.774 (11)

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

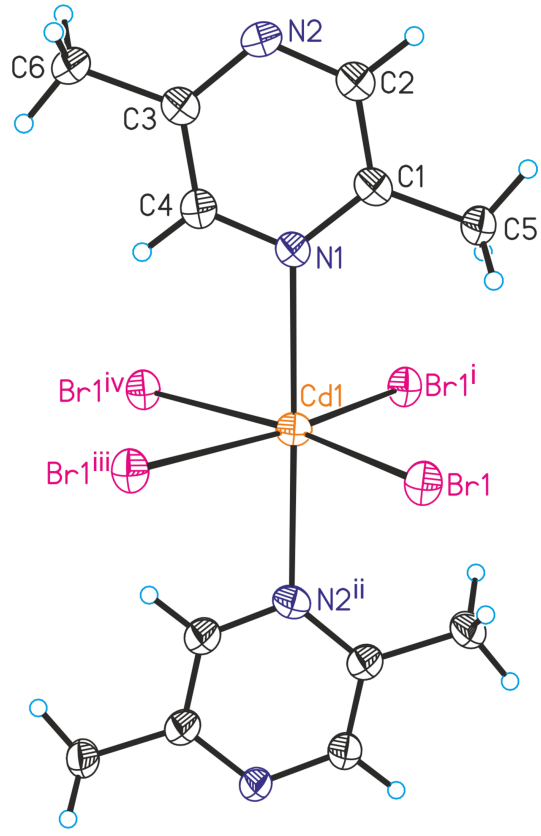


Figure 1
The crystal structure of (**I**) with labeling and displacement ellipsoids drawn at the 50% probability level. Symmetry codes for the generation of equivalent atoms: (i) $-x+1, y, z$; (ii) $x, y+\frac{1}{2}, -z+\frac{3}{2}$; (iii) $-x+\frac{3}{2}, y, -z+\frac{3}{2}$; (iv) $x-\frac{1}{2}, y, -z+\frac{3}{2}$; (v) $x+\frac{1}{2}, y, -z+\frac{3}{2}$.

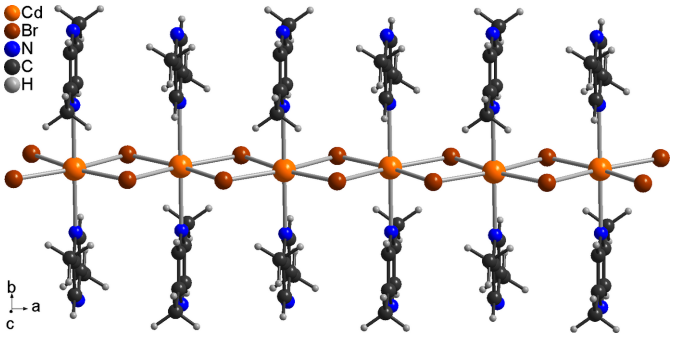


Figure 2
Crystal structure of (**I**) with view of part of one [100] chain.

such as CdX_2(pyrazine) (X = Cl, Br, I) (Bailey & Pennington, 1997; Pickardt & Staub, 1997). It is also noted that the crystal structure of the title compound is completely different from the iodide analogue CdI_2(2,5-dimethylpyrazine) already reported in the literature (EHEQUG; Rogers, 2020).

3. Supramolecular features

The layers in (**I**) are stacked in the crystallographic *c*-axis direction such that the methyl groups of neighboring layers point towards each along the *a*-axis direction or that they are shifted relative to each other along the *b*-axis direction so that the methyl groups are opposite to the bromide anions (Fig. 4). In the crystal structure of (**I**) a number of intermolecular C—H···Br contacts are observed but for all of them the H···Br distances are very long and the C—H···Br angles are far from linear, indicating that these are only very weak interactions (Table 2).

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···Br1^{vi}	0.95	3.02	3.624 (5)	123
C2—H2···Br1^{vii}	0.95	3.02	3.624 (5)	123
C4—H4···Br1^{i}	0.95	3.04	3.622 (5)	121
C4—H4···Br1^{iv}	0.95	3.04	3.622 (5)	121
C5—H5*B*···Br1	0.98	2.83	3.658 (5)	142
C5—H5*C*···Br1^{iii}	0.98	2.83	3.658 (5)	142
C6—H6*B*···Br1^{viii}	0.98	2.86	3.674 (5)	141
C6—H6*C*···Br1^{ix}	0.98	2.86	3.674 (5)	141

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

4. Database survey

As mentioned in the *Chemical context* section, only one cadmium halide compound with 2,5-dimethylpyrazine is reported as a private communication in the CCDC database [CSD Version 5.43, September 2024 (Groom *et al.*, 2016), search with CONQUEST (Bruno *et al.*, 2002)]. However, a number of compounds with other twofold positively charged transition-metal cations, halide anions and 2,5-dimethylpyrazine are known. This include the two isotypic compounds MBr$_2$(2,5-dimethylpyrazine), in which the metal cations are square-planar coordinated by two bromide anions and two 2,5-dimethylpyrazine ligands and linked into chains by the neutral coligands [M = Ni (BRMPYN; Ayres *et al.*, 1964) and M = Cu (DOVNUY; Butcher *et al.*, 2009)]. The same structure is also observed in $CuCl_2$(2,5-dimethylpyrazine) (RAZYEX; Awwadi *et al.*, 2005), but this compound is not isotypic to the bromide compounds mentioned before.

Several compounds are reported with Zn^{II} in which the Zn^{II} cations are tetrahedrally coordinated, including ZnX_2(2,5-dimethylpyrazine) in which the Zn^{II} cations are linked into chains by the 2,5-dimethylpyrazine ligands (X = Cl, DOPYAJ, X = Br, DOPYIR, X = I, DOPZAK; Wriedt *et al.*, 2009). In (ZnX_2)$_2$(2,5-dimethylpyrazine)$_3$ dinuclear complexes are formed in which the 2,5-dimethylpyrazine acts as bridging and terminal ligands (X = Cl, DOPYEN, X = Br, DOPYOX; Wriedt *et al.*, 2009). In $ZnBr_2$(2,5-dimethylpyrazine)$_2$-2,5-di-

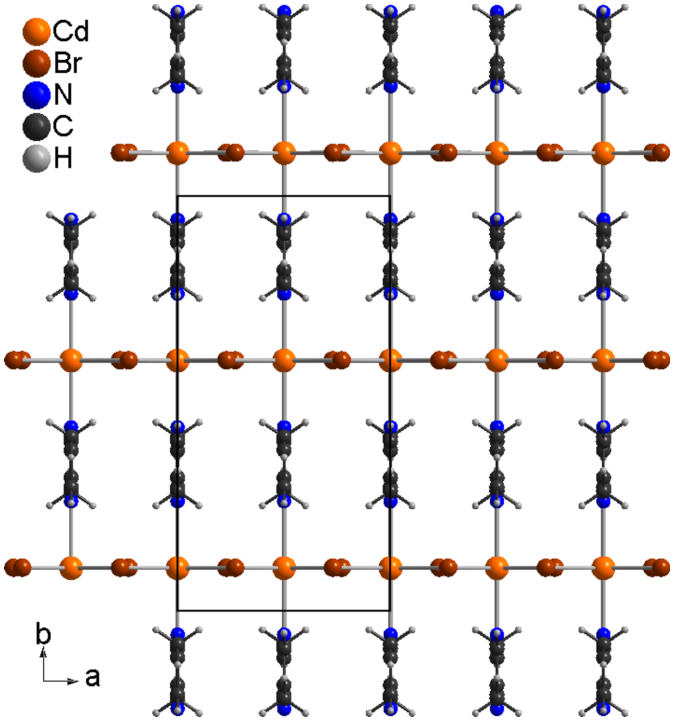


Figure 3
Crystal structure of (**I**) with view along the crystallographic *c*-axis direction.

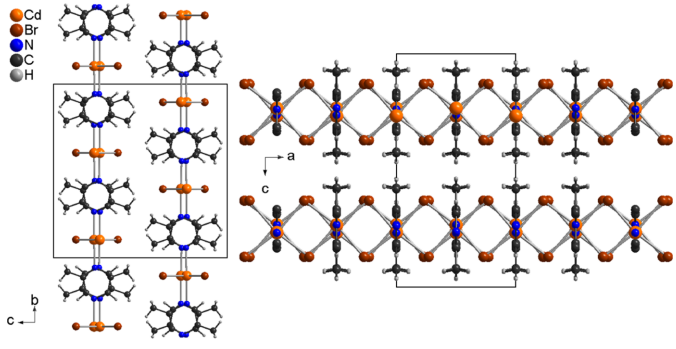


Figure 4
Crystal structure of (**I**) with view along the crystallographic *a*- (left) and *b*-axis (right) directions.

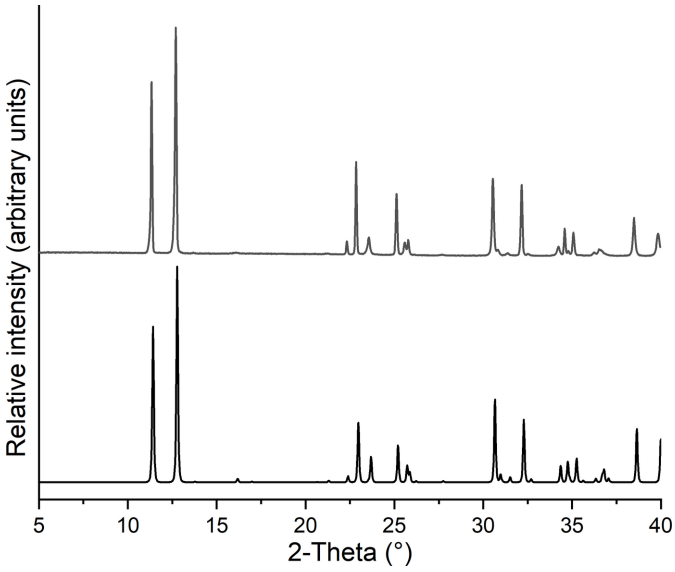


Figure 5
Experimental (top) and calculated X-ray powder pattern (bottom) for (**I**).

methylpyrazine solvate, discrete complexes are observed (DOPYUD; Wriedt *et al.*, 2009). Discrete complexes are also observed in ZnI_2(2,5-dimethylpyrazine)$_2$ (DOPZEO; Wriedt *et al.*, 2009). Additional compounds are reported with Cu^{II} cations, including $CuBr_2$(2,5-dimethylpyrazine)(acetonitrile), in which the Cu^{II} cations are fivefold coordinated by two chloride anions, one acetonitrile ligand and two bridging 2,5-dimethylpyrazine ligands that link the cations into chains (MEVRAG; Näther & Greve, 2001).

Finally, two compounds with the composition (HgX_2)$_2$(2,5-dimethylpyrazine) (X = Cl, QUMVIE, X = Br, QUMTUO; Mahmoudi & Morsali, 2009) are also reported, and show a topology similar to that of the title compound.

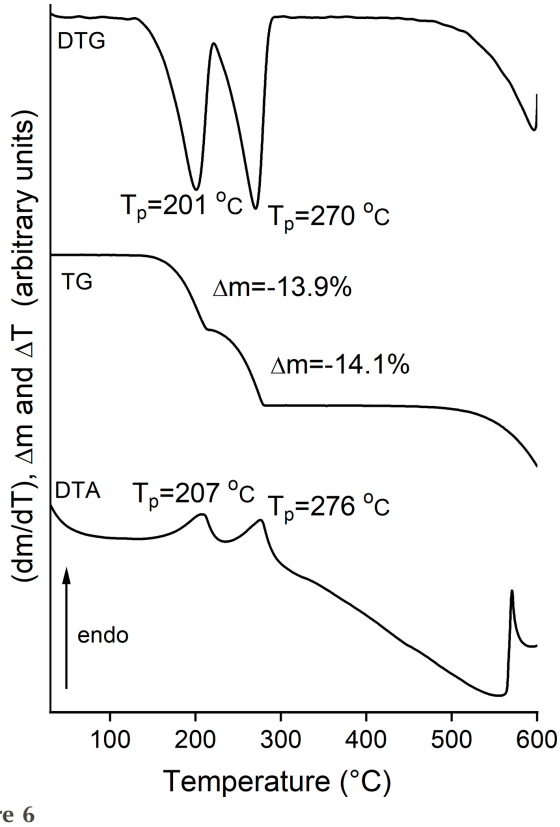


Figure 6
DTG, TG and DTA curves for (**I**) measured with a heating rate of 4°C min^{-1}. The mass loss is given in % and the peak temperature in °C.

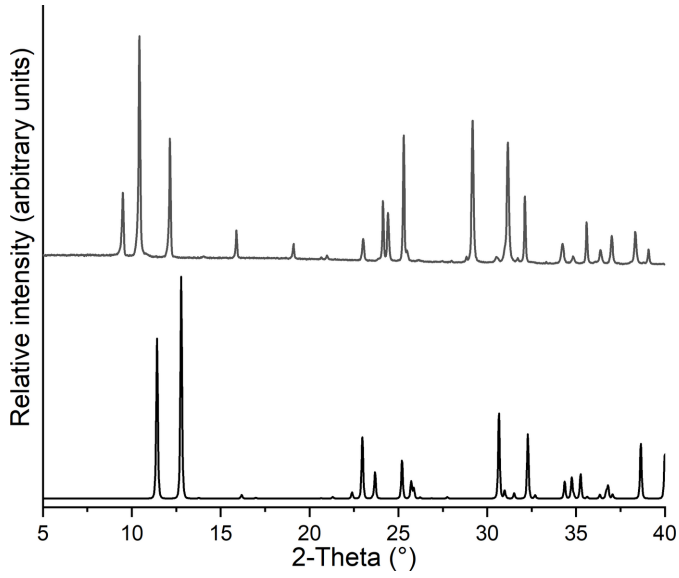


Figure 7
Experimental X-ray powder pattern of the residue obtained after the first mass loss in a TG measurement for (**I**) (top) and calculated powder pattern for (**I**) (bottom).

5. Additional investigations

Comparison of the the experimental X-ray powder pattern of the sample with that calculated for the title compound from single-crystal data shows that a pure crystalline phase has been obtained (Fig. 5).

Thermogravimetry and differential thermoanalysis (TG-DTA) measurements reveal that (**I**) decomposes in two steps that are accompanied with endothermic events in the DTA curve at peak temperatures of 207 and 276°C (Fig. 6). The experimental mass losses of the first and second thermogravimetric step of 13.9 and 14.1% are in good agreement with those calculated for the removal of a half 2,5-dimethylpyrazine ligand in each step ($\Delta m_{calc.}$ = 14.2%). Therefore, one can assume that after the first mass loss a compound with the composition ($CdBr_2$)$_2$(2,5-dimethylpyrazine) is formed, which decomposes into $CdBr_2$ upon further heating.

To prove that a new crystalline phase had formed, the residue obtained after the first mass loss was investigated by powder X-ray diffraction, which shows that a compound with very good crystallinity was obtained with a powder pattern completely different from that of the title compound (Fig. 7). Unfortunately, indexing of this powder pattern failed, so that no structural information is available. However, it can be assumed that a more condensed $CdBr_2$ network formed.

6. Synthesis and crystallization

$CdBr_2$ and 2,5-dimethylpyrazine were purchased from Sigma-Aldrich. 136.1 mg (0.5 mmol) of $CdBr_2$ and 54.1 mg of (0.5 mmol) 2,5-dimethylpyrazine were reacted in 2 ml of water for 2 d at 353 K, which led to the formation of colorless crystals suitable for single crystal X-ray diffraction.

The PXRD measurements were performed with Cu $K\alpha_1$ radiation (λ = 1.540598 Å) using a Stoe Transmission Powder Diffraction System (STADI P) equipped with a MYTHEN 1K detector and a Johansson-type Ge(111) monochromator. Thermogravimetry and differential thermoanalysis (TG-DTA) experiments were performed in a dynamic nitrogen atmosphere in Al_2O_3 crucibles with 8°C min^{-1} using a STA-PT 1000 thermobalance from Linseis. The TG-DTA instrument was calibrated using standard reference materials.

7. 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 $U_{iso}(H) = 1.2U_{eq}(C)$ (1.5 for methyl H atoms).

Table 3
Experimental details.

Crystal data	
Chemical formula	$[CdBr_2(C_6H_8N_2)]$
M_r	380.36
Crystal system, space group	Orthorhombic, *Cmce*
Temperature (K)	170
a, *b*, *c* (Å)	7.9334 (2), 15.4735 (6), 15.4898 (6)
V (Å^3)	1901.49 (11)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	10.64
Crystal size (mm)	0.14 × 0.11 × 0.07
Data collection	
Diffractometer	Stoe *IPDS2*
Absorption correction	Numerical
T_{min}, T_{max}	0.193, 0.276
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14714, 1238, 1082
R_{int}	0.039
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.661
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.033, 0.088, 1.13
No. of reflections	1238
No. of parameters	64
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.99, −0.84

Computer programs: *X-AREA* (Stoe, 2008), *SHELXT2014/4* (Sheldrick, 2015*a*), *SHELXL2016/6* (Sheldrick, 2015*b*), *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. (2025). E**81**, 29-33 [https://doi.org/10.1107/S2056989024011824]

Synthesis, crystal structure and thermal properties of poly[di-μ-bromido-(μ-2,5-dimethylpyrazine)cadmium(II)]

Christian Näther

Computing details

Poly[di-μ-bromido-(μ-2,5-dimethylpyrazine)cadmium(II)]

Crystal data

$[CdBr_2(C_6H_8N_2)]$
M_r = 380.36
Orthorhombic, *Cmce*
a = 7.9334 (2) Å
b = 15.4735 (6) Å
c = 15.4898 (6) Å
V = 1901.49 (11) Å^3
Z = 8
$F(000)$ = 1408
D_x = 2.657 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 15283 reflections
θ = 5.3–57.8°
μ = 10.64 mm^{-1}
T = 170 K
Block, colorless
0.14 × 0.11 × 0.07 mm

Data collection

Stoe IPDS-2 diffractometer
ω scans
Absorption correction: numerical
T_{min} = 0.193, T_{max} = 0.276
14714 measured reflections
1238 independent reflections
1082 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 28.0°, θ_{min} = 2.6°
h = −10→10
k = −20→20
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.088
S = 1.13
1238 reflections
64 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0592P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.99 e Å^{-3}
$\Delta\rho_{min}$ = −0.84 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}	Occ. (<1)
Cd1	0.500000	0.60333 (2)	0.76619 (2)	0.02282 (15)	
Br1	0.77081 (5)	0.60437 (3)	0.87036 (2)	0.02692 (15)	
N1	0.500000	0.4430 (3)	0.7622 (3)	0.0250 (9)	
C1	0.500000	0.3874 (3)	0.8292 (4)	0.0275 (11)	
C2	0.500000	0.2984 (4)	0.8119 (4)	0.0294 (12)	
H2	0.500000	0.259776	0.859575	0.035*	
N2	0.500000	0.2645 (3)	0.7328 (3)	0.0263 (10)	
C3	0.500000	0.3214 (4)	0.6659 (3)	0.0267 (11)	
C4	0.500000	0.4088 (4)	0.6818 (4)	0.0264 (11)	
H4	0.500000	0.447104	0.633895	0.032*	
C5	0.500000	0.4195 (4)	0.9195 (3)	0.0350 (14)	
H5A	0.500000	0.370280	0.959327	0.052*	
H5B	0.600860	0.454687	0.929396	0.052*	0.5
H5C	0.399140	0.454687	0.929396	0.052*	0.5
C6	0.500000	0.2890 (4)	0.5746 (4)	0.0350 (14)	
H6A	0.500000	0.338159	0.534803	0.052*	
H6B	0.600860	0.253755	0.564744	0.052*	0.5
H6C	0.399140	0.253755	0.564744	0.052*	0.5

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0223 (2)	0.0213 (2)	0.0248 (2)	0.000	0.000	0.00021 (14)
Br1	0.0231 (2)	0.0340 (3)	0.0237 (2)	−0.00048 (15)	0.00010 (13)	−0.00062 (14)
N1	0.031 (2)	0.022 (2)	0.022 (2)	0.000	0.000	0.0015 (16)
C1	0.031 (3)	0.025 (3)	0.026 (3)	0.000	0.000	0.0040 (19)
C2	0.036 (3)	0.026 (3)	0.026 (2)	0.000	0.000	0.003 (2)
N2	0.030 (2)	0.021 (2)	0.028 (2)	0.000	0.000	−0.0030 (17)
C3	0.029 (3)	0.025 (3)	0.026 (2)	0.000	0.000	0.002 (2)
C4	0.028 (3)	0.028 (3)	0.023 (2)	0.000	0.000	0.0009 (19)
C5	0.057 (4)	0.026 (3)	0.022 (2)	0.000	0.000	−0.001 (2)
C6	0.056 (4)	0.023 (3)	0.026 (2)	0.000	0.000	−0.004 (2)

Geometric parameters (Å, º)

Cd1—Br1	2.6869 (4)	C2—N2	1.332 (7)
Cd1—Br1^{i}	2.7893 (4)	N2—C3	1.360 (7)
Cd1—Br1^{ii}	2.6869 (4)	C3—C4	1.374 (8)
Cd1—Br1^{iii}	2.7893 (4)	C3—C6	1.500 (7)
Cd1—N1	2.482 (5)	C4—H4	0.9500
Cd1—N2^{iv}	2.494 (5)	C5—H5A	0.9800
N1—C1	1.347 (7)	C5—H5B	0.9800
N1—C4	1.353 (7)	C5—H5C	0.9800
C1—C2	1.404 (8)	C6—H6A	0.9800
C1—C5	1.484 (8)	C6—H6B	0.9800

C2—H2	0.9500	C6—H6C	0.9800
Br1—Cd1—Br1^{ii}	106.18 (2)	N2—C2—C1	124.2 (5)
Br1—Cd1—Br1^{iii}	86.222 (11)	N2—C2—H2	117.9
Br1^{ii}—Cd1—Br1^{i}	86.222 (11)	C2—N2—Cd1^{vi}	112.8 (4)
Br1^{i}—Cd1—Br1^{iii}	81.37 (2)	C2—N2—C3	116.5 (5)
Br1^{ii}—Cd1—Br1^{iii}	167.574 (18)	C3—N2—Cd1^{vi}	130.7 (3)
Br1—Cd1—Br1^{i}	167.574 (18)	N2—C3—C4	120.0 (5)
N1—Cd1—Br1^{iii}	89.25 (8)	N2—C3—C6	120.1 (5)
N1—Cd1—Br1^{ii}	91.20 (6)	C4—C3—C6	119.9 (5)
N1—Cd1—Br1	91.20 (6)	N1—C4—C3	123.4 (5)
N1—Cd1—Br1^{i}	89.25 (8)	N1—C4—H4	118.3
N1—Cd1—N2^{iv}	178.93 (15)	C3—C4—H4	118.3
N2^{iv}—Cd1—Br1^{ii}	89.45 (6)	C1—C5—H5A	109.5
N2^{iv}—Cd1—Br1	89.45 (6)	C1—C5—H5B	109.5
N2^{iv}—Cd1—Br1^{i}	89.94 (8)	C1—C5—H5C	109.5
N2^{iv}—Cd1—Br1^{iii}	89.94 (8)	H5A—C5—H5B	109.5
Cd1—Br1—Cd1^{v}	93.774 (11)	H5A—C5—H5C	109.5
C1—N1—Cd1	128.2 (4)	H5B—C5—H5C	109.5
C1—N1—C4	117.3 (5)	C3—C6—H6A	109.5
C4—N1—Cd1	114.4 (4)	C3—C6—H6B	109.5
N1—C1—C2	118.6 (5)	C3—C6—H6C	109.5
N1—C1—C5	120.8 (5)	H6A—C6—H6B	109.5
C2—C1—C5	120.6 (5)	H6A—C6—H6C	109.5
C1—C2—H2	117.9	H6B—C6—H6C	109.5
Cd1—N1—C1—C2	180.0	C1—C2—N2—C3	0.0
Cd1—N1—C1—C5	0.0	C2—N2—C3—C4	0.0
Cd1—N1—C4—C3	180.0	C2—N2—C3—C6	180.0
Cd1^{vi}—N2—C3—C4	180.0	N2—C3—C4—N1	0.0
Cd1^{vi}—N2—C3—C6	0.0	C4—N1—C1—C2	0.0
N1—C1—C2—N2	0.0	C4—N1—C1—C5	180.0
C1—N1—C4—C3	0.0	C5—C1—C2—N2	180.0
C1—C2—N2—Cd1^{vi}	180.0	C6—C3—C4—N1	180.0

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···Br1^{vii}	0.95	3.02	3.624 (5)	123
C2—H2···Br1^{viii}	0.95	3.02	3.624 (5)	123
C4—H4···Br1^{i}	0.95	3.04	3.622 (5)	121
C4—H4···Br1^{iii}	0.95	3.04	3.622 (5)	121
C5—H5*B*···Br1	0.98	2.83	3.658 (5)	142
C5—H5*C*···Br1^{ii}	0.98	2.83	3.658 (5)	142

C6—H6*B*···Br1^{vi}	0.98	2.86	3.674 (5)	141
C6—H6*C*···Br1^{ix}	0.98	2.86	3.674 (5)	141

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