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Syntheses and structures of bis(2-aminopyrimidine-κN^1)dichloridozinc(II) (orthorhombic polymorph) and bis(2-aminopyrimidine-κN^1)diiodidozinc(II)

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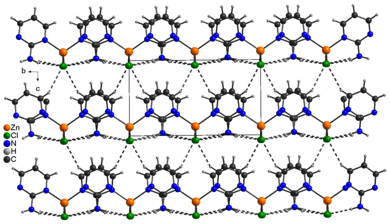
The title compounds, $[ZnCl_2(C_4H_5N_3)_2]$ (**1**) and $[ZnI_2(C_4H_5N_3)_2]$ (**2**) ($C_4H_5N_3$ = 2-aminopyrimidine), were prepared from a solvent mixture of trichloromethane and methanol and structurally characterized. The asymmetric unit of **1** consists of one Zn^{II} cation that is situated on a twofold rotation axis and one chloride anion as well as one 2-aminopyrimidine ligand in general positions. The asymmetric unit of **2** is built up of one Zn^{II} cation, two iodide anions and two 2-aminopyrimidine ligands, all of them located in general positions. In both compounds, the metal cations are tetrahedrally coordinated by two halide anions and two 2-aminopyrimidine ligands. In compound **1**, the discrete complexes are linked by N—H⋯Cl hydrogen bonds into layers that are further connected by weak C—H⋯Cl interactions. In compound **2**, the complexes are connected *via* N—H⋯I hydrogen bonds into layers that are further linked by a number of N—H⋯I and C—H⋯I hydrogen bonds. Compound **1** represents a second polymorphic modification of $ZnCl_2(C_4H_5N_3)_2$ that crystallizes in the orthorhombic non-centrosymmetric space group *Pba*2, whereas the known form crystallizes in the monoclinic, centrosymmetric space group *C*2/*c* [Lin & Zeng (2007). *Acta Cryst.* E**63**, m1597].

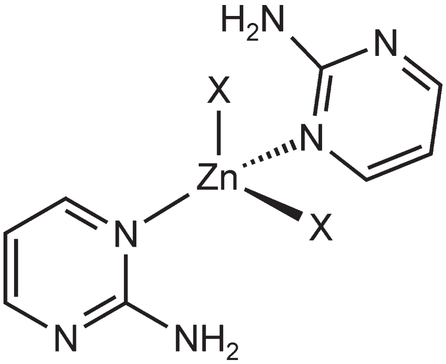
1. Chemical context

Investigations on the synthesis and crystal structures of new coordination compounds is still a major field in inorganic chemistry. Our interest is focused on coordination compounds based on transition-metal halides and N-donor coligands. In the beginning, we concentrated on compounds based on univalent cations such as Cu^I because they show a versatile structural behavior that can be traced back to the fact that the metal cations are frequently linked by bridging halide anions (Kromp & Sheldrick, 1999; Peng *et al.*, 2010; Näther *et al.*, 2001, 2002). Moreover, multiple compounds with a different ratio between the metal halide and the coligand are often observed (Näther & Jess, 2002; Näther *et al.*, 2003). In further work, we investigated coordination compounds with twofold positively charged metal cations such as Zn^{II} or Cd^{II}, but compared to the copper(I) halides these show a limited structural variability (Bhosekar *et al.*, 2006; Neumann *et al.*, 2018*a*,*b*). Such compounds, however, are of interest because of their luminescence properties (Zeng *et al.*, 2010; Neumann *et al.*, 2018*a*,*b*; Jess *et al.*, 2020; Kokina *et al.*, 2020).

In the course of our systematic investigations, we became interested in 2-aminopyrimidine ($C_4H_5N_3$) as coligand. On the one hand, the coordination of a metal cation might be more difficult, because of steric interference from the neighbouring amino group, but on the other strong hydrogen bonding can be expected.



In this context it is noted that two compounds with the composition $ZnCl_2(C_4H_5N_3)_2$ (CSD refcode YIDPAD; Lin & Zeng, 2007) and $ZnBr_2(C_4H_5N_3)_2$ (LOBPOI; Qu *et al.*, 2008) are already reported in the CSD (Version 5.43, 2025; Groom *et al.*, 2016), as found using a CONQUEST (Bruno *et al.*, 2002) search. Both of them consist of discrete neutral complexes that are linked by intermolecular hydrogen bonds. In the course of our investigations, we obtained crystals of the missing compound with ZnI_2, and with $ZnCl_2$ we obtained crystals of a second polymorph of $ZnCl_2(C_4H_5N_3)_2$ (Lin & Zeng, 2007).



X = Cl (**1**), X = I (**2**)

2. Structural commentary

$ZnCl_2(C_4H_5N_3)_2$ (**1**) represents a second polymorphic modification of the form that is already reported in the literature (Lin & Zeng, 2007). In contrast to the reported form that crystallizes in the centrosymmetric monoclinic space group *C*2/*c*, compound **1** crystallizes in the non-centrosymmetric orthorhombic space group *Pba*2. The asymmetric unit of **1** consists of one Zn^{II} cation located on a twofold rotation axis and one chloride anion and one 2-aminopyrimidine ligand in general positions (Fig. 1). In the crystal structure, the Zn^{II} cations are fourfold coordinated by two symmetry-related halide anions and two symmetry-related 2-aminopyrimidine ligands (Fig. 1). Bond lengths and angles show that the tetrahedra are only slightly distorted (Table 1). The overall geometry is very similar to the form reported in the literature (Lin & Zeng, 2007). Compound **1** was crystallized from the mixed solvents of methanol and trichloromethane (see *Synthesis and crystallization*) whereas the form reported by Lin & Zeng was crystallized from an ethanol solution.

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

Zn1—N1	2.028 (3)	Zn1—Cl1	2.2613 (10)
$N1^i$—Zn1—N1	111.5 (2)	N1—Zn1—Cl1	111.64 (9)
N1—Zn1—$Cl1^i$	105.22 (9)	$Cl1^i$—Zn1—Cl1	111.79 (6)

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

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

Zn1—N11	2.040 (3)	Zn1—I2	2.5686 (6)
Zn1—N1	2.052 (4)	Zn1—I1	2.5948 (6)
N11—Zn1—N1	103.25 (14)	N11—Zn1—I1	109.47 (10)
N11—Zn1—I2	110.46 (10)	N1—Zn1—I1	114.82 (10)
N1—Zn1—I2	107.01 (10)	I2—Zn1—I1	111.50 (2)

The iodide compound $ZnI_2(C_4H_5N_3)_2$ (**2**) is not isotypic to any of the zinc(II) halide compounds known in the literature and also not to **1**. Its asymmetric unit is built up of one Zn^{II} cation as well as two crystallographically independent iodide anions and 2-aminopyrimidine ligands that are located in general positions (Fig. 2). As in **1**, the Zn^{II} cations are fourfold coordinated by two iodide anions and two 2-aminopyrimidine ligands within slightly distorted tetrahedra (Fig. 2 and Table 2).

3. Supramolecular features

In the extended structure of **1**, the discrete complexes are linked *via* N—H···Cl hydrogen bonds between the amino H

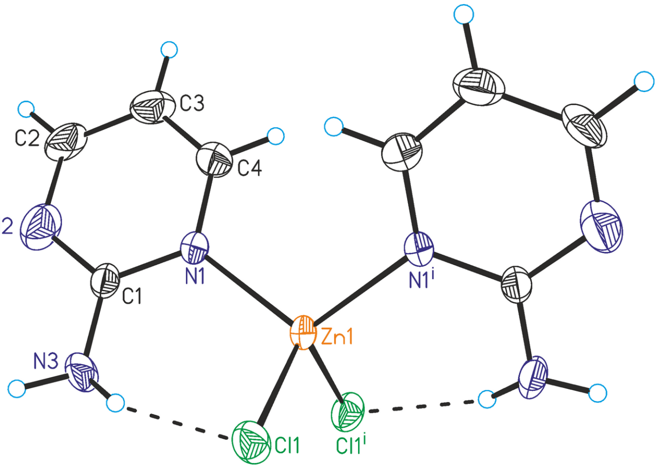


Figure 1
The molecular structure of **1** with displacement ellipsoids drawn at the 50% probability level and intramolecular N—H···Cl hydrogen bonding shown as dashed lines. Symmetry code: (i) $-x+1, -y+1, z$.

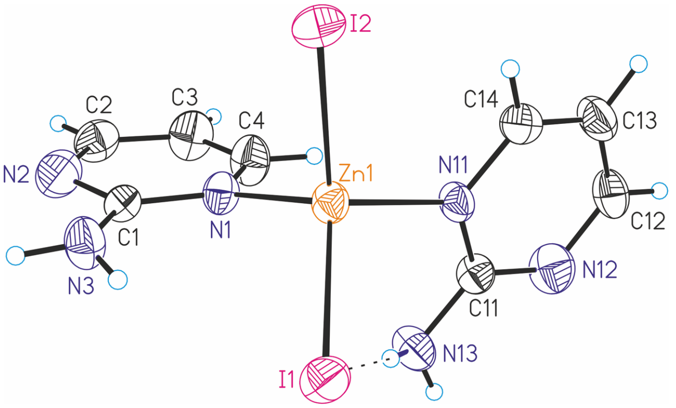


Figure 2
The molecular structure of **2** with displacement ellipsoids drawn at the 50% probability level and the intramolecular N—H···I hydrogen bonding shown as a dashed line.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···Cl1$^{\rm ii}$	0.91 (2)	2.52 (3)	3.431 (4)	177 (5)
N3—H3*B*···Cl1	0.92 (2)	2.43 (3)	3.311 (4)	162 (4)
C2—H2···Cl1$^{\rm iii}$	0.94	2.92	3.772 (5)	152

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···I1	0.88 (2)	2.96 (3)	3.742 (4)	150 (4)
N3—H3*B*···I1$^{\rm i}$	0.89 (2)	3.03 (2)	3.922 (4)	173 (5)
C2—H2···I2$^{\rm ii}$	0.94	3.31	3.982 (5)	130
C4—H4···N11	0.94	2.67	3.275 (6)	123
N13—H13*A*···I1	0.90	2.84	3.738 (4)	173
N13—H13*B*···I2$^{\rm iii}$	0.90	2.81	3.693 (4)	169
C13—H13···I2$^{\rm iv}$	0.94	3.10	4.001 (5)	162
C14—H14···I2	0.94	3.14	3.815 (5)	130

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

atom and the chloride anions (Fig. 3). One of these H atoms acts as donor for an intramolecular, the second for an intermolecular hydrogen bond. The H···Cl distances are relatively short and the N—H···Cl angles close to linear indicate strong hydrogen bonding (Table 3). In this way, layers are formed, that lie parallel to the *ab* plane with the hydrogen bonds pointed in the direction of the crystallographic *b* axis (Fig. 3). These layers are further linked by C—H···Cl hydrogen bonds between one of the H atoms of the six-membered rings and the chloride anions (Fig. 4 and Table 3). From Fig. 4 it may be seen that all the pyrimidine rings point in the crystallographic *c*-axis direction, clearly proving the non-centrosymmetry of this structure (Fig. 4).

The structure of **1** is completely different from that of the other polymorph already reported in the literature. In this modification, each complex is linked to neighbouring complexes by centrosymmetric pairs of N—H···N hydrogen bonds (Fig. 5). The second N—H H atom is only involved in intramolecular N—H···Cl hydrogen bonding but in contrast to the form presented here, the N—H···N and N—H···Cl angles are far from linear, surprisingly indicating weaker interactions. Finally, in contrast to the title polymorph, in the known form the complexes are linked into chains that propagate in the *c*-axis direction (Fig. 5).

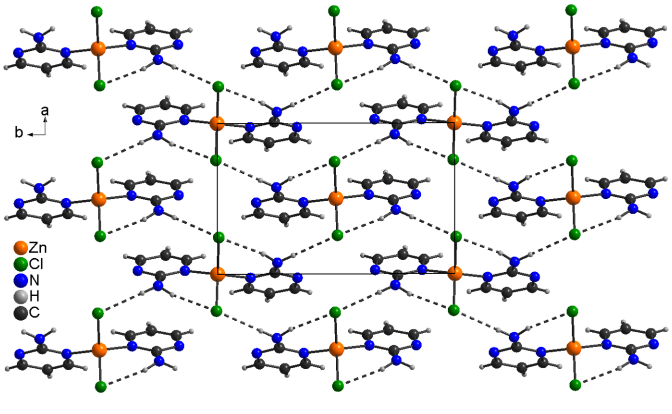


Figure 3
Crystal structure of **1** with a view onto the layers formed by intermolecular N—H···Cl hydrogen bonds (shown as dashed lines).

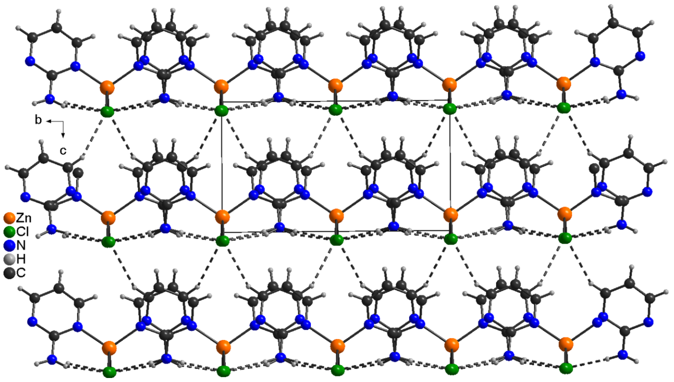


Figure 4
Crystal structure of **1** with a view along the *a*-axis direction showing the non-centrosymmetry of this structure. Intermolecular hydrogen bonds are shown as dashed lines.

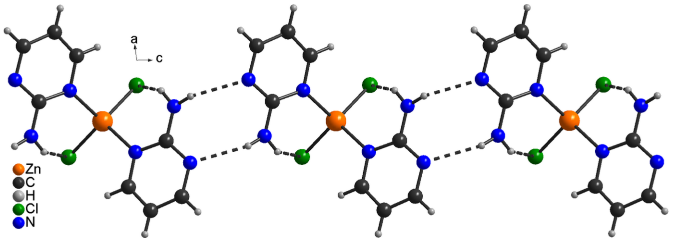


Figure 5
Crystal structure of the second polymorph of **1** already reported in the literature (Lin & Zeng, 2007) with intermolecular N—H···N and N—H···Cl hydrogen bonds shown as dashed lines.

In the iodide compound **2**, the discrete complexes are linked by intermolecular N—H···I hydrogen bonds into layers that

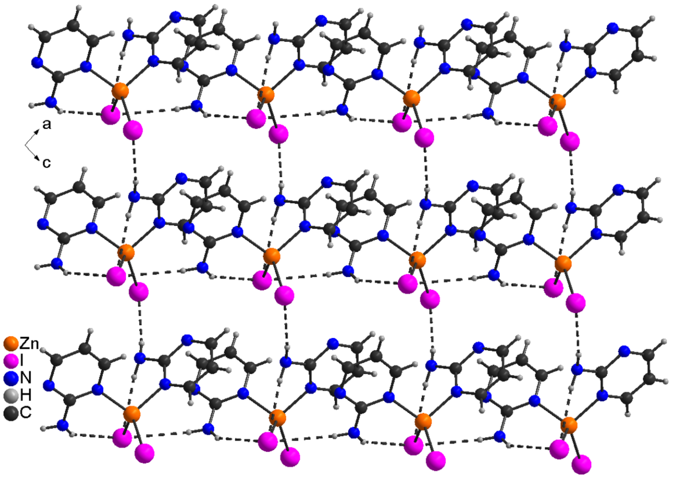


Figure 6
Crystal structure of **2** along the *b*-axis direction with a view onto the layers and intermolecular N—H···I hydrogen bonds shown as dashed lines.

Table 5
Experimental details.

	1	**2**
Crystal data		
Chemical formula	$[ZnCl_2(C_4H_5N_3)_2]$	$[ZnI_2(C_4H_5N_3)_2]$
M_r	326.49	509.39
Crystal system, space group	Orthorhombic, *Pba*2	Monoclinic, $P2_1/n$
Temperature (K)	220	220
a, b, c (Å)	7.6628 (7), 12.0590 (8), 6.8735 (4)	9.5469 (6), 15.3764 (13), 10.1518 (6)
α, β, γ (°)	90, 90, 90	90, 95.884 (7), 90
V (Å^3)	635.15 (8)	1482.40 (18)
Z	2	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	2.34	5.81
Crystal size (mm)	0.18 × 0.16 × 0.14	0.16 × 0.10 × 0.06
Data collection		
Diffractometer	Stoe *IPDS1*	Stoe *IPDS1*
Absorption correction	Numerical (*X-RED* and *X-SHAPE*; Stoe, 2008)	Numerical (*X-RED* and *X-SHAPE*; Stoe, 2008)
T_{min}, T_{max}	0.636, 0.842	0.296, 0.471
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5690, 1490, 1251	14800, 3491, 2946
R_{int}	0.045	0.091
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.660	0.661
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.032, 0.080, 1.00	0.036, 0.094, 1.03
No. of reflections	1490	3491
No. of parameters	87	163
No. of restraints	3	2
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.49, −0.43	1.17, −1.28
Absolute structure	Flack x determined using 505 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)	–
Absolute structure parameter	0.007 (13)	–

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

in this compound are parallel to the *bc* plane (Fig. 6). As in compound **1**, one amine H atom is involved in an intramolecular hydrogen bond, whereas the second H atom shows intermolecular hydrogen bonding. Bond lengths and angles also indicate a significant interaction (Table 4). These layers are further linked by pairs of C—H⋯I interactions between the iodide anions and the H atoms of the pyrimidine rings (Fig. 7).

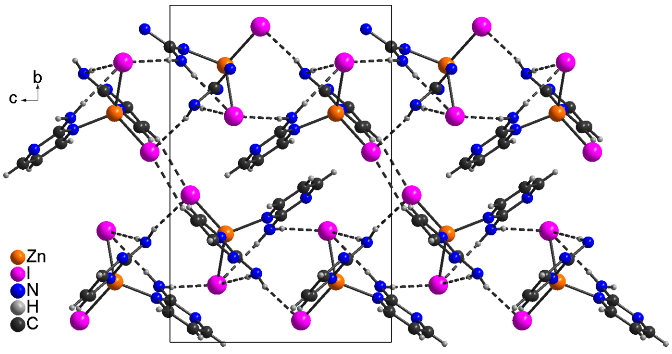


Figure 7
Crystal structure of **2** with a view along the *a*-axis direction and intermolecular hydrogen bonds shown as dashed lines.

4. Database survey

A search in the CSD (Version 5.43, 2025; Groom *et al.*, 2016) using CONQUEST (Bruno *et al.*, 2002) revealed that two Zn halide coordination compounds with the composition $ZnCl_2(C_4H_5N_3)_2$ (Lin & Zeng, 2007) and $ZnBr_2(C_4H_5N_3)_2$ (Qu *et al.*, 2008) are already reported (see above). There are additional Zn compounds with different anions that are related to the title compounds, including $(Zn(NCS)_2(C_4H_5N_3)_2$ (Jin *et al.*, 2010), $(Zn(NO_3)_2(C_4H_5N_3)_2(H_2O)$ (Gao & Ng, 2010) and $(Zn(C_{11}H_5O_2F_3)_2(C_4H_5N_3)_2$ (Perdih, 2016) that also consists of discrete complexes. There is also a compound with mixed hydroxide nitrate anions that forms a polymeric structure (Kang *et al.*, 2011).

Finally, it is noted that some compounds are reported in which the 2-aminopyrimidine ligands are protonated, but none of them contain zinc(II) as cation. These include, for example, 2-amino-1,3-dihydropyrimidiniumtetrabromocopper(II) (Pon *et al.*, 1997), 2-aminopyrimidiniumtetrabromocobalt(II) monohydrate (Masaki *et al.*, 2002), 2-amino-1,3-dihydropyrimidiniumtetraaquadibromomanganese(II) dibromide (Lee *et al.*, 2003) and 2-amino-1,3-dihydropyrimidiniumtetraaquadibromonickel(II) dibromide (Masaki *et al.*, 2002). In three additional compounds, the 2-aminopyridine ligand is also protonated and act as counter-cation for Mo and W cluster compounds (Chen *et al.*, 2015; Xiao *et al.*, 2018).

5. Synthesis and crystallization

Zinc chloride and zinc iodide as well as 2-aminopyrimidine were purchased from Sigma-Aldrich.

To prepare **1**, 0.500 mmol (68.1 mg) of zinc chloride and 1.00 mmol (95.1 mg) of 2-aminopyrimidine were reacted in a solvent mixture of 1 ml of trichloromethane and 1 ml of methanol. Within 3 d, crystals suitable for single crystal X-ray diffraction were obtained in the form of colorless blocks.

Compound **2** was prepared by reacting 0.500 mmol (159.6 mg) of zinc iodide and 1.00 mmol (95.1 mg) of 2-aminopyrimidine in a solvent mixture of 3 ml of trichloromethane and 3 ml of methanol. Within 3 d, colorless blocks suitable for single crystal X-ray diffraction were obtained.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 5. The C—H hydrogen atoms were positioned with idealized geometry and were refined as riding atoms with $U_{\rm iso}(\rm H) = 1.2U_{\rm eq}(\rm C)$. The N—H H atoms were located in difference maps and were refined isotropically with restraints (DFIX).

Acknowledgements

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supporting information

Acta Cryst. (2026). E**82**, 300-304   [https://doi.org/10.1107/S2056989026001878]

Syntheses and structures of bis(2-aminopyrimidine-κN^1)dichloridozinc(II) (orthorhombic polymorph) and bis(2-aminopyrimidine-κN^1)diiodidozinc(II)

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Computing details

Bis(2-aminopyrimidine-κN^1)dichloridozinc(II) (1)

Crystal data

$[ZnCl_2(C_4H_5N_3)_2]$
M_r = 326.49
Orthorhombic, *Pba*2
a = 7.6628 (7) Å
b = 12.0590 (8) Å
c = 6.8735 (4) Å
V = 635.15 (8) Å^3
Z = 2
F(000) = 328
D_x = 1.707 Mg m^{-3}
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 6615 reflections
θ = 3.0–28.0°
μ = 2.34 mm^{-1}
T = 220 K
Block, colorless
0.18 × 0.16 × 0.14 mm

Data collection

Stoe IPDS-1
diffractometer
Phi scans
Absorption correction: numerical
(X-Red and X-Shape; Stoe, 2008)
T_{min} = 0.636, T_{max} = 0.842
5690 measured reflections
1490 independent reflections
1251 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 28.0°, θ_{min} = 3.2°
$h = -10 \rightarrow 10$
$k = -15 \rightarrow 15$
$l = -8 \rightarrow 9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.080
S = 1.00
1490 reflections
87 parameters
3 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent
and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0537P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 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: 0.038 (7)
Absolute structure: Flack x determined using
505 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.007 (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	$U_{\rm iso}$*/$U_{\rm eq}$
Zn1	0.500000	0.500000	0.88265 (9)	0.0219 (2)
Cl1	0.74418 (15)	0.50555 (6)	1.06713 (13)	0.0302 (3)
N1	0.4752 (4)	0.6381 (3)	0.7166 (5)	0.0222 (7)
N2	0.4748 (6)	0.8362 (4)	0.6738 (8)	0.0446 (12)
N3	0.5753 (6)	0.7516 (3)	0.9660 (7)	0.0349 (9)
H3A	0.623 (6)	0.819 (3)	0.998 (8)	0.035 (12)*
H3B	0.634 (5)	0.692 (3)	1.018 (7)	0.029 (12)*
C1	0.5104 (5)	0.7413 (4)	0.7842 (6)	0.0232 (8)
C2	0.4046 (7)	0.8250 (4)	0.4924 (8)	0.0388 (11)
H2	0.378192	0.888020	0.417373	0.047*
C3	0.3723 (6)	0.7190 (4)	0.4194 (6)	0.0372 (11)
H3	0.328392	0.709206	0.292874	0.045*
C4	0.4057 (6)	0.6306 (3)	0.5345 (7)	0.0304 (9)
H4	0.379338	0.559649	0.486091	0.036*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0307 (3)	0.0128 (3)	0.0223 (3)	−0.0020 (2)	0.000	0.000
Cl1	0.0370 (6)	0.0213 (5)	0.0322 (6)	0.0024 (4)	−0.0098 (4)	−0.0014 (5)
N1	0.0293 (18)	0.0158 (14)	0.0215 (17)	−0.0022 (11)	−0.0010 (13)	0.0017 (13)
N2	0.058 (3)	0.029 (2)	0.047 (3)	0.0026 (17)	0.004 (2)	0.008 (2)
N3	0.058 (2)	0.0152 (14)	0.032 (2)	−0.0020 (19)	−0.011 (2)	−0.0034 (14)
C1	0.0279 (19)	0.0170 (18)	0.025 (2)	−0.0020 (15)	0.0059 (17)	0.0000 (16)
C2	0.055 (3)	0.030 (2)	0.031 (2)	0.008 (2)	−0.002 (2)	0.0150 (19)
C3	0.046 (2)	0.042 (2)	0.024 (3)	0.005 (2)	−0.0037 (18)	0.0048 (18)
C4	0.035 (2)	0.030 (2)	0.026 (2)	−0.0036 (16)	−0.0062 (18)	−0.0002 (16)

Geometric parameters (Å, º)

Zn1—N1$^{\rm i}$	2.028 (3)	N3—C1	1.351 (6)
Zn1—N1	2.028 (3)	N3—H3A	0.91 (2)
Zn1—Cl1$^{\rm i}$	2.2612 (10)	N3—H3B	0.92 (2)
Zn1—Cl1	2.2613 (10)	C2—C3	1.396 (7)
N1—C1	1.355 (6)	C2—H2	0.9400
N1—C4	1.363 (6)	C3—C4	1.352 (6)
N2—C2	1.365 (7)	C3—H3	0.9400
N2—C1	1.401 (6)	C4—H4	0.9400

N1^{i}—Zn1—N1	111.5 (2)	N3—C1—N1	118.4 (4)
N1^{i}—Zn1—Cl1^{i}	111.64 (9)	N3—C1—N2	119.8 (4)
N1—Zn1—Cl1^{i}	105.22 (9)	N1—C1—N2	121.7 (4)
N1^{i}—Zn1—Cl1	105.22 (9)	N2—C2—C3	119.3 (4)
N1—Zn1—Cl1	111.64 (9)	N2—C2—H2	120.4
Cl1^{i}—Zn1—Cl1	111.79 (6)	C3—C2—H2	120.4
C1—N1—C4	117.0 (3)	C4—C3—C2	118.6 (4)
C1—N1—Zn1	122.8 (3)	C4—C3—H3	120.7
C4—N1—Zn1	119.9 (3)	C2—C3—H3	120.7
C2—N2—C1	119.4 (4)	C3—C4—N1	124.0 (4)
C1—N3—H3A	117 (3)	C3—C4—H4	118.0
C1—N3—H3B	118 (3)	N1—C4—H4	118.0
H3A—N3—H3B	114 (4)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···Cl1^{ii}	0.91 (2)	2.52 (3)	3.431 (4)	177 (5)
N3—H3*B*···Cl1	0.92 (2)	2.43 (3)	3.311 (4)	162 (4)
C2—H2···Cl1^{iii}	0.94	2.92	3.772 (5)	152

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

Bis(2-aminopyrimidine-κ*N*^{1})diiodidozinc(II) (2)

Crystal data

$[ZnI_2(C_4H_5N_3)_2]$
$M_r = 509.39$
Monoclinic, $P2_1/n$
$a = 9.5469$ (6) Å
$b = 15.3764$ (13) Å
$c = 10.1518$ (6) Å
$\beta = 95.884$ (7)°
$V = 1482.40$ (18) Å^3
$Z = 4$

$F(000) = 944$
$D_x = 2.282$ Mg m^{-3}
Mo *Kα* radiation, $\lambda = 0.71073$ Å
Cell parameters from 8000 reflections
$\theta = 10.4–25.7°$
$\mu = 5.81$ mm^{-1}
$T = 220$ K
Block, colorless
0.16 × 0.10 × 0.06 mm

Data collection

Stoe IPDS-1 diffractometer
Phi scans
Absorption correction: numerical (X-Red and X-Shape; Stoe, 2008)
$T_{min} = 0.296$, $T_{max} = 0.471$
14800 measured reflections

3491 independent reflections
2946 reflections with $I > 2\sigma(I)$
$R_{int} = 0.091$
$\theta_{max} = 28.0°$, $\theta_{min} = 2.4°$
$h = -12\rightarrow12$
$k = -20\rightarrow20$
$l = -13\rightarrow13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.094$
$S = 1.03$

3491 reflections
163 parameters
2 restraints
Primary atom site location: dual
Hydrogen site location: mixed

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0549P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.17$ e Å^{-3}
$\Delta\rho_{min} = -1.28$ e Å^{-3}
Extinction correction: SHELXL-2016/6 (Sheldrick 2015b), Fc*=kFc[1+0.001xFc$^2\lambda^3$/sin(2θ)]$^{-1/4}$
Extinction coefficient: 0.0054 (4)

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}
Zn1	0.75540 (4)	0.82087 (3)	0.75052 (5)	0.02767 (14)
I1	0.86634 (3)	0.67008 (2)	0.71225 (3)	0.03788 (12)
I2	0.83722 (3)	0.93595 (2)	0.59175 (3)	0.03509 (12)
N1	0.7972 (4)	0.8692 (2)	0.9389 (3)	0.0299 (7)
N2	0.9550 (5)	0.9284 (3)	1.1144 (5)	0.0474 (10)
N3	1.0345 (4)	0.8344 (3)	0.9503 (5)	0.0391 (9)
H3A	1.031 (5)	0.792 (2)	0.892 (4)	0.033 (13)*
H3B	1.113 (4)	0.837 (4)	1.006 (5)	0.049 (16)*
C1	0.9279 (4)	0.8763 (3)	1.0011 (4)	0.0293 (8)
C2	0.8455 (5)	0.9696 (3)	1.1649 (5)	0.0407 (10)
H2	0.861854	1.004769	1.240675	0.049*
C3	0.7096 (5)	0.9592 (4)	1.1032 (6)	0.0460 (11)
H3	0.632564	0.985892	1.137634	0.055*
C4	0.6905 (5)	0.9095 (3)	0.9917 (5)	0.0403 (10)
H4	0.598736	0.902899	0.949621	0.048*
N11	0.5413 (3)	0.8105 (2)	0.7281 (4)	0.0286 (7)
N12	0.3223 (4)	0.7503 (3)	0.7851 (5)	0.0480 (10)
N13	0.5463 (4)	0.7037 (3)	0.8897 (4)	0.0405 (9)
H13A	0.627117	0.693806	0.853657	0.061*
H13B	0.493126	0.664756	0.928267	0.061*
C11	0.4698 (4)	0.7547 (3)	0.8001 (4)	0.0296 (8)
C12	0.2495 (4)	0.8033 (3)	0.6940 (5)	0.0370 (10)
H12	0.150638	0.801076	0.681757	0.044*
C13	0.3224 (5)	0.8608 (3)	0.6193 (5)	0.0397 (10)
H13	0.273687	0.898093	0.557058	0.048*
C14	0.4642 (5)	0.8618 (3)	0.6384 (5)	0.0371 (9)
H14	0.512675	0.899989	0.586882	0.044*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0211 (2)	0.0315 (2)	0.0306 (3)	−0.00168 (16)	0.00331 (19)	0.00062 (17)
I1	0.02970 (17)	0.03171 (17)	0.0529 (2)	0.00108 (10)	0.00748 (13)	−0.00385 (11)
I2	0.03910 (19)	0.02980 (17)	0.03796 (19)	−0.00264 (10)	0.01170 (13)	0.00272 (10)

N1	0.0257 (16)	0.0353 (18)	0.0290 (18)	−0.0031 (13)	0.0035 (14)	−0.0019 (13)
N2	0.048 (2)	0.045 (2)	0.049 (3)	−0.0071 (18)	0.003 (2)	−0.0010 (18)
N3	0.0285 (19)	0.046 (2)	0.042 (2)	0.0032 (15)	−0.0006 (17)	−0.0062 (17)
C1	0.0274 (19)	0.0267 (19)	0.033 (2)	−0.0041 (14)	0.0008 (16)	0.0029 (15)
C2	0.049 (3)	0.036 (2)	0.037 (2)	−0.0031 (19)	0.006 (2)	−0.0065 (19)
C3	0.042 (3)	0.049 (3)	0.048 (3)	0.003 (2)	0.009 (2)	−0.013 (2)
C4	0.027 (2)	0.049 (3)	0.045 (3)	0.0028 (18)	0.0058 (19)	−0.012 (2)
N11	0.0200 (15)	0.0340 (17)	0.0314 (19)	−0.0005 (12)	0.0000 (14)	0.0044 (13)
N12	0.034 (2)	0.055 (3)	0.055 (3)	−0.0010 (17)	0.0069 (19)	0.000 (2)
N13	0.0268 (18)	0.050 (2)	0.044 (2)	−0.0027 (15)	0.0034 (16)	0.0186 (18)
C11	0.0246 (19)	0.034 (2)	0.031 (2)	−0.0015 (14)	0.0058 (16)	0.0016 (15)
C12	0.0203 (19)	0.052 (3)	0.038 (3)	0.0063 (17)	0.0002 (17)	−0.004 (2)
C13	0.034 (2)	0.043 (3)	0.040 (3)	0.0090 (18)	−0.0064 (19)	0.0030 (19)
C14	0.034 (2)	0.034 (2)	0.043 (3)	−0.0013 (17)	−0.0001 (19)	0.0050 (18)

Geometric parameters (Å, º)

Zn1—N11	2.040 (3)	C3—H3	0.9400
Zn1—N1	2.052 (4)	C4—H4	0.9400
Zn1—I2	2.5686 (6)	N11—C11	1.356 (5)
Zn1—I1	2.5948 (6)	N11—C14	1.361 (6)
N1—C1	1.344 (5)	N12—C12	1.368 (6)
N1—C4	1.349 (6)	N12—C11	1.403 (6)
N2—C2	1.367 (7)	N13—C11	1.356 (6)
N2—C1	1.403 (6)	N13—H13A	0.9000
N3—C1	1.351 (6)	N13—H13B	0.9001
N3—H3A	0.876 (19)	C12—C13	1.396 (7)
N3—H3B	0.89 (2)	C12—H12	0.9400
C2—C3	1.391 (7)	C13—C14	1.348 (6)
C2—H2	0.9400	C13—H13	0.9400
C3—C4	1.363 (7)	C14—H14	0.9400
N11—Zn1—N1	103.25 (14)	N1—C4—C3	123.1 (4)
N11—Zn1—I2	110.46 (10)	N1—C4—H4	118.5
N1—Zn1—I2	107.01 (10)	C3—C4—H4	118.5
N11—Zn1—I1	109.47 (10)	C11—N11—C14	117.3 (4)
N1—Zn1—I1	114.82 (10)	C11—N11—Zn1	122.9 (3)
I2—Zn1—I1	111.50 (2)	C14—N11—Zn1	119.8 (3)
C1—N1—C4	118.6 (4)	C12—N12—C11	118.6 (4)
C1—N1—Zn1	123.4 (3)	C11—N13—H13A	104.5
C4—N1—Zn1	117.0 (3)	C11—N13—H13B	112.8
C2—N2—C1	119.2 (4)	H13A—N13—H13B	127.6
C1—N3—H3A	129 (4)	N11—C11—N13	117.5 (4)
C1—N3—H3B	111 (4)	N11—C11—N12	121.8 (4)
H3A—N3—H3B	115 (5)	N13—C11—N12	120.7 (4)
N1—C1—N3	118.8 (4)	N12—C12—C13	119.9 (4)
N1—C1—N2	121.0 (4)	N12—C12—H12	120.1
N3—C1—N2	120.2 (4)	C13—C12—H12	120.1

N2—C2—C3	119.5 (4)	C14—C13—C12	118.5 (4)
N2—C2—H2	120.3	C14—C13—H13	120.7
C3—C2—H2	120.3	C12—C13—H13	120.7
C4—C3—C2	118.5 (5)	C13—C14—N11	123.8 (4)
C4—C3—H3	120.7	C13—C14—H14	118.1
C2—C3—H3	120.7	N11—C14—H14	118.1

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···I1	0.88 (2)	2.96 (3)	3.742 (4)	150 (4)
N3—H3*B*···I1^{i}	0.89 (2)	3.03 (2)	3.922 (4)	173 (5)
C2—H2···I2^{ii}	0.94	3.31	3.982 (5)	130
C4—H4···N11	0.94	2.67	3.275 (6)	123
N13—H13*A*···I1	0.90	2.84	3.738 (4)	173
N13—H13*B*···I2^{iii}	0.90	2.81	3.693 (4)	169
C13—H13···I2^{iv}	0.94	3.10	4.001 (5)	162
C14—H14···I2	0.94	3.14	3.815 (5)	130

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