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Syntheses and crystal structures of dichlorido(2,6-dimethylpyrazine-κN)(methanol-κO)zinc(II), dibromido(2,6-dimethylpyrazine-κN)(methanol-κO)zinc(II) and aqua(2,6-dimethylpyrazine-κN)-diiodidozinc(II)

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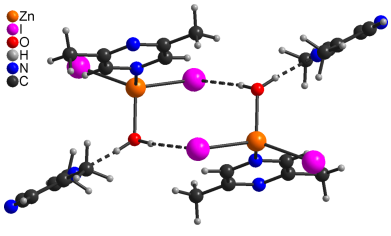
Three new compounds with the compositions $[ZnCl_2(C_6H_8N_2)(CH_3OH)]$ (**1**), $[ZnBr_2(C_6H_8N_2)(CH_3OH)]$ (**2**) and $[ZnI_2(C_6H_8N_2)(H_2O)]$ (**3**) were prepared ($C_6H_8N_2$ = 2,6-dimethylpyrazine). The asymmetric unit of each compound consists of one Zn^{II} cation, two halide anions, one 2,6-dimethylpyrazine ligand and one methanol (**1** and **2**) or water molecule (**3**), with all atoms located in general positions. Compounds **1** and **2** are not isostructural. In the crystal structures, the metal cations are fourfold coordinated by two halide anions, one 2,6-dimethylpyrazine ligand and one methanol or water molecule within a slightly distorted tetrahedral geometry. In **1** and **2** the discrete complexes are linked into chains *via* O—H···O hydrogen bonds between the O—H H atom of the methanol molecule and the 2,6-dimethylpyrazine N atom that is not involved in the metal coordination. These chains are further linked by weak C—H···Cl (**1**) or C—H···Br (**2**) interactions. In **3**, two complexes are linked by pairwise O—H···I hydrogen bonds into centrosymmetric dimeric units that are further connected by strong O—H···O hydrogen bonding between the second water H atom and the 2,6-dimethylpyrazine N-atom that is adjacent to the two methyl groups.

1. Chemical context

Coordination compounds based on transition metal halides and N-donor coligands shows versatile structural behavior, which is especially the case for Cu^{I} halides (Kromp & Sheldrick, 1999; Peng *et al.*, 2010; Li *et al.*, 2005; Näther *et al.*, 2001, 2002). For one definite N-donor ligand and one definite halide anion, compounds of a different ratio between the metal halide and the coligand are observed in many cases (Näther & Jess, 2002).

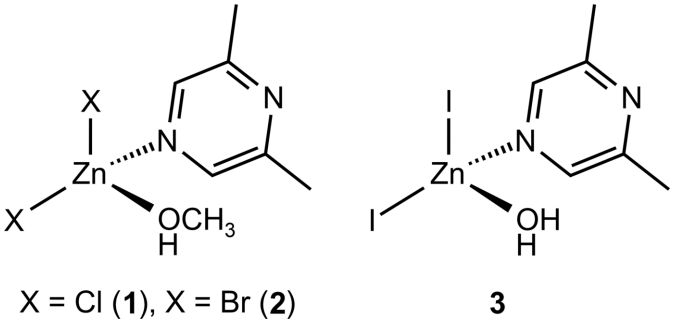
In contrast, compounds based on twofold positively charged cations such as Zn^{II} show a limited structural behavior because in most cases only a tetrahedral coordination is observed, leading to discrete complexes if monocoordinating coligands are used. However, there are a few examples for polymeric compounds, in which the Zn^{II} cations are in an octahedral coordination and linked into chains by μ-1,1-bridging halide anions (Pickardt & Staub, 1997; Saha *et al.*, 2017). Nevertheless, even for metals showing tetrahedral coordination, compounds with a different stoichiometry and more condensed networks can be obtained if bridging instead of monocoordinating coligands such as, for example, pyrazine are used. With this ligand, compounds with the composition $ZnX_2(pyrazine)_2$ (X = Cl, Br) and $ZnX_2(pyrazine)$ (X = Cl, Br,



I) have been reported (Bhosekar *et al.*, 2006; Bourne *et al.*, 200; Pickardt & Staub, 1997; Song *et al.*, 2004). In all of these compounds, the pyrazine ligand acts as bridging ligand.

In the course of our systematic investigations in this area, we became interested in ZnX_2 compounds based on 2,3-dimethylpyrazine. Because the methyl group is adjacent to the N atom, coordination of metal cations might be more difficult. In contrast to the pyrazine compounds, when $ZnCl_2$ and 2,3-dimethylpyrazine were reacted, two compounds with the composition $ZnCl_2$(2,3-dimethylpyrazine)$_2$ and $ZnCl_2$(2,3-dimethylpyrazine) were observed (Näther & Bhosekar, 2025*a*). The 2,3-dimethylpyrazine-rich compound consists of discrete tetrahedral complexes, in which the coligand is only terminally coordinated, whereas in the 2,3-dimethylpyrazine deficient compound the tetrahedra are linked into chains by bridging 2,3-dimethylpyrazine ligands. The corresponding bromide compounds $ZnBr_2$(2,3-dimethylpyrazine)$_2$ (Yang *et al.*, 2025) and $ZnBr_2$(2,3-dimethylpyrazine) (Näther & Bhosekar, 2025*b*) have also been reported. With ZnI_2, only the 2,3-dimethylpyrazine-deficient compound ZnI_2(2,3-dimethylpyrazine was found, which forms discrete complexes and which is isotypic to $ZnBr_2$(2,3-dimethylpyrazine) (Näther & Bhosekar, 2026).

Based on these results, we decided to prepare compounds with 2,6-dimethylpyrazine ($C_6H_8N_2$), in which one of the N atoms is adjacent to both methyl groups, which make a metal coordination even more difficult. In this context, it is noted that one compound with the composition ZnI_2(2,6-dimethylpyrazine)$_2$ is already reported, which consists of discrete complexes in which the metal cations are coordinated by two iodide anions and two terminal 2,6-dimethylpyrazine ligands (Lee *et al.*, 2008). As expected, the 2,6-dimethylpyrazine ligand coordinates with the N atom that is not adjacent to the two methyl groups. As part of these investigations, we prepared and isolated crystals of the three title compounds, which were characterized by single crystal X-ray diffraction.



X = Cl (**1**), X = Br (**2**) **3**

2. Structural commentary

The asymmetric units of $ZnCl_2(C_6H_8N_2)(CH_3OH)$ (**1**) and of $ZnBr_2(C_6H_8N_2)(CH_3OH)$ (**2**) consist of one Zn^{II} cation, two crystallographically independent halide anions, one 2,6-dimethylpyrazine ligand and one methanol molecule, with all atoms lying on general crystallographic positions (Fig. 1). Compounds **1** (space group $P\overline{1}$) and **2** (space group $P2_1/n$) are not isostructural.

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

Zn1—Cl1	2.2088 (11)	Zn1—O1	2.024 (3)
Zn1—Cl2	2.2008 (10)	Zn1—N2	2.064 (3)
Cl2—Zn1—Cl1	122.64 (4)	O1—Zn1—N2	102.15 (11)
O1—Zn1—Cl1	106.68 (9)	N2—Zn1—Cl1	108.38 (9)
O1—Zn1—Cl2	104.91 (9)	N2—Zn1—Cl2	110.06 (9)

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

Zn1—Br1	2.3533 (5)	Zn1—O1	2.003 (2)
Zn1—Br2	2.3334 (5)	Zn1—N2	2.075 (3)
Br2—Zn1—Br1	123.16 (2)	O1—Zn1—N2	103.06 (11)
O1—Zn1—Br1	110.09 (9)	N2—Zn1—Br1	105.94 (7)
O1—Zn1—Br2	101.02 (7)	N2—Zn1—Br2	111.81 (8)

Table 3
Selected geometric parameters (Å, °) for **3**.

Zn1—I1	2.5557 (5)	Zn1—O1	2.022 (3)
Zn1—I2	2.5352 (5)	Zn1—N2	2.077 (3)
I2—Zn1—I1	121.276 (18)	O1—Zn1—N2	97.32 (12)
O1—Zn1—I1	103.93 (8)	N2—Zn1—I1	113.23 (9)
O1—Zn1—I2	112.16 (8)	N2—Zn1—I2	106.39 (9)

In the crystal structures, the metal cations are tetrahedrally coordinated by two halide anions, one methanol molecule and one 2,6-dimethylpyrazine ligand that is coordinated by the N atom that is not adjacent to the methyl groups (Fig. 1). Bond lengths and angles shows that the tetrahedra are strongly distorted with the halide–Zn–halide angles showing the largest values (Tables 1 and 2).

The asymmetric unit of $ZnI_2(C_6H_8N_2)(H_2O)$ (**3**) consists of one Zn^{II} cation, two iodide anions, one 2,6-dimethylpyrazine ligand and one water molecule in general positions (Fig. 2).

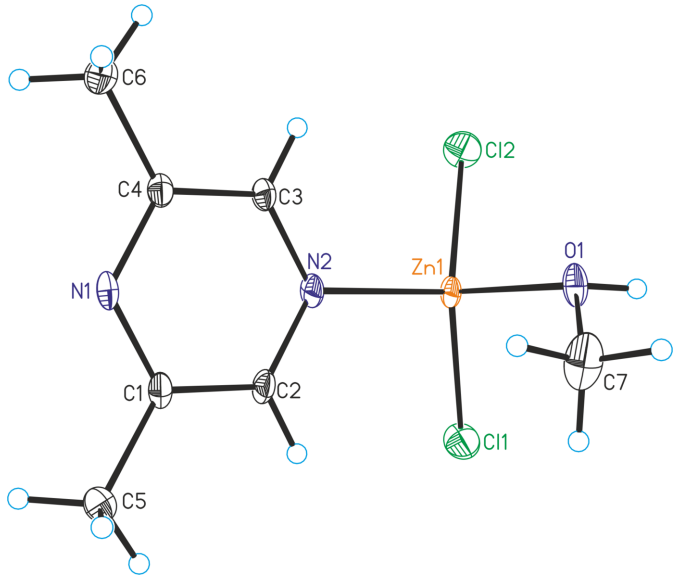


Figure 1
Crystal structures of **1** with labeling and displacement ellipsoids drawn at the 50% probability level.

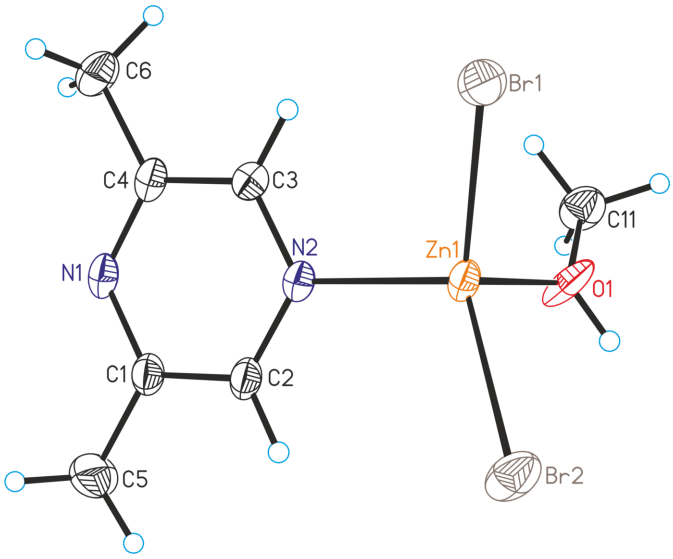


Figure 2
Crystal structures of **2** with labeling and displacement ellipsoids drawn at the 50% probability level.

The metal cations are fourfold coordinated by two halide anions, one 2,6-dimethylpyrazine ligand and one water molecule (Fig. 1: bottom). As in compounds **1** and **2**, the coordination polyhedra can be described as strongly distorted tetrahedra (Table 3).

As expected, in all three compounds the 2,6-dimethylpyrazine ligand is coordinated to the zinc cations with the N2 nitrogen atom that is not adjacent to the two methyl groups because of steric crowding and this might also be the reason why no compounds with bridging 2,6-dimethylpyrazine ligands were isolated. This is in contrast to, for example, compounds

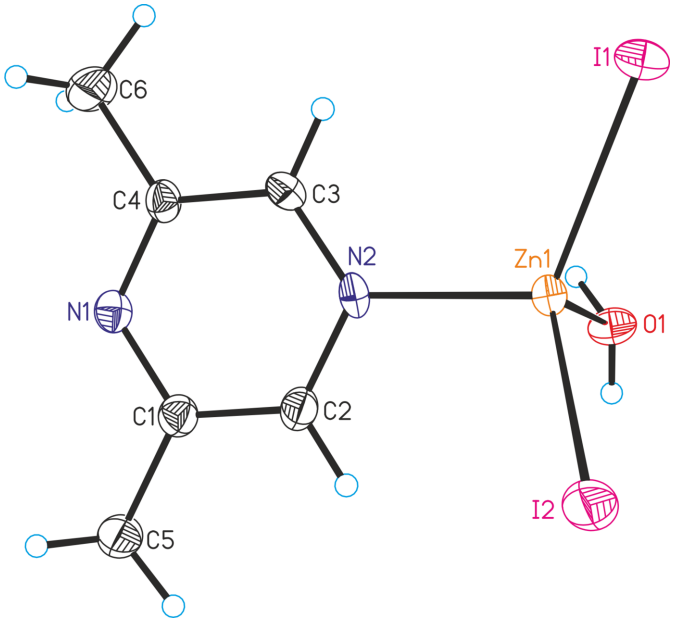


Figure 3
Crystal structure of **3** with labeling and displacement ellipsoids drawn at the 50% probability level.

Table 4
Hydrogen-bond geometry (Å, °) for **1**.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1^{i}	0.84 (2)	1.90 (2)	2.738 (4)	173 (5)
C3—H3···Cl2^{ii}	0.95	2.86	3.721 (4)	152
C5—H5*B*···Cl1^{iii}	0.98	2.84	3.721 (4)	150
C5—H5*C*···Cl1^{iv}	0.98	2.88	3.842 (4)	168
C6—H6*A*···Cl2^{iv}	0.98	2.98	3.929 (4)	163
C6—H6*B*···Cl2^{ii}	0.98	2.82	3.767 (4)	163
C7—H7*A*···Cl2^{v}	0.98	2.98	3.876 (5)	153

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

Table 5
Hydrogen-bond geometry (Å, °) for **2**.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1^{i}	0.83 (2)	1.84 (2)	2.677 (3)	178 (5)
C11—H11*A*···Br2^{ii}	0.98	3.13	3.767 (4)	124
C11—H11*C*···Br1^{iii}	0.98	2.88	3.807 (4)	157
C2—H2···Br1^{iv}	0.95	3.12	3.994 (3)	153
C3—H3···Br1	0.95	3.05	3.626 (3)	121
C5—H5*B*···Br1^{iv}	0.98	2.95	3.903 (4)	166

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

with 2,3-dimethylpyrazine such as $ZnCl_2$(2,3-dimethylpyrazine) (Näther & Bhosekar, 2025*a*) and $ZnBr_2$(2,3-dimethylpyrazine) (Näther & Bhosekar, 2025*b*) in which the metal centers are linked by the 2,3-dimethylpyrazine ligands.

3. Supramolecular features

In compound **1** and **2**, the discrete complexes are linked *via* O—H···N hydrogen bonds between the hydroxyl H atom of the methanol molecule and the 2,6-dimethylpyrazine N atom that is not involved in the metal coordination (Fig. 3 and Tables 4 and 5). The O—H···N bond angles are close to linear and the H···N distances below 2 Å, indicating strong hydrogen bonds (Tables 4 and 5). The geometry of the chains in **1** and **2** is slightly different because of a different rotation of the methanol molecule and the 2,6 dimethylpyrazine ligands.

These chains are interlinked by a number of C—H···Cl and C—H···Br hydrogen bonds. The C—H···X angles (X = Cl, Br), especially for the chloride compound, are mostly close to

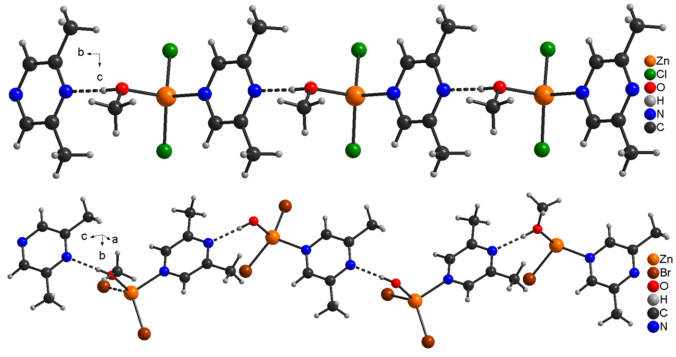


Figure 4
Crystal structure of **1** (top) and **2** (bottom) with view of a part of a chain. Intermolecular O—H···N hydrogen bonds are shown as dashed lines.

Table 6
Hydrogen-bond geometry (Å, °) for **3**.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···I1^{i}	0.86 (2)	2.70 (2)	3.555 (3)	172 (5)
O1—H1B···N1^{ii}	0.85 (2)	1.87 (2)	2.708 (4)	172 (5)
C2—H2···I2	0.95	3.22	3.776 (4)	119
C5—H5A···I2^{iii}	0.98	3.25	4.207 (5)	165

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

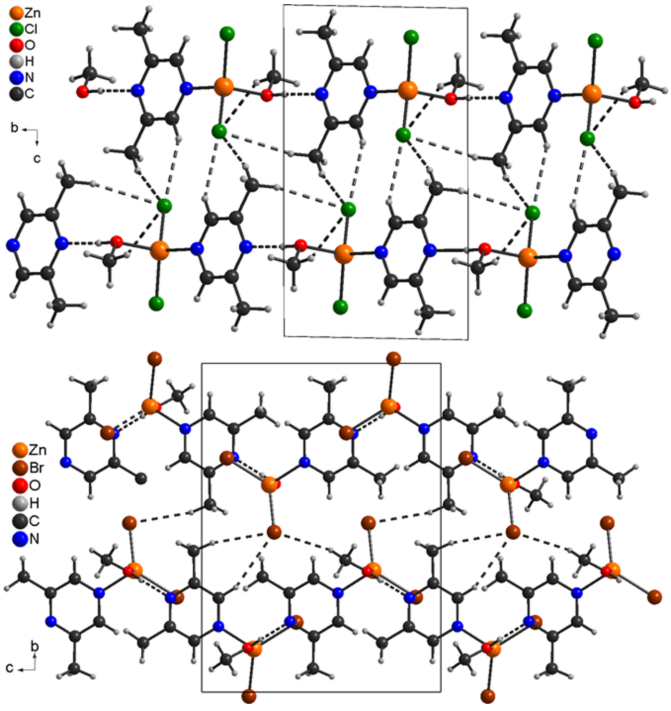


Figure 5
Crystal structure of **1** (top) and **2** (bottom) with view along the crystallographic *a*-axis direction and hydrogen bonds shown as dashed lines.

linear, indicating stronger interactions (Figs. 4 and 5 and Tables 4 and 5).

In compound **3**, two complexes are linked into dimers by centrosymmetric pairs of O—H···I hydrogen bonds between one of the water H atoms and the iodide anions, generating

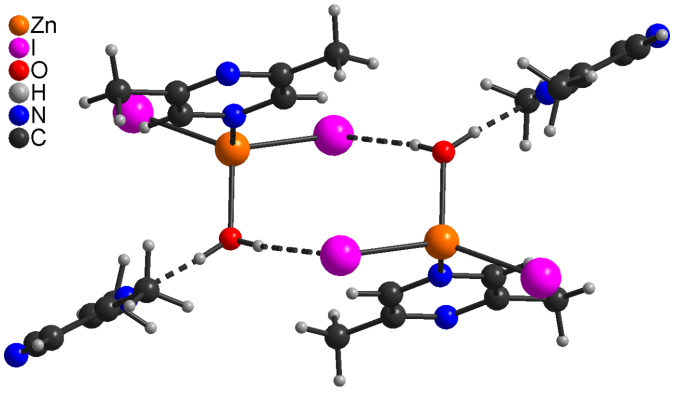


Figure 6
Crystal structure of **3** with view of a dimeric unit and C—H···I and O—H···N hydrogen bonds shown as dashed lines.

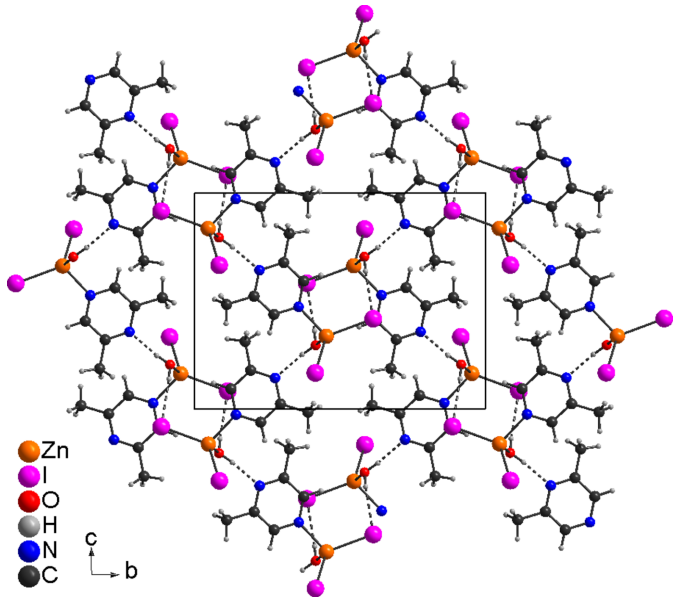


Figure 7
Crystal structure of **3** with view along the crystallographic *a*-axis direction and intermolecular hydrogen bonding shown as dashed lines.

eight-membered rings. The O—H···I angle of 172 (5)° and the H···I distance of only 2.70 (2) Å indicate relatively strong hydrogen bonding (Fig. 6 and Table 6). These dimers are linked by strong O—H···N hydrogen bonds between the second water H atom and the 2,6-dimethylpyrazine ligands that are not involved in the metal coordination (Fig. 7 and Table 6). There are additional C—H···I interactions with much longer H···I distances indicating only weak interactions.

4. Database survey

A literature search revealed that only one coordination compound with Zn halides and 2,6-dimethylpyrazine is reported in the CSD (Version 5.43, 2025; Groom *et al.*, 2016) using CONQUEST (Bruno *et al.*, 2002). This is ZnI_2(2,6-dimethylpyrazine)$_2$ (CSD refcode XIYGIW; Lee *et al.*, 2008), in which the Zn cations are coordinated by two iodide anions and two terminal 2,6-dimethylpyrazine ligands into discrete complexes. Many more compounds are reported with pyrazine. These include $ZnCl_2$(pyrazine)$_2$ (REMPAB, Bhosekar *et al.*, 2006) and $ZnBr_2$(pyrazine)$_2$ (EBOLAI, Bourne *et al.*, 2001 and EBOLAI01, Bhosekar *et al.*, 2006) and ZnX_2(pyrazine) [X = Cl (TISTAQ, Pickardt & Staub, 1996), Br (EBOKUB, Bourne *et al.*, 2001) and I (ISOPOV, Song *et al.*, 2004 and ISOPOV01, Bhosekar *et al.*, 2006)].

5. Synthesis and crystallization

General

Zinc chloride, zinc bromide and zinc iodide as well as 2,6-dimethylpyrazine were purchased from Sigma-Aldrich.

Synthesis of 1

0.500 mmol (68.1 mg) of zinc chloride and 1.00 mmol (108.1 mg 2,6-of dimethylpyrazine were reacted in 3 ml of

Table 7
Experimental details.

	1	2	3
Crystal data			
Chemical formula	$[ZnCl_2(C_6H_8N_2)(CH_4O)]$	$[ZnBr_2(C_6H_8N_2)(CH_4O)]$	$[ZnI_2(C_6H_8N_2)(H_2O)]$
M_r	276.46	365.38	445.33
Crystal system, space group	Triclinic, $P\overline{1}$	Monoclinic, $P2_1/n$	Monoclinic, $P2_1/n$
Temperature (K)	170	170	170
a, b, c (Å)	6.0481 (6), 7.4627 (7), 12.9967 (13)	7.1931 (5), 15.2428 (9), 11.4186 (6)	7.3914 (5), 14.7767 (8), 10.9917 (7)
α, β, γ (°)	89.945 (12), 85.471 (12), 74.710 (11)	90, 103.937 (7), 90	90, 94.883 (8), 90
V (Å^3)	563.96 (10)	1215.11 (13)	1196.16 (13)
Z	2	4	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	2.62	8.57	7.18
Crystal size (mm)	0.22 × 0.18 × 0.16	0.12 × 0.10 × 0.08	0.12 × 0.08 × 0.06
Data collection			
Diffractometer	Stoe IPDS2	Stoe IPDS2	Stoe IPDS2
Absorption correction	Numerical (*X-RED* and *X-SHAPE*; Stoe, 2008)	Numerical (*X-RED* and *X-SHAPE*; Stoe, 2008)	Numerical (*X-RED* and *X-SHAPE*; Stoe, 2008)
T_{min}, T_{max}	0.655, 0.765	0.236, 0.357	0.295, 0.510
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5812, 2675, 2223	10027, 2943, 2434	12550, 2880, 2477
R_{int}	0.048	0.031	0.040
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.660	0.662	0.661
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.046, 0.132, 1.05	0.031, 0.078, 1.02	0.028, 0.070, 1.03
No. of reflections	2675	2943	2880
No. of parameters	125	125	118
No. of restraints	1	1	3
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	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.36, −1.32	0.47, −0.61	0.78, −0.93

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

methanol. Within 2 d, crystals were obtained suitable for single crystal X-ray diffraction.

Synthesis of 2

0.500 mmol (112.6 mg) of zinc bromide and 1.00 mmol (108.1 mg) of 2,6-dimethylpyrazine were reacted in 3 ml of methanol. Within 3 d, crystals were obtained suitable for single crystal X-ray diffraction.

Synthesis of 3

0.500 mmol (159.6 mg) of zinc iodide and 1.00 mmol (108.1 mg) of 2,6-dimethylpyrazine were reacted in 3 mL of a water/methanol mixture (1:1). Within 2 d, crystals were obtained suitable for single crystal X-ray diffraction.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 7. 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).

Acknowledgements

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References

Bhosekar, G., Jess, I. & Näther, C. (2006). *Inorg. Chem.* **45**, 6508–6515.
Bourne, S. A., Kilkenny, M. & Nassimbeni, L. R. (2001). *J. Chem. Soc. Dalton Trans.* pp. 1176–1179.
Brandenburg, K. (1999). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Bruno, I. J., Cole, J. C., Edgington, P. R., Kessler, M., Macrae, C. F., McCabe, P., Pearson, J. & Taylor, R. (2002). *Acta Cryst.* B**58**, 389–397.
Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.
Kromp, T. & Sheldrick, W. S. (1999). *Z. Naturforsch. B* **54**, 1175–1180.
Lee, S. H., Kim, S.-H., Kim, P.-G., Kim, C. & Kim, Y. (2008). *Acta Cryst.* E**64**, m511.
Li, D., Shi, W. J. & Hou, L. (2005). *Inorg. Chem.* **44**, 3907–3913.
Näther, C. & Bhosekar, G. (2025*a*). *Acta Cryst.* E**81**, 694–698.
Näther, C. & Bhosekar, G. (2025*b*). *Acta Cryst.* E**81**, 928–931.
Näther, C. & Bhosekar, G. (2026). *Acta Cryst.* E**82**, 244–248.
Näther, C., Greve, J. & Jess, I. (2002). *Solid State Sci.* **4**, 813–820.
Näther, C. & Jess, I. (2002). *J. Solid State Chem.* **169**, 103–112.
Näther, C., Jess, I. & Greve, J. (2001). *Polyhedron* **20**, 1017–1022.
Peng, R., Li, M. & Li, D. (2010). *Coord. Chem. Rev.* **254**, 1–18.
Pickardt, J. & Staub, B. (1996). *Z. Naturforsch* B**51**, 947–951.
Pickardt, J. & Staub, B. (1997). *Z. Naturforsch* B**52**, 1456–1460.
Saha, B. K., Rather, S. A. & Saha, A. (2017). *Eur. J. Inorg. Chem.* 3390–3394.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.

Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Song, Y., Niu, Y., Hou, H. & Zhu, Y. (2004). *J. Mol. Struct.* **689**, 69–74.
Stoe (2008). *X-AREA X-RED* and *X-SHAPE*. Stoe & Cie, Darmstadt, Germany.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.
Yang, C., Zheng, J., Xu, C., Xiao, C., Chang, Y., Zhou, L. & Gong, X. (2025). *Chem. Commun.* **61**, 4379–4382.

supporting information

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Syntheses and crystal structures of dichlorido(2,6-dimethylpyrazine-κ*N*)(methanol-κ*O*)zinc(II), dibromido(2,6-dimethylpyrazine-κ*N*)(methanol-κ*O*)zinc(II) and aqua(2,6-dimethylpyrazine-κ*N*)diiodidozinc(II)

Christian Näther

Computing details

Dichlorido(2,6-dimethylpyrazine-κ*N*)(methanol-κ*O*)zinc(II) (1)

Crystal data

$[ZnCl_2(C_6H_8N_2)(CH_4O)]$
M_r = 276.46
Triclinic, $P\overline{1}$
a = 6.0481 (6) Å
b = 7.4627 (7) Å
c = 12.9967 (13) Å
α = 89.945 (12)°
β = 85.471 (12)°
γ = 74.710 (11)°
V = 563.96 (10) Å^3
Z = 2
$F(000)$ = 280
D_x = 1.628 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2716 reflections
θ = 2.9–28.1°
μ = 2.62 mm^{-1}
T = 170 K
Block, colorless
0.22 × 0.18 × 0.16 mm

Data collection

Stoe IPDS-2 diffractometer
Graphite monochromator
ω scans
Absorption correction: numerical (X-Red and X-Shape; Stoe, 2008)
T_{min} = 0.655, T_{max} = 0.765
5812 measured reflections
2675 independent reflections
2223 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
θ_{max} = 28.0°, θ_{min} = 2.8°
h = −7→7
k = −9→9
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.132
S = 1.05
2675 reflections
125 parameters
1 restraint
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0889P)^2 + 0.0814P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.36 e Å^{-3}
$\Delta\rho_{min}$ = −1.32 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: 0.028 (5)

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}
Zn1	1.02256 (6)	0.32540 (5)	0.25117 (3)	0.01229 (18)
Cl1	1.18124 (16)	0.30675 (14)	0.09118 (8)	0.0246 (3)
Cl2	1.21156 (16)	0.35079 (14)	0.38598 (8)	0.0241 (3)
O1	0.9178 (4)	0.0914 (4)	0.2745 (2)	0.0172 (6)
H1	1.028 (6)	−0.005 (5)	0.270 (4)	0.026*
N1	0.2974 (5)	0.7935 (4)	0.2674 (2)	0.0124 (6)
N2	0.7144 (5)	0.5283 (4)	0.2586 (2)	0.0133 (6)
C1	0.3971 (6)	0.7158 (5)	0.1768 (3)	0.0132 (7)
C2	0.6088 (6)	0.5818 (5)	0.1728 (3)	0.0139 (7)
H2	0.678622	0.528008	0.108048	0.017*
C3	0.6139 (6)	0.6067 (5)	0.3488 (3)	0.0140 (7)
H3	0.687547	0.570667	0.410353	0.017*
C4	0.4018 (6)	0.7410 (5)	0.3542 (3)	0.0133 (7)
C5	0.2791 (7)	0.7769 (6)	0.0814 (3)	0.0215 (8)
H5A	0.144983	0.726829	0.079890	0.032*
H5B	0.385738	0.730979	0.020628	0.032*
H5C	0.229148	0.912884	0.080948	0.032*
C6	0.2844 (7)	0.8266 (6)	0.4547 (3)	0.0221 (8)
H6A	0.237284	0.962092	0.448915	0.033*
H6B	0.390538	0.792852	0.509089	0.033*
H6C	0.148516	0.781027	0.472088	0.033*
C7	0.7388 (7)	0.0526 (6)	0.2186 (4)	0.0287 (10)
H7A	0.594142	0.147234	0.236440	0.043*
H7B	0.720038	−0.070144	0.237140	0.043*
H7C	0.780465	0.054397	0.144286	0.043*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0077 (2)	0.0089 (2)	0.0179 (3)	0.00237 (15)	−0.00194 (15)	−0.00016 (15)
Cl1	0.0228 (5)	0.0263 (5)	0.0199 (5)	−0.0002 (4)	0.0051 (4)	0.0030 (4)
Cl2	0.0205 (5)	0.0272 (5)	0.0253 (5)	−0.0052 (4)	−0.0105 (4)	−0.0016 (4)
O1	0.0106 (12)	0.0105 (12)	0.0289 (15)	0.0007 (9)	−0.0032 (11)	0.0025 (11)
N1	0.0081 (13)	0.0080 (13)	0.0199 (16)	0.0000 (10)	−0.0013 (11)	0.0022 (11)
N2	0.0076 (13)	0.0114 (14)	0.0179 (15)	0.0028 (11)	−0.0016 (11)	0.0002 (11)
C1	0.0111 (15)	0.0083 (15)	0.0196 (18)	−0.0010 (12)	−0.0038 (13)	0.0000 (13)
C2	0.0110 (15)	0.0099 (16)	0.0181 (17)	0.0020 (12)	−0.0011 (13)	−0.0018 (13)
C3	0.0119 (15)	0.0114 (16)	0.0160 (17)	0.0024 (13)	−0.0030 (13)	0.0004 (13)
C4	0.0123 (16)	0.0104 (15)	0.0157 (17)	−0.0007 (12)	−0.0004 (13)	0.0012 (13)

C5	0.0200 (18)	0.0208 (19)	0.0194 (19)	0.0038 (15)	−0.0077 (15)	−0.0019 (15)
C6	0.0184 (18)	0.023 (2)	0.0178 (19)	0.0062 (15)	0.0004 (15)	−0.0009 (15)
C7	0.0178 (19)	0.020 (2)	0.049 (3)	−0.0050 (16)	−0.0101 (18)	−0.0034 (19)

Geometric parameters (Å, º)

Zn1—Cl1	2.2088 (11)	C3—H3	0.9500
Zn1—Cl2	2.2008 (10)	C3—C4	1.401 (5)
Zn1—O1	2.024 (3)	C4—C6	1.495 (5)
Zn1—N2	2.064 (3)	C5—H5A	0.9800
O1—H1	0.841 (19)	C5—H5B	0.9800
O1—C7	1.439 (5)	C5—H5C	0.9800
N1—C1	1.339 (5)	C6—H6A	0.9800
N1—C4	1.343 (5)	C6—H6B	0.9800
N2—C2	1.337 (5)	C6—H6C	0.9800
N2—C3	1.338 (5)	C7—H7A	0.9800
C1—C2	1.398 (4)	C7—H7B	0.9800
C1—C5	1.491 (5)	C7—H7C	0.9800
C2—H2	0.9500		
Cl2—Zn1—Cl1	122.64 (4)	N1—C4—C3	119.8 (3)
O1—Zn1—Cl1	106.68 (9)	N1—C4—C6	118.4 (3)
O1—Zn1—Cl2	104.91 (9)	C3—C4—C6	121.8 (3)
O1—Zn1—N2	102.15 (11)	C1—C5—H5A	109.5
N2—Zn1—Cl1	108.38 (9)	C1—C5—H5B	109.5
N2—Zn1—Cl2	110.06 (9)	C1—C5—H5C	109.5
Zn1—O1—H1	113 (4)	H5A—C5—H5B	109.5
C7—O1—Zn1	121.7 (2)	H5A—C5—H5C	109.5
C7—O1—H1	107 (3)	H5B—C5—H5C	109.5
C1—N1—C4	119.4 (3)	C4—C6—H6A	109.5
C2—N2—Zn1	120.4 (2)	C4—C6—H6B	109.5
C2—N2—C3	118.5 (3)	C4—C6—H6C	109.5
C3—N2—Zn1	121.1 (2)	H6A—C6—H6B	109.5
N1—C1—C2	120.1 (3)	H6A—C6—H6C	109.5
N1—C1—C5	118.6 (3)	H6B—C6—H6C	109.5
C2—C1—C5	121.3 (3)	O1—C7—H7A	109.5
N2—C2—C1	121.0 (3)	O1—C7—H7B	109.5
N2—C2—H2	119.5	O1—C7—H7C	109.5
C1—C2—H2	119.5	H7A—C7—H7B	109.5
N2—C3—H3	119.5	H7A—C7—H7C	109.5
N2—C3—C4	121.1 (3)	H7B—C7—H7C	109.5
C4—C3—H3	119.5		
Zn1—N2—C2—C1	178.4 (3)	C1—N1—C4—C6	−178.6 (3)
Zn1—N2—C3—C4	−178.3 (3)	C2—N2—C3—C4	0.5 (5)
N1—C1—C2—N2	0.4 (6)	C3—N2—C2—C1	−0.4 (5)
N2—C3—C4—N1	−0.4 (6)	C4—N1—C1—C2	−0.3 (5)
N2—C3—C4—C6	178.5 (4)	C4—N1—C1—C5	−179.6 (3)

C1—N1—C4—C3	0.4 (5)	C5—C1—C2—N2	179.6 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1^{i}	0.84 (2)	1.90 (2)	2.738 (4)	173 (5)
C3—H3···Cl2^{ii}	0.95	2.86	3.721 (4)	152
C5—H5*B*···Cl1^{iii}	0.98	2.84	3.721 (4)	150
C5—H5*C*···Cl1^{iv}	0.98	2.88	3.842 (4)	168
C6—H6*A*···Cl2^{iv}	0.98	2.98	3.929 (4)	163
C6—H6*B*···Cl2^{ii}	0.98	2.82	3.767 (4)	163
C7—H7*A*···Cl2^{v}	0.98	2.98	3.876 (5)	153

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

Dibromido(2,6-dimethylpyrazine-κ*N*)(methanol-κ*O*)zinc(II) (2)

Crystal data

$[ZnBr_2(C_6H_8N_2)(CH_4O)]$
M_r = 365.38
Monoclinic, $P2_1/n$
a = 7.1931 (5) Å
b = 15.2428 (9) Å
c = 11.4186 (6) Å
β = 103.937 (7)°
V = 1215.11 (13) Å^3
Z = 4
F(000) = 704
D_x = 1.997 Mg m^{-3}
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 8000 reflections
θ = 7.2–27.3°
μ = 8.57 mm^{-1}
T = 170 K
Block, colorless
0.12 × 0.10 × 0.08 mm

Data collection

Stoe IPDS-2 diffractometer
Graphite monochromator
ω scans
Absorption correction: numerical (X-Red and X-Shape; Stoe, 2008)
T_{min} = 0.236, T_{max} = 0.357
10027 measured reflections
2943 independent reflections
2434 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 28.1°, θ_{min} = 2.3°
h = −9→9
k = −20→20
l = −13→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.078
S = 1.02
2943 reflections
125 parameters
1 restraint
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0515P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.47 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: 0.0084 (7)

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}
Zn1	0.62772 (5)	0.63072 (2)	0.71740 (3)	0.01889 (11)
Br1	0.73136 (5)	0.48630 (2)	0.69719 (3)	0.02990 (12)
Br2	0.72234 (5)	0.71163 (3)	0.89530 (3)	0.03381 (12)
O1	0.3423 (3)	0.6336 (2)	0.6914 (2)	0.0344 (6)
H1	0.308 (7)	0.660 (3)	0.747 (4)	0.052*
C11	0.1921 (5)	0.5986 (3)	0.6012 (3)	0.0309 (7)
H11A	0.107236	0.646053	0.562825	0.046*
H11B	0.119366	0.556534	0.637516	0.046*
H11C	0.245122	0.568677	0.540544	0.046*
N1	0.7234 (4)	0.78592 (19)	0.3686 (2)	0.0220 (5)
N2	0.6734 (4)	0.69914 (17)	0.5698 (2)	0.0188 (5)
C1	0.7187 (4)	0.8310 (2)	0.4688 (3)	0.0228 (6)
C2	0.6960 (4)	0.7861 (2)	0.5705 (3)	0.0217 (6)
H2	0.696644	0.817979	0.642087	0.026*
C3	0.6748 (4)	0.6556 (2)	0.4683 (3)	0.0213 (6)
H3	0.656328	0.593891	0.465830	0.026*
C4	0.7024 (4)	0.6984 (2)	0.3666 (3)	0.0229 (6)
C5	0.7385 (7)	0.9290 (2)	0.4656 (4)	0.0410 (9)
H5A	0.861314	0.944069	0.447765	0.062*
H5B	0.733555	0.953631	0.544044	0.062*
H5C	0.633628	0.953363	0.402749	0.062*
C6	0.7132 (6)	0.6496 (3)	0.2544 (3)	0.0341 (8)
H6A	0.656530	0.685392	0.183474	0.051*
H6B	0.642639	0.594258	0.250431	0.051*
H6C	0.847488	0.637298	0.255916	0.051*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.01907 (18)	0.02417 (19)	0.01512 (19)	−0.00124 (13)	0.00745 (13)	0.00053 (13)
Br1	0.0435 (2)	0.02313 (17)	0.02577 (19)	0.00434 (13)	0.01359 (15)	0.00339 (13)
Br2	0.02469 (18)	0.0514 (2)	0.02468 (19)	−0.00688 (15)	0.00469 (13)	−0.01538 (15)
O1	0.0184 (10)	0.0626 (18)	0.0240 (12)	−0.0024 (11)	0.0089 (9)	−0.0233 (12)
C11	0.0277 (16)	0.039 (2)	0.0248 (17)	−0.0036 (14)	0.0036 (13)	−0.0066 (15)
N1	0.0188 (12)	0.0312 (14)	0.0174 (13)	−0.0020 (10)	0.0072 (10)	0.0038 (11)
N2	0.0192 (12)	0.0229 (12)	0.0159 (12)	−0.0003 (10)	0.0070 (10)	0.0019 (10)
C1	0.0231 (15)	0.0269 (16)	0.0204 (15)	−0.0034 (12)	0.0092 (12)	0.0013 (12)
C2	0.0214 (14)	0.0276 (16)	0.0180 (15)	−0.0034 (12)	0.0090 (12)	0.0003 (12)
C3	0.0229 (14)	0.0224 (15)	0.0200 (15)	−0.0008 (11)	0.0077 (12)	−0.0015 (12)

C4	0.0206 (14)	0.0301 (16)	0.0204 (15)	−0.0008 (12)	0.0095 (12)	0.0012 (12)
C5	0.065 (3)	0.0275 (18)	0.034 (2)	−0.0106 (18)	0.0197 (19)	0.0004 (16)
C6	0.047 (2)	0.037 (2)	0.0227 (17)	−0.0013 (17)	0.0177 (16)	−0.0036 (15)

Geometric parameters (Å, º)

Zn1—Br1	2.3533 (5)	C1—C2	1.391 (4)
Zn1—Br2	2.3334 (5)	C1—C5	1.503 (5)
Zn1—O1	2.003 (2)	C2—H2	0.9500
Zn1—N2	2.075 (3)	C3—H3	0.9500
O1—H1	0.833 (19)	C3—C4	1.387 (4)
O1—C11	1.406 (4)	C4—C6	1.499 (5)
C11—H11A	0.9800	C5—H5A	0.9800
C11—H11B	0.9800	C5—H5B	0.9800
C11—H11C	0.9800	C5—H5C	0.9800
N1—C1	1.342 (4)	C6—H6A	0.9800
N1—C4	1.343 (4)	C6—H6B	0.9800
N2—C2	1.335 (4)	C6—H6C	0.9800
N2—C3	1.337 (4)		
Br2—Zn1—Br1	123.16 (2)	N2—C2—C1	121.4 (3)
O1—Zn1—Br1	110.09 (9)	N2—C2—H2	119.3
O1—Zn1—Br2	101.02 (7)	C1—C2—H2	119.3
O1—Zn1—N2	103.06 (11)	N2—C3—H3	119.2
N2—Zn1—Br1	105.94 (7)	N2—C3—C4	121.7 (3)
N2—Zn1—Br2	111.81 (8)	C4—C3—H3	119.2
Zn1—O1—H1	112 (4)	N1—C4—C3	119.4 (3)
C11—O1—Zn1	132.8 (2)	N1—C4—C6	118.6 (3)
C11—O1—H1	115 (4)	C3—C4—C6	122.0 (3)
O1—C11—H11A	109.5	C1—C5—H5A	109.5
O1—C11—H11B	109.5	C1—C5—H5B	109.5
O1—C11—H11C	109.5	C1—C5—H5C	109.5
H11A—C11—H11B	109.5	H5A—C5—H5B	109.5
H11A—C11—H11C	109.5	H5A—C5—H5C	109.5
H11B—C11—H11C	109.5	H5B—C5—H5C	109.5
C1—N1—C4	119.8 (3)	C4—C6—H6A	109.5
C2—N2—Zn1	122.5 (2)	C4—C6—H6B	109.5
C2—N2—C3	118.1 (3)	C4—C6—H6C	109.5
C3—N2—Zn1	119.4 (2)	H6A—C6—H6B	109.5
N1—C1—C2	119.5 (3)	H6A—C6—H6C	109.5
N1—C1—C5	117.8 (3)	H6B—C6—H6C	109.5
C2—C1—C5	122.7 (3)		
Zn1—N2—C2—C1	−177.3 (2)	C1—N1—C4—C6	−178.5 (3)
Zn1—N2—C3—C4	179.2 (2)	C2—N2—C3—C4	1.2 (5)
N1—C1—C2—N2	−1.9 (5)	C3—N2—C2—C1	0.6 (5)
N2—C3—C4—N1	−1.8 (5)	C4—N1—C1—C2	1.3 (4)
N2—C3—C4—C6	177.1 (3)	C4—N1—C1—C5	−178.7 (3)

C1—N1—C4—C3	0.5 (4)	C5—C1—C2—N2	178.1 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1^{i}	0.83 (2)	1.84 (2)	2.677 (3)	178 (5)
C11—H11*A*···Br2^{ii}	0.98	3.13	3.767 (4)	124
C11—H11*C*···Br1^{iii}	0.98	2.88	3.807 (4)	157
C2—H2···Br1^{iv}	0.95	3.12	3.994 (3)	153
C3—H3···Br1	0.95	3.05	3.626 (3)	121
C5—H5*B*···Br1^{iv}	0.98	2.95	3.903 (4)	166

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

Aqua(2,6-dimethylpyrazine-κ*N*)diiodidozinc(II) (3)

Crystal data

$[ZnI_2(C_6H_8N_2)(H_2O)]$
M_r = 445.33
Monoclinic, $P2_1/n$
a = 7.3914 (5) Å
b = 14.7767 (8) Å
c = 10.9917 (7) Å
β = 94.883 (8)°
V = 1196.16 (13) Å^3
Z = 4
F(000) = 816
D_x = 2.473 Mg m^{-3}
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 7998 reflections
θ = 8.5–27.1°
μ = 7.18 mm^{-1}
T = 170 K
Block, colorless
0.12 × 0.08 × 0.06 mm

Data collection

Stoe IPDS-2 diffractometer
Graphite monochromator
ω scans
Absorption correction: numerical (X-Red and X-Shape; Stoe, 2008)
T_{min} = 0.295, T_{max} = 0.510
12550 measured reflections
2880 independent reflections
2477 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 28.0°, θ_{min} = 2.3°
h = −9→9
k = −19→19
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.070
S = 1.02
2880 reflections
118 parameters
3 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0479P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.78 e Å^{-3}
$\Delta\rho_{min}$ = −0.93 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: 0.0043 (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}
Zn1	0.73068 (6)	0.45260 (3)	0.33652 (4)	0.01746 (11)
I1	0.70914 (3)	0.61402 (2)	0.41751 (2)	0.02247 (9)
I2	0.92934 (4)	0.41488 (2)	0.16648 (2)	0.03004 (10)
O1	0.4691 (4)	0.41616 (19)	0.2948 (3)	0.0225 (6)
H1A	0.417 (7)	0.412 (3)	0.361 (3)	0.034*
H1B	0.433 (7)	0.371 (2)	0.252 (4)	0.034*
N1	0.8726 (4)	0.2232 (2)	0.6430 (3)	0.0184 (6)
N2	0.7913 (4)	0.3577 (2)	0.4732 (3)	0.0183 (6)
C1	0.8679 (5)	0.2047 (3)	0.5226 (3)	0.0208 (7)
C2	0.8277 (5)	0.2728 (2)	0.4380 (3)	0.0211 (7)
H2	0.825714	0.259317	0.353358	0.025*
C3	0.7957 (5)	0.3750 (2)	0.5925 (3)	0.0185 (7)
H3	0.770384	0.434435	0.619252	0.022*
C4	0.8369 (5)	0.3069 (2)	0.6790 (3)	0.0187 (7)
C5	0.9078 (7)	0.1104 (3)	0.4843 (4)	0.0292 (9)
H5A	1.024937	0.091071	0.524392	0.044*
H5B	0.912702	0.108462	0.395508	0.044*
H5C	0.811997	0.069732	0.507787	0.044*
C6	0.8398 (8)	0.3260 (3)	0.8127 (4)	0.0356 (10)
H6A	0.762378	0.282163	0.850627	0.053*
H6B	0.794385	0.387313	0.824971	0.053*
H6C	0.964498	0.320920	0.850212	0.053*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0199 (2)	0.01571 (19)	0.0166 (2)	0.00201 (15)	0.00033 (16)	0.00198 (15)
I1	0.02262 (14)	0.01846 (13)	0.02691 (14)	−0.00292 (9)	0.00547 (10)	−0.00573 (9)
I2	0.03415 (17)	0.03106 (16)	0.02667 (15)	0.00725 (11)	0.01290 (11)	0.00196 (10)
O1	0.0219 (14)	0.0237 (13)	0.0218 (13)	−0.0040 (11)	0.0014 (11)	−0.0067 (11)
N1	0.0185 (15)	0.0168 (14)	0.0198 (15)	−0.0022 (12)	0.0012 (12)	0.0032 (11)
N2	0.0176 (15)	0.0172 (14)	0.0196 (14)	0.0044 (12)	−0.0009 (12)	0.0056 (12)
C1	0.0211 (18)	0.0201 (17)	0.0208 (17)	−0.0003 (14)	−0.0008 (14)	0.0002 (14)
C2	0.0241 (19)	0.0201 (17)	0.0183 (17)	0.0001 (14)	−0.0032 (15)	0.0011 (14)
C3	0.0184 (17)	0.0157 (15)	0.0217 (17)	0.0034 (13)	0.0036 (14)	−0.0006 (13)
C4	0.0197 (18)	0.0195 (17)	0.0170 (16)	0.0022 (14)	0.0029 (13)	0.0048 (13)
C5	0.043 (3)	0.0177 (17)	0.0255 (19)	0.0012 (17)	−0.0035 (18)	−0.0024 (15)
C6	0.059 (3)	0.032 (2)	0.0159 (19)	0.008 (2)	0.0074 (19)	0.0014 (16)

Geometric parameters (Å, º)

Zn1—I1	2.5557 (5)	C1—C5	1.492 (5)
Zn1—I2	2.5352 (5)	C2—H2	0.9500
Zn1—O1	2.022 (3)	C3—H3	0.9500
Zn1—N2	2.077 (3)	C3—C4	1.400 (5)
O1—H1A	0.858 (19)	C4—C6	1.495 (5)
O1—H1B	0.849 (19)	C5—H5A	0.9800
N1—C1	1.349 (5)	C5—H5B	0.9800
N1—C4	1.331 (5)	C5—H5C	0.9800
N2—C2	1.347 (5)	C6—H6A	0.9800
N2—C3	1.334 (5)	C6—H6B	0.9800
C1—C2	1.385 (5)	C6—H6C	0.9800
I2—Zn1—I1	121.276 (18)	N2—C3—H3	119.5
O1—Zn1—I1	103.93 (8)	N2—C3—C4	121.0 (3)
O1—Zn1—I2	112.16 (8)	C4—C3—H3	119.5
O1—Zn1—N2	97.32 (12)	N1—C4—C3	120.2 (3)
N2—Zn1—I1	113.23 (9)	N1—C4—C6	118.7 (3)
N2—Zn1—I2	106.39 (9)	C3—C4—C6	121.0 (3)
Zn1—O1—H1A	108 (3)	C1—C5—H5A	109.5
Zn1—O1—H1B	126 (4)	C1—C5—H5B	109.5
H1A—O1—H1B	106 (4)	C1—C5—H5C	109.5
C4—N1—C1	119.4 (3)	H5A—C5—H5B	109.5
C2—N2—Zn1	117.2 (2)	H5A—C5—H5C	109.5
C3—N2—Zn1	124.6 (2)	H5B—C5—H5C	109.5
C3—N2—C2	118.2 (3)	C4—C6—H6A	109.5
N1—C1—C2	119.8 (3)	C4—C6—H6B	109.5
N1—C1—C5	118.5 (3)	C4—C6—H6C	109.5
C2—C1—C5	121.6 (3)	H6A—C6—H6B	109.5
N2—C2—C1	121.3 (3)	H6A—C6—H6C	109.5
N2—C2—H2	119.3	H6B—C6—H6C	109.5
C1—C2—H2	119.3		
Zn1—N2—C2—C1	−179.4 (3)	C1—N1—C4—C6	179.0 (4)
Zn1—N2—C3—C4	179.7 (3)	C2—N2—C3—C4	0.0 (5)
N1—C1—C2—N2	−0.6 (6)	C3—N2—C2—C1	0.3 (6)
N2—C3—C4—N1	0.0 (6)	C4—N1—C1—C2	0.6 (6)
N2—C3—C4—C6	−179.3 (4)	C4—N1—C1—C5	−179.8 (4)
C1—N1—C4—C3	−0.3 (5)	C5—C1—C2—N2	179.8 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···I1^{i}	0.86 (2)	2.70 (2)	3.555 (3)	172 (5)
O1—H1*B*···N1^{ii}	0.85 (2)	1.87 (2)	2.708 (4)	172 (5)

C2—H2···I2	0.95	3.22	3.776 (4)	119
C5—H5*A*···I2^{iii}	0.98	3.25	4.207 (5)	165

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